



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 03:11 AM BST

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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

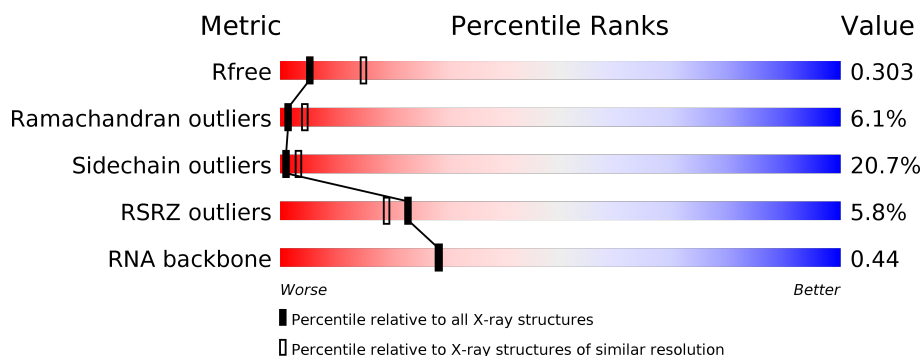
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

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.





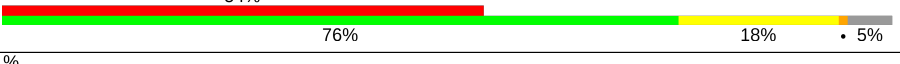
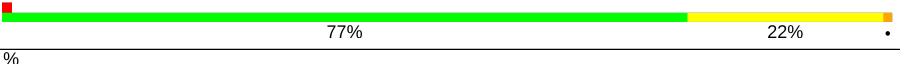
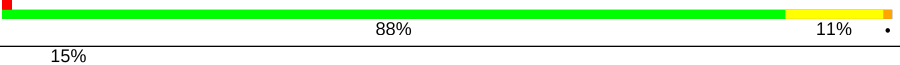



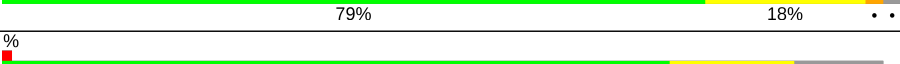
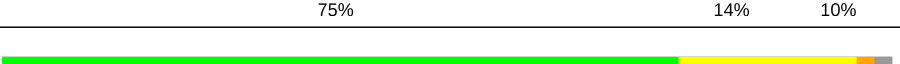
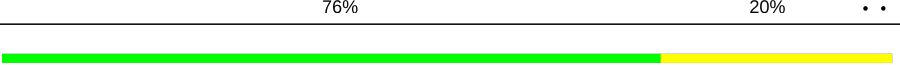
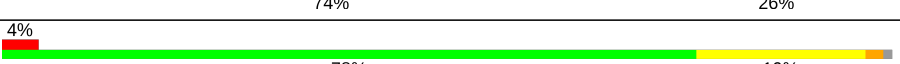
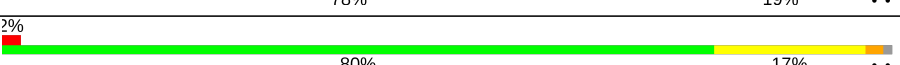
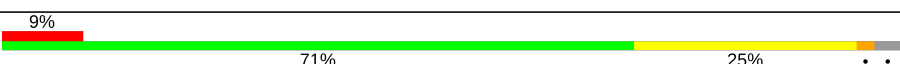

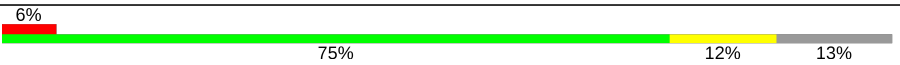



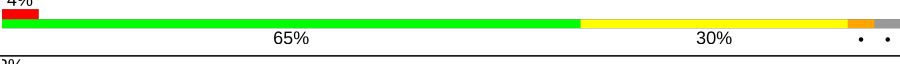

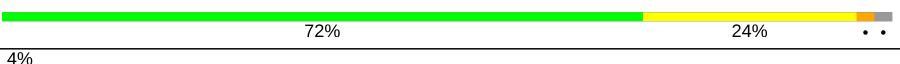



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2915	<div> <div>3%</div> <div>60% 32% 6% .</div> </div>
2	B	122	<div> <div>78% 19% . .</div> </div>
3	D	276	<div> <div>% 76% 22% .</div> </div>
4	E	206	<div> <div>2% 81% 17% . .</div> </div>
5	F	205	<div> <div>81% 17% . .</div> </div>
6	G	182	<div> <div>3% 74% 24% . .</div> </div>

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Mol	Chain	Length	Quality of chain
7	H	180	
8	J	173	
9	K	147	
10	N	140	
11	O	122	
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	

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

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Mol	Chain	Length	Quality of chain
57	y	679	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	PSU	x	32	-	-	-	X
33	MIA	x	37	-	-	-	X
33	5MU	x	54	-	-	-	X
33	PSU	x	55	-	-	-	X
33	4SU	x	8	-	-	-	X
58	MG	A	3011	-	-	-	X
58	MG	A	3056	-	-	-	X
58	MG	A	3058	-	-	-	X
58	MG	A	3132	-	-	-	X
58	MG	A	3152	-	-	-	X
58	MG	A	3160	-	-	-	X
58	MG	A	3161	-	-	-	X
58	MG	A	3165	-	-	-	X
58	MG	A	3213	-	-	-	X
58	MG	A	3226	-	-	-	X
58	MG	A	3282	-	-	-	X
58	MG	A	3608	-	-	-	X
58	MG	B	214	-	-	-	X
58	MG	P	201	-	-	-	X
58	MG	U	203	-	-	-	X
58	MG	a	3323	-	-	-	X
58	MG	a	3390	-	-	-	X
58	MG	x	3002	-	-	-	X
58	MG	x	3003	-	-	-	X

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 152111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

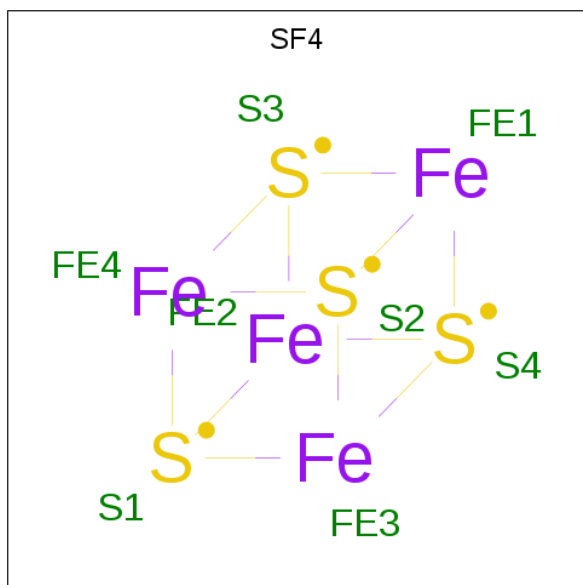
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y	1	Total 1	Zn 1	0	0
59	6	1	Total 1	Zn 1	0	0
59	4	1	Total 1	Zn 1	0	0

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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		

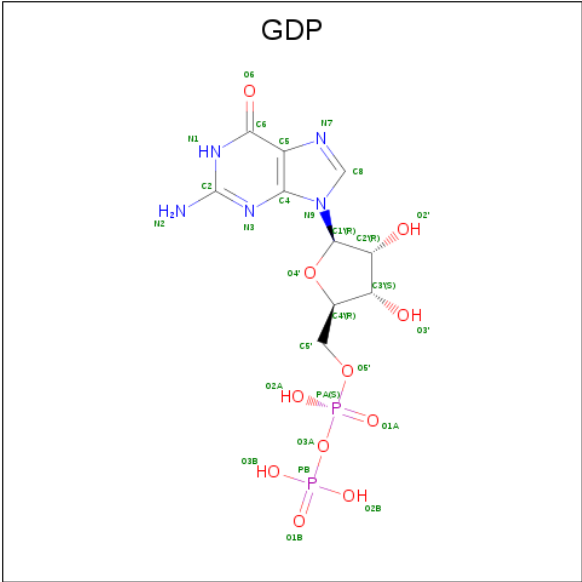
- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).





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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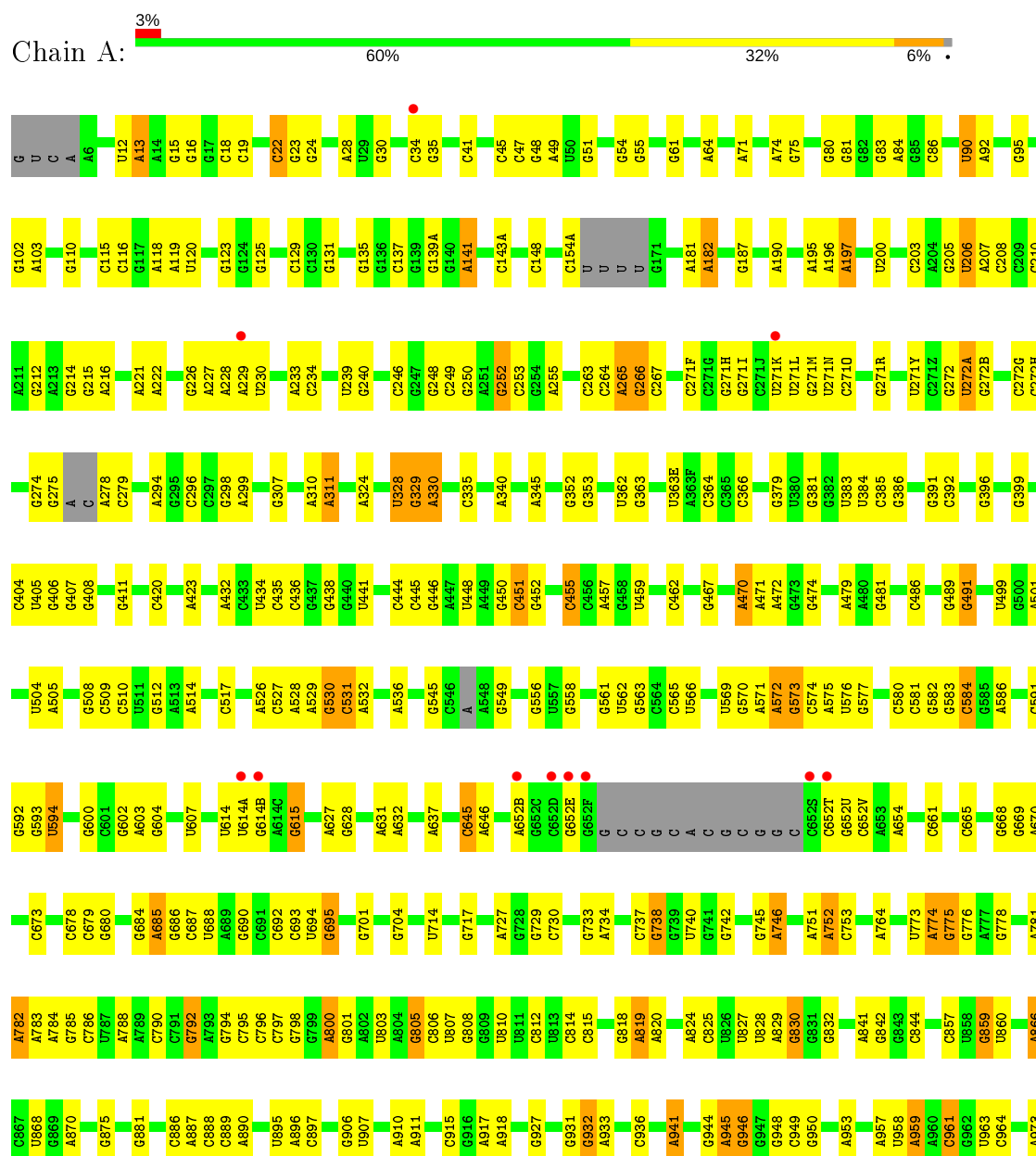
*Continued from previous page...*

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

### 3 Residue-property plots [i](#)

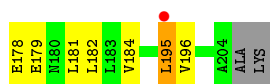
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 23S Ribosomal RNA



A2199	A2134	C2065	C1988	C1914	C1782	G1667	A1572	A1460	A1353	G1245	C1145	G1051	G974
C2200	A2135	G2069	G1989	A1918	A1787	A1668	U1578	G1461	U1357	A1246	G1149	C1052	C975
C2201	C2136	G2070	C1990	A1919	C1787	A1669	U1578	C1467	G1358	A1247		A1053	G975A
C2202	C2137	G2071	U1991	A1920	C1790	U1673	G1581		A1359	G1250	C1152	A1054	C976
U2203	C2138	A2072	G1992	G1921	A1791	C1672	C1582	A1471	A1360	C1251	C1153	G1055	G977
C2205	C2139	C2073	U1993		G1792	G1674	A1583		G1363	G1252	G1154	G1058	G978
G2206	C2140		C1996	C1924	C1793			U1481	C1362	A1253	A1155	G1059	G979
G2207	G2141		G1997	U1794	U1794	A1677	C1584	G1482	C1363	G1256	A1156	G1060	A990
G2223	C2143	C2078	G1998	A1927	C1795	U1680	C1586	G1491	C1364	C1257	U1157	U1061	A981
G2224	U2144	U2079	C1999	G1929	U1796	G1681	C1587	A1490	G1365	G1257	C1161	U1062	A982
A2225	C2145	G2080	G2000	G1930	C1797	G1681	C1588	G1492	A1365			G1062	A983
C2226	C2146		A2001	U1931	U1798		G1595	G1492	G1368	G1271	A1067	A984	A984
	G2147	C2084		G1932	G1799	C1691		C1493	G1369	A1272	C1166	G1068	C985
G2228	G2148	G2087	G2011	A1933	C1800	C1694	C1599		U1372	U1273		G1069	C986
G2229	G2149	G2088	U2011	G1933	G1801	G1695	G1500		A1373	A1274	G1171	A1070	A990
G2230	G2151		G2018	C1934	A1802	G1696	C1501		A1275	A1276	G1173		C991
	G2152	U2091	A2019	G1935	A1812	G1697	A1508		A1378	A1276	A1174	A1073	
U2233	G2153	A2092	A2020	A1936	G1813	C1698	A1509		A1379	G1277	U1175		A996
G2234	G2154	G2093	C2021	A1937	G1813	G1699	A1610		G1380	A1278	A1177		G997
G2235	G2155	G2094	U2022	A1938		U1700	G1613		A1384	G1285		C1076	
G2236	G2156	C2095	G2023	U1939	G1816	A1701	C1509		G1385			U1077	
G2238	G2157	U2096	G2024	U1940	G1817	G1702	A1514		C1386	G1289	G1191	C1078	
G2239	G2158	C2097	C2025	C1942	U1820		G1617			G1289		U1083	G1005
	G2159	U2098	C2026	U1943	A1821	G1705	A1618		A1395	G1299		A1084	G1006
G2242	G2160		G2027	U1944	G1822		G1619		A1398	U1300	U1198	A1085	C1007
U2243	C2161		U2028		G1823	G1721	G1620		C1398	A1301	U1199		G1008
	G2162	U2102	G2029	G1950	C1827	U1722	U1621			C1305		U1088	U1012
G2246	C2163	C2103	A2030	U1951	G1827	U1739	G1920		A1404	C1306	C1202	G1089	C1013
	G2164	G2104	A2031	A1952	G1828	G1740	U1622		U1405	A1307	G1203		U1014
U2249	G2165	C2105	G2032	A1953	A1829		G1628		U1406	A1308	A1204	A1095	G1015
G2250	U2166	G2106	A2033	G1954	C1837	C1745	U1629		G1433	G1309	U1205		G1016
G2251	U2167	U2034	G2033	U1955	C1837	C1745A	A1631A		G1436	G1310	G1207	U1108	G1017
G2252	C2168	C2108	G2035	U1956	C1838	G1746	G1632		U1437		G1208	G1110	U1019
G2253	A2169	U2109		C1957	G1838	G1747	G1633			U1313	G1209	A1111	A1020
	A2170	G2110	G2038	G1958	G1842		A1634		G1446	C1314	A1210	G1112	A1021
	A2171	C2111	C2039	G1959		C1751	A1637		U1420		U1211		G1022
U2257	U2172	G2112	C2040	A1960	A1847	G1756	A1637		G1424	C1320	G1115		U1025
	A2173	U2113		C1961		U1757	G1644			A1321		U1026	U1027
C2261	C2174	G2115	C2043	C1962	G1877	G1758	C1645		A1427	A1322	C1119		G1030
U2262	C2175	G2116		U1963	G1878		G1646		C1428			G1123	
	C2176	G2117	U2047	G1964	A1889	G1761	C1645		G1429	G1325	G1218	G1124	
U2265	C2177	U2118	G2048	C1965	A1895	A1762	G1647		C1430	G1328	A1227		U1033
A2268	C2178	U2119	G2049	A1966	G1896	G1763	G1648		G1436	U1329	C1222	A1127	G1034
	C2179	A2180	C2050	C1967	G1897	G1764	G1649		C1437		C1224	A1128	U1035
G2271	U2180	G2121	A2051	A1970	U1898		G1650			G1332	G1227	A1129	G1036
U2272	G2181	U2122	G2052	A1971	U1898	C1767	G1651					U1130	
A2273	G2182	G2123	G2053	A1972	G1899		A1652			G1338	G1230	G1131	G1037
U2274	C2183	G2124	A2054	A1973	A1900		G1653		A1445	G1339	C1135		G1038
C2275	G2184	G2125	C2055		A1901	G1772	A1654		G1450		C1136	C1041	
G2276	C2185	A2057	G2056	A1977	C1902	A1773	A1655		C1450A	A1342	C1230	G1042	
	G2186	A2126	G2057	G1978	G1903	C1774	C1656			G1343	G1137		
G2279	G2187	G2127	A2058	A1979	G1903	U1775	C1657				G1236	G1138	
	C2188	C2128	A2059	C1979	G1906	G1776							
U2189	U2189	C2129	A2060	G1980		U1778							
C2283	G2190	U2130	G2061	A1981		U1778							
C2284		G2131	A2062	C1982		U1779							
C2285		U2197	C2063	C1983		U1780							
A2286						A1569			G1455		G1239	A1142A	A1045
A2287						A1571			G1459		G1244	A1143	G1046
												G1144	





- Molecule 5: 50S ribosomal protein L4

Chain F: 81% 17% ..



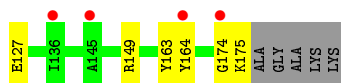
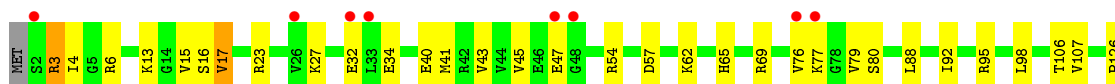
- Molecule 6: 50S ribosomal protein L5

Chain G: 3% 74% 24% ..



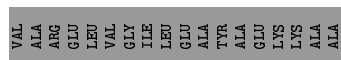
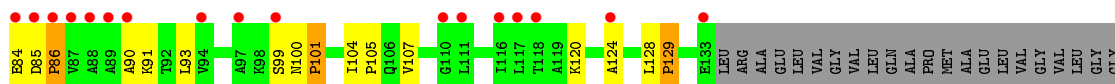
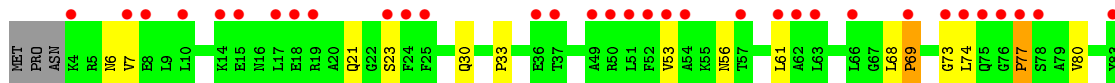
- Molecule 7: 50S ribosomal protein L6

Chain H: 7% 76% 20% ..

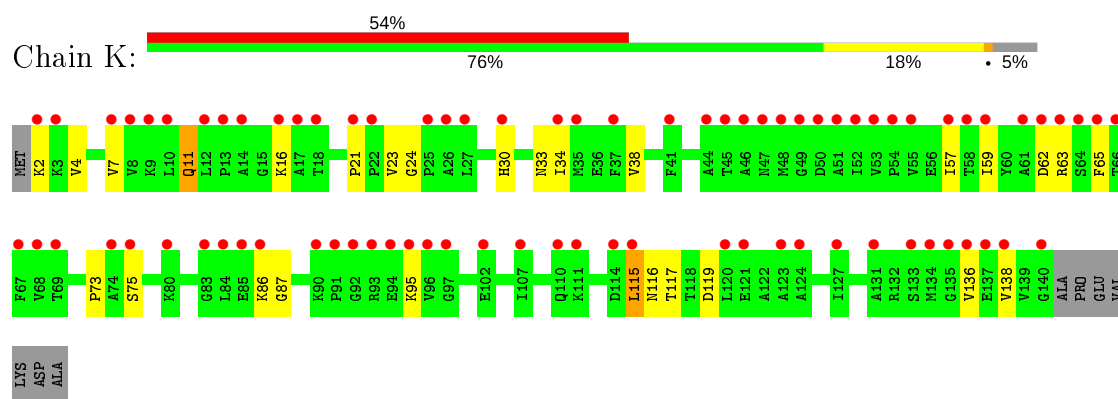


- Molecule 8: 50S ribosomal protein L10

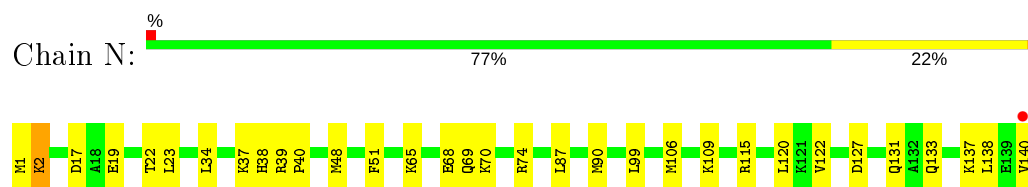
Chain J: 29% 57% 15% 25%



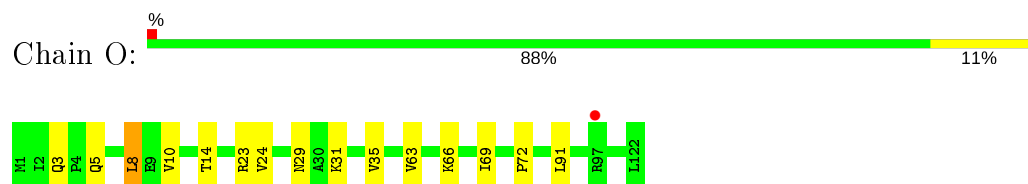
- Molecule 9: 50S ribosomal protein L11



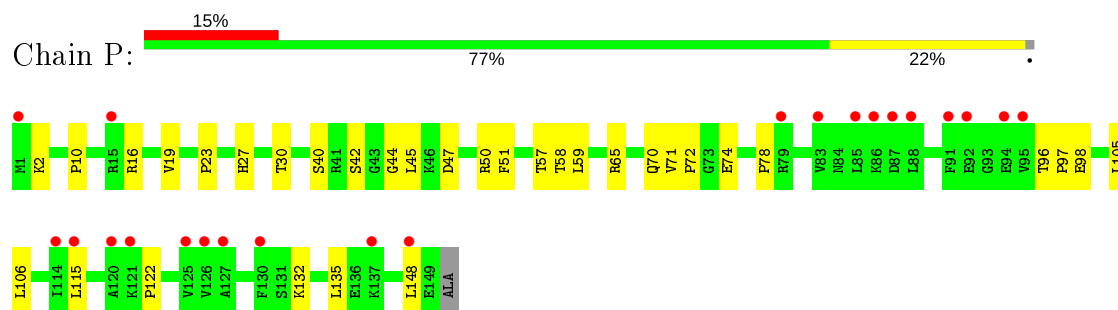
- Molecule 10: 50S ribosomal protein L13



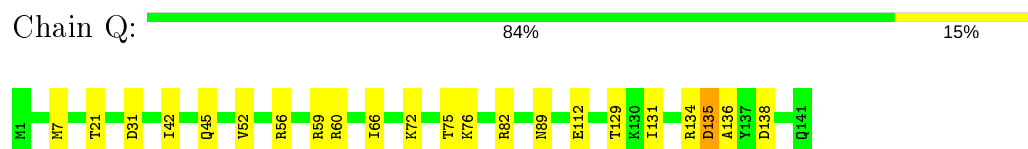
- Molecule 11: 50S ribosomal protein L14



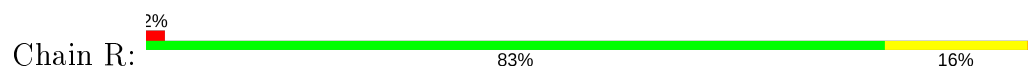
- Molecule 12: 50S ribosomal protein L15

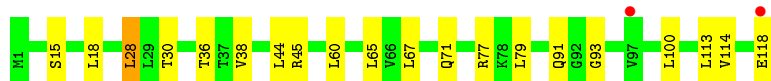


- Molecule 13: 50S ribosomal protein L16

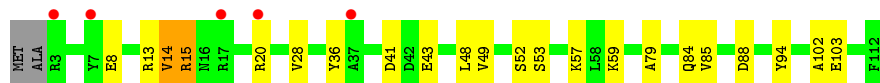
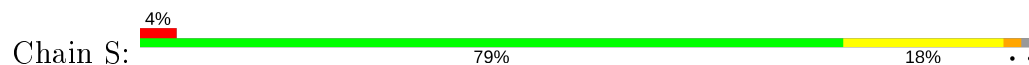


- Molecule 14: 50S ribosomal protein L17

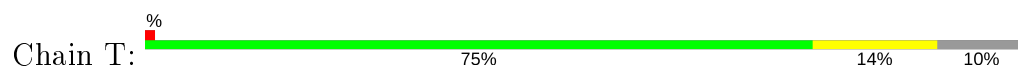




- Molecule 15: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L19



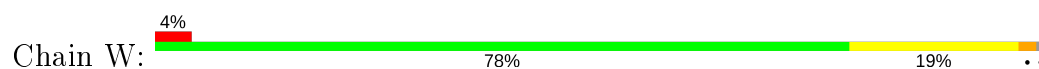
- Molecule 17: 50S ribosomal protein L20



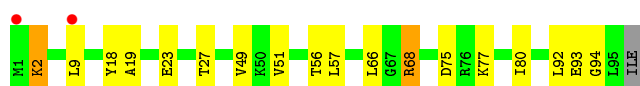
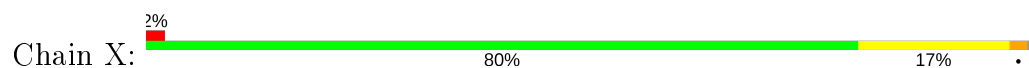
- Molecule 18: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L22

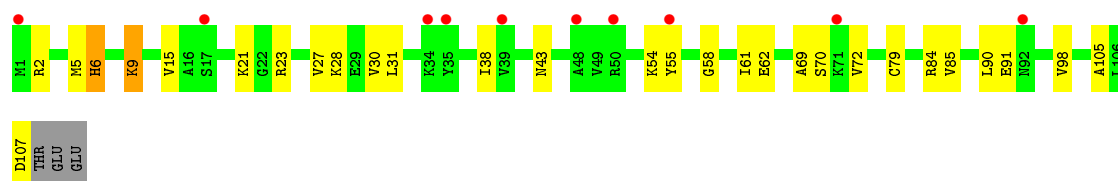


- Molecule 20: 50S ribosomal protein L23

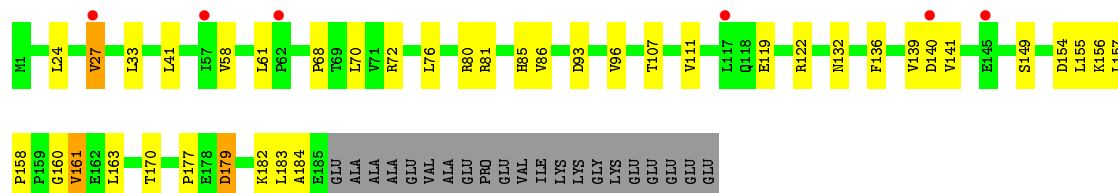


- Molecule 21: 50S ribosomal protein L24





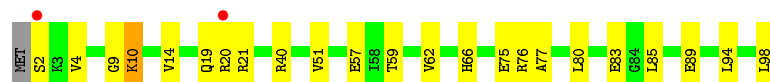
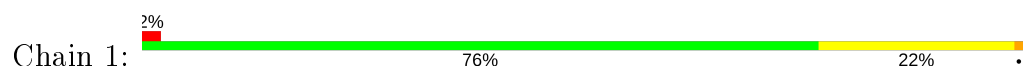
- Molecule 22: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L27



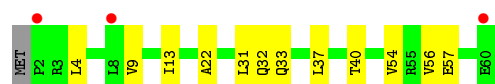
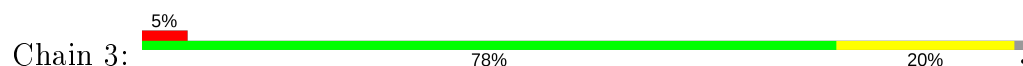
- Molecule 24: 50S ribosomal protein L28



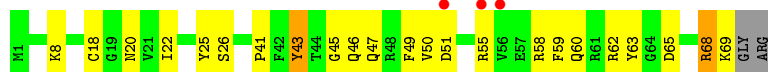
- Molecule 25: 50S ribosomal protein L29



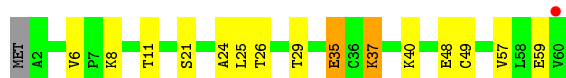
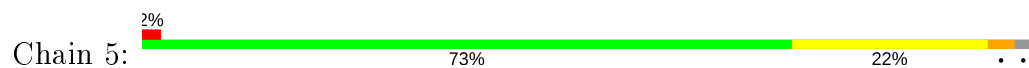
- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L31



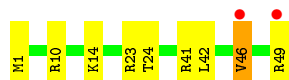
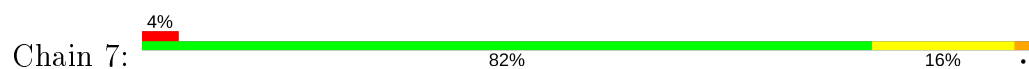
- Molecule 28: 50S ribosomal protein L32



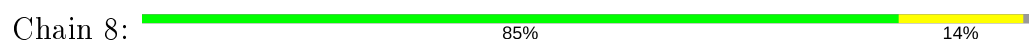
- Molecule 29: 50S ribosomal protein L33



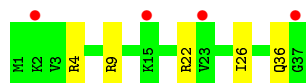
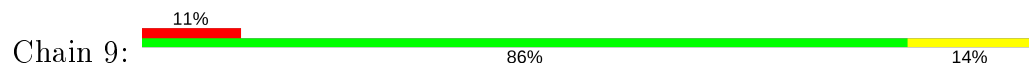
- Molecule 30: 50S ribosomal protein L34



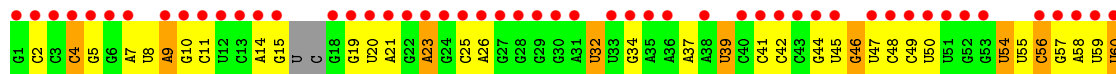
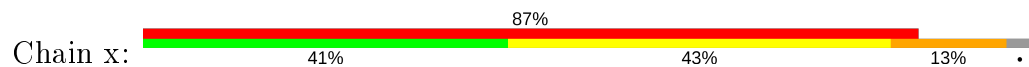
- Molecule 31: 50S ribosomal protein L35

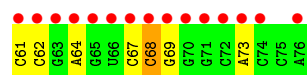


- Molecule 32: 50S ribosomal protein L36



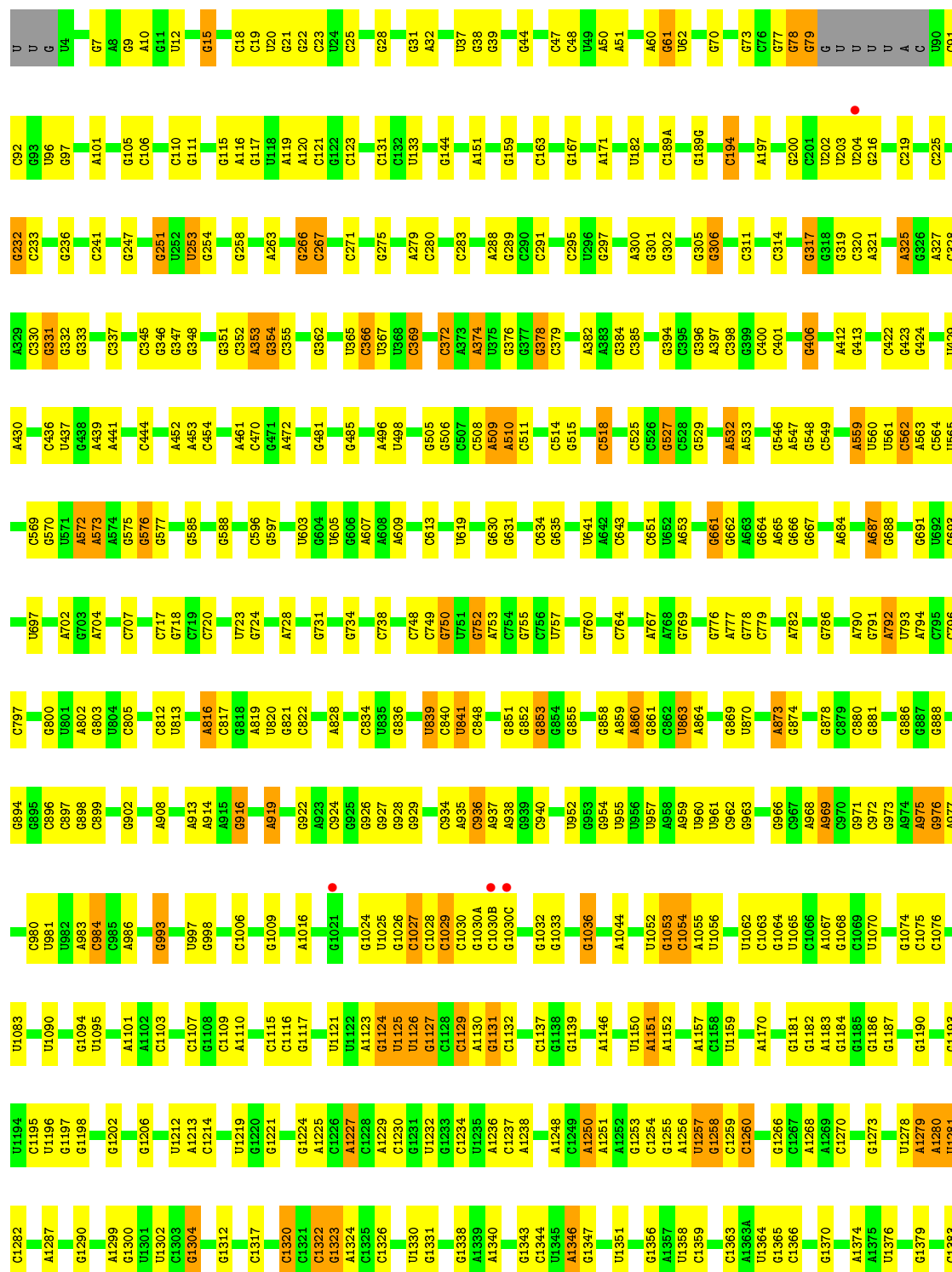
- Molecule 33: E-site tRNA

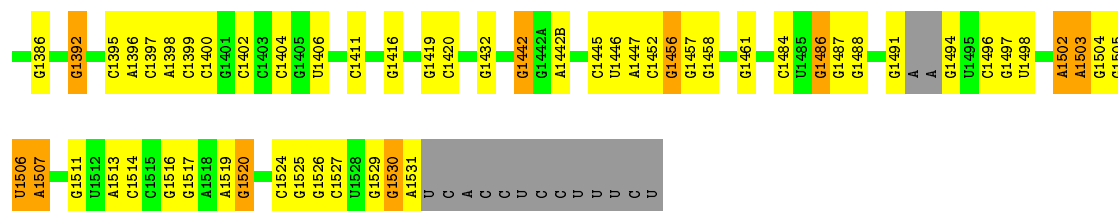




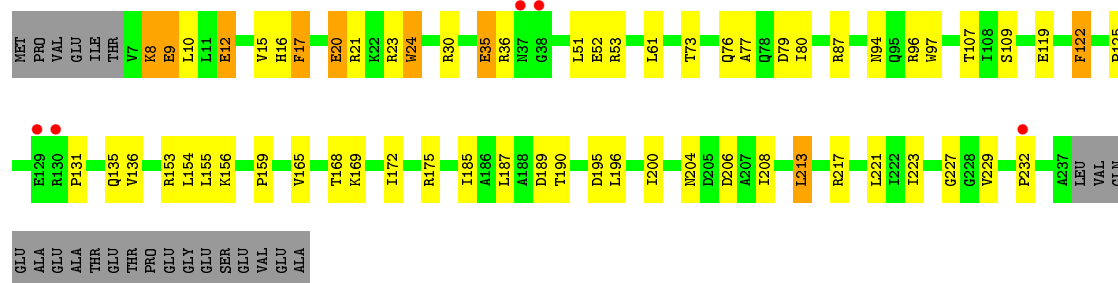
● Molecule 34: 16S Ribosomal RNA

Chain a: 63% 30% 6%

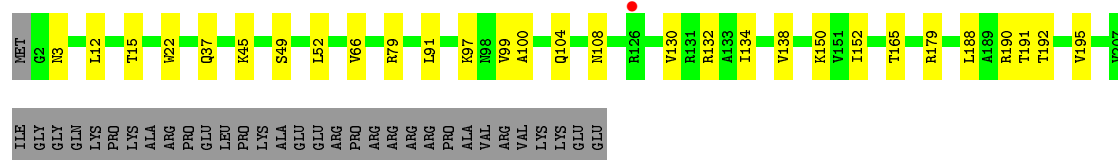




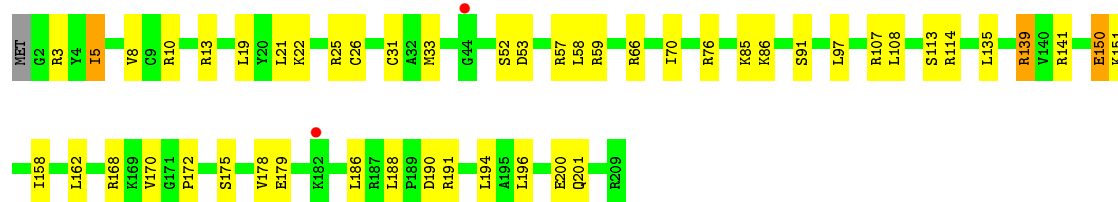
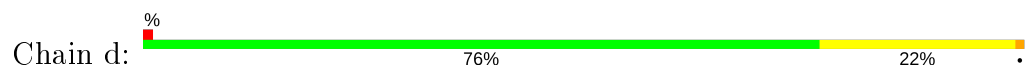
• Molecule 35: 30S ribosomal protein S2



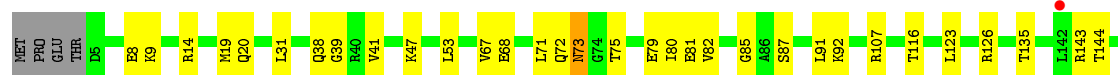
• Molecule 36: 30S ribosomal protein S3

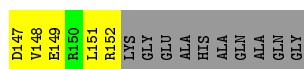


• Molecule 37: 30S ribosomal protein S4

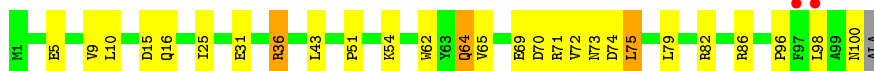


• Molecule 38: 30S ribosomal protein S5

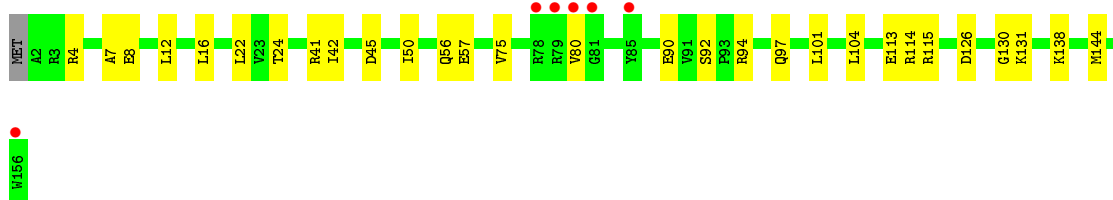
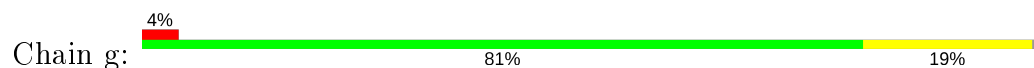




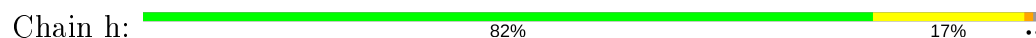
- Molecule 39: 30S ribosomal protein S6



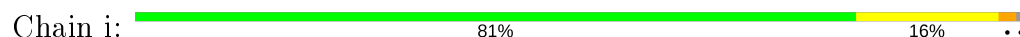
- Molecule 40: 30S ribosomal protein S7



- Molecule 41: 30S ribosomal protein S8



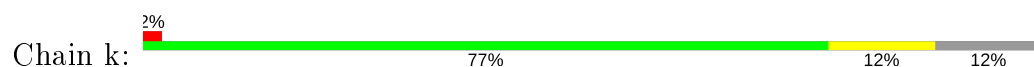
- Molecule 42: 30S ribosomal protein S9



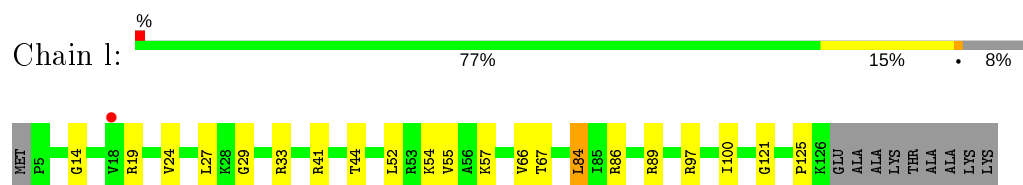
- Molecule 43: 30S ribosomal protein S10



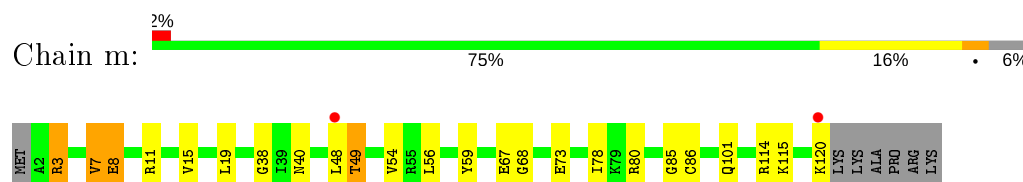
- Molecule 44: 30S ribosomal protein S11



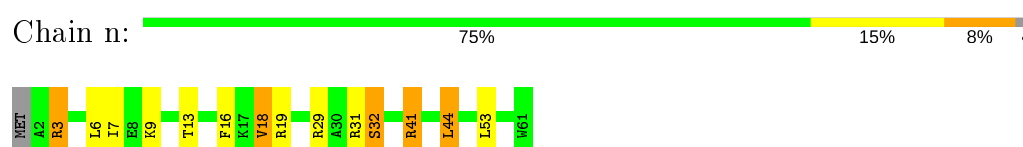
- Molecule 45: 30S ribosomal protein S12



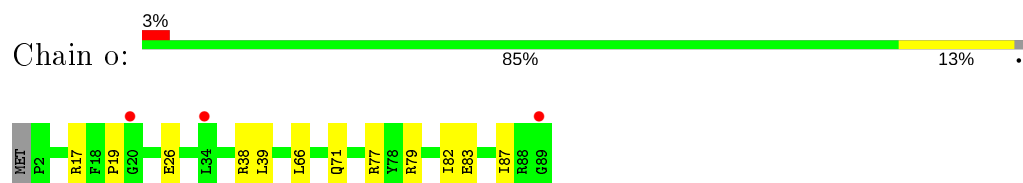
- Molecule 46: 30S ribosomal protein S13



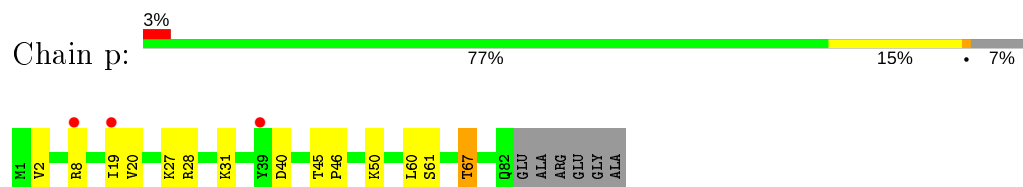
- Molecule 47: 30S ribosomal protein S14 type Z



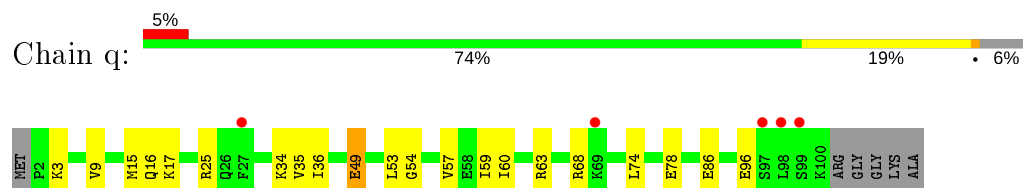
- Molecule 48: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S16

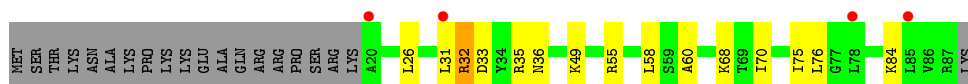


- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18





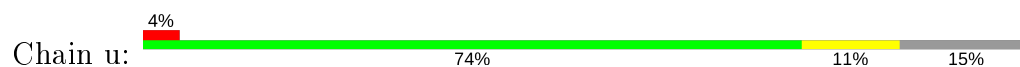
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



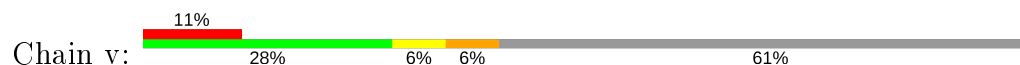
- Molecule 54: 30S ribosomal protein Thx



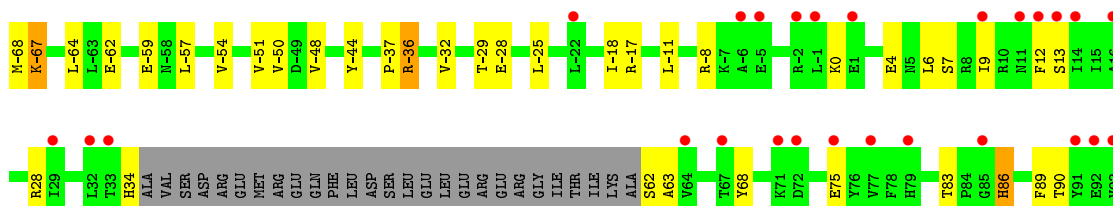
- Molecule 55: P-site tRNA



- Molecule 56: mRNA



- Molecule 57: 50S ribosomal protein L9, Elongation factor 4







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.238 , 0.304 0.239 , 0.303	Depositor DCC
$R_{free}$ test set	29295 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 66.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	152111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	2	7
4	E	202/206 (98%)	165 (82%)	27 (13%)	10 (5%)	2	7
5	F	201/205 (98%)	152 (76%)	37 (18%)	12 (6%)	1	4
6	G	179/182 (98%)	143 (80%)	25 (14%)	11 (6%)	1	4
7	H	172/180 (96%)	128 (74%)	34 (20%)	10 (6%)	1	5
8	J	128/173 (74%)	69 (54%)	31 (24%)	28 (22%)	0	0
9	K	137/147 (93%)	94 (69%)	33 (24%)	10 (7%)	1	3
10	N	138/140 (99%)	106 (77%)	24 (17%)	8 (6%)	1	5
11	O	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	4	15
12	P	147/150 (98%)	108 (74%)	29 (20%)	10 (7%)	1	3
13	Q	139/141 (99%)	122 (88%)	12 (9%)	5 (4%)	3	14
14	R	116/118 (98%)	92 (79%)	21 (18%)	3 (3%)	5	20
15	S	108/112 (96%)	77 (71%)	20 (18%)	11 (10%)	0	1
16	T	129/146 (88%)	113 (88%)	15 (12%)	1 (1%)	19	51
17	U	114/118 (97%)	92 (81%)	16 (14%)	6 (5%)	2	6
18	V	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	1	1
19	W	110/113 (97%)	86 (78%)	14 (13%)	10 (9%)	1	1
20	X	93/96 (97%)	73 (78%)	12 (13%)	8 (9%)	1	2
21	Y	105/110 (96%)	82 (78%)	12 (11%)	11 (10%)	0	1
22	Z	183/206 (89%)	145 (79%)	24 (13%)	14 (8%)	1	2
23	0	72/85 (85%)	65 (90%)	6 (8%)	1 (1%)	11	36
24	1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	4
25	2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	10	34
26	3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	14
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	2
29	6	51/54 (94%)	43 (84%)	6 (12%)	2 (4%)	3	12
30	7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	7	26
31	8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
32	9	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	4	18
35	b	229/256 (90%)	167 (73%)	41 (18%)	21 (9%)	1	1
36	c	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	3	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	d	206/209 (99%)	163 (79%)	33 (16%)	10 (5%)	2	8
38	e	146/162 (90%)	108 (74%)	30 (20%)	8 (6%)	2	5
39	f	98/101 (97%)	70 (71%)	20 (20%)	8 (8%)	1	2
40	g	153/156 (98%)	123 (80%)	26 (17%)	4 (3%)	5	20
41	h	135/138 (98%)	115 (85%)	18 (13%)	2 (2%)	10	34
42	i	125/128 (98%)	98 (78%)	17 (14%)	10 (8%)	1	2
43	j	94/105 (90%)	73 (78%)	12 (13%)	9 (10%)	0	1
44	k	112/129 (87%)	88 (79%)	20 (18%)	4 (4%)	3	14
45	l	120/132 (91%)	106 (88%)	9 (8%)	5 (4%)	3	10
46	m	117/126 (93%)	91 (78%)	16 (14%)	10 (8%)	1	2
47	n	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	6
48	o	86/89 (97%)	69 (80%)	15 (17%)	2 (2%)	6	23
49	p	80/88 (91%)	61 (76%)	17 (21%)	2 (2%)	5	21
50	q	97/105 (92%)	78 (80%)	13 (13%)	6 (6%)	1	4
51	r	66/88 (75%)	57 (86%)	6 (9%)	3 (4%)	2	9
52	s	81/93 (87%)	64 (79%)	9 (11%)	8 (10%)	0	1
53	t	94/106 (89%)	74 (79%)	10 (11%)	10 (11%)	0	1
54	u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
57	y	640/679 (94%)	534 (83%)	67 (10%)	39 (6%)	1	4
All	All	6466/6910 (94%)	5145 (80%)	924 (14%)	397 (6%)	1	4

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%)	0	2
4	E	164/166 (99%)	134 (82%)	30 (18%)	1	5
5	F	160/162 (99%)	133 (83%)	27 (17%)	2	6
6	G	143/156 (92%)	103 (72%)	40 (28%)	0	1
7	H	144/148 (97%)	115 (80%)	29 (20%)	1	4
9	K	104/111 (94%)	84 (81%)	20 (19%)	1	4
10	N	118/119 (99%)	93 (79%)	25 (21%)	1	3
11	O	100/100 (100%)	89 (89%)	11 (11%)	6	19
12	P	115/116 (99%)	93 (81%)	22 (19%)	1	4
13	Q	111/111 (100%)	93 (84%)	18 (16%)	2	7
14	R	101/101 (100%)	83 (82%)	18 (18%)	2	5
15	S	87/88 (99%)	74 (85%)	13 (15%)	3	9
16	T	115/127 (91%)	95 (83%)	20 (17%)	2	6
17	U	93/94 (99%)	72 (77%)	21 (23%)	1	2
18	V	80/82 (98%)	63 (79%)	17 (21%)	1	3
19	W	90/92 (98%)	74 (82%)	16 (18%)	2	5
20	X	77/78 (99%)	65 (84%)	12 (16%)	2	8
21	Y	85/91 (93%)	66 (78%)	19 (22%)	1	2
22	Z	156/179 (87%)	127 (81%)	29 (19%)	1	5
23	0	59/67 (88%)	50 (85%)	9 (15%)	2	8
24	1	80/83 (96%)	62 (78%)	18 (22%)	1	2
25	2	65/67 (97%)	50 (77%)	15 (23%)	1	2
26	3	51/52 (98%)	42 (82%)	9 (18%)	2	5
27	4	60/63 (95%)	46 (77%)	14 (23%)	1	2
28	5	51/52 (98%)	39 (76%)	12 (24%)	1	2
29	6	51/52 (98%)	38 (74%)	13 (26%)	0	1
30	7	42/42 (100%)	33 (79%)	9 (21%)	1	3
31	8	53/55 (96%)	44 (83%)	9 (17%)	2	6
32	9	34/34 (100%)	30 (88%)	4 (12%)	5	16
35	b	193/220 (88%)	144 (75%)	49 (25%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	c	142/188 (76%)	121 (85%)	21 (15%)	3	9
37	d	169/181 (93%)	129 (76%)	40 (24%)	1	2
38	e	113/123 (92%)	83 (74%)	30 (26%)	0	1
39	f	83/90 (92%)	62 (75%)	21 (25%)	0	2
40	g	118/127 (93%)	93 (79%)	25 (21%)	1	3
41	h	114/119 (96%)	91 (80%)	23 (20%)	1	4
42	i	90/99 (91%)	76 (84%)	14 (16%)	2	8
43	j	65/92 (71%)	49 (75%)	16 (25%)	0	2
44	k	82/99 (83%)	71 (87%)	11 (13%)	4	11
45	l	97/109 (89%)	82 (84%)	15 (16%)	2	8
46	m	89/101 (88%)	73 (82%)	16 (18%)	1	5
47	n	49/50 (98%)	36 (74%)	13 (26%)	0	1
48	o	78/80 (98%)	68 (87%)	10 (13%)	4	13
49	p	69/74 (93%)	56 (81%)	13 (19%)	1	4
50	q	94/97 (97%)	78 (83%)	16 (17%)	2	6
51	r	59/77 (77%)	46 (78%)	13 (22%)	1	3
52	s	68/80 (85%)	50 (74%)	18 (26%)	0	1
53	t	69/82 (84%)	58 (84%)	11 (16%)	2	7
54	u	18/22 (82%)	15 (83%)	3 (17%)	2	6
57	y	289/560 (52%)	193 (67%)	96 (33%)	0	0
All	All	4952/5576 (89%)	3927 (79%)	1025 (21%)	1	3

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	4SU	w	8	55	14,21,22	1.20	1 (7%)	15,30,33	1.51	2 (13%)
33	MIA	x	37	33	18,24,32	1.16	2 (11%)	18,35,47	1.24	2 (11%)
33	PSU	x	55	33	17,21,22	1.63	3 (17%)	20,30,33	3.05	6 (30%)
55	5MU	w	54	55	15,22,23	1.05	2 (13%)	16,32,35	1.90	1 (6%)
33	5MU	x	54	33	15,22,23	1.12	1 (6%)	16,32,35	1.98	2 (12%)
33	PSU	x	32	33	17,21,22	1.46	2 (11%)	20,30,33	3.17	6 (30%)
55	PSU	w	32	55	17,21,22	1.52	3 (17%)	20,30,33	3.34	6 (30%)
55	PSU	w	39	55	17,21,22	1.55	3 (17%)	20,30,33	2.82	6 (30%)
55	MIA	w	37	55	24,31,32	2.75	5 (20%)	26,44,47	3.57	7 (26%)
55	PSU	w	55	55	17,21,22	1.59	3 (17%)	20,30,33	2.89	6 (30%)
55	F3O	w	76	55,58	30,36,37	1.04	1 (3%)	33,51,54	1.58	5 (15%)
33	4SU	x	8	33	14,21,22	1.31	1 (7%)	15,30,33	1.39	2 (13%)
33	PSU	x	39	33	17,21,22	1.52	2 (11%)	20,30,33	3.24	7 (35%)
33	7MG	x	46	33	22,26,27	1.68	4 (18%)	28,39,42	3.20	12 (42%)
55	7MG	w	46	55	22,26,27	1.72	4 (18%)	28,39,42	2.67	8 (28%)

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	4SU	w	8	55	-	0/5/25/26	0/2/2/2
33	MIA	x	37	33	-	3/3/25/34	0/3/3/3
33	PSU	x	55	33	-	0/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/5/25/26	0/2/2/2
33	5MU	x	54	33	-	3/5/25/26	0/2/2/2
33	PSU	x	32	33	-	2/7/25/26	0/2/2/2
55	PSU	w	32	55	-	0/7/25/26	0/2/2/2
55	PSU	w	39	55	-	0/7/25/26	0/2/2/2
55	MIA	w	37	55	-	4/11/33/34	0/3/3/3
55	PSU	w	55	55	-	0/7/25/26	0/2/2/2
55	F3O	w	76	55,58	-	6/15/37/38	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	4SU	x	8	33	-	0/5/25/26	0/2/2/2
33	PSU	x	39	33	-	2/7/25/26	0/2/2/2
33	7MG	x	46	33	-	4/7/37/38	0/3/3/3
55	7MG	w	46	55	-	1/7/37/38	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	37	MIA	C2-S10	-9.18	1.67	1.75
55	w	37	MIA	C13-C14	7.75	1.54	1.32
55	w	46	7MG	C6-C5	5.33	1.48	1.41
33	x	55	PSU	C5-C1'	-4.75	1.48	1.52
33	x	46	7MG	C5-C4	4.38	1.47	1.39

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	37	MIA	C11-S10-C2	-15.14	90.96	102.27
33	x	46	7MG	N3-C4-N9	11.28	141.39	126.91
55	w	32	PSU	N1-C2-N3	-9.58	120.81	128.43
33	x	39	PSU	N1-C2-N3	-8.88	121.37	128.43
33	x	32	PSU	N1-C2-N3	-8.75	121.47	128.43

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	x	37	MIA	C3'-C4'-C5'-O5'
33	x	54	5MU	C2'-C1'-N1-C6
33	x	54	5MU	C3'-C4'-C5'-O5'
33	x	32	PSU	O4'-C4'-C5'-O5'
55	w	37	MIA	C5-C6-N6-C12

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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	0,12,12	0.00	-	-		
61	GDP	y	703	58	24,30,30	1.31	2 (8%)	31,47,47	1.95	8 (25%)

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	-	-	0/6/5/5
61	GDP	y	703	58	-	1/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	y	703	GDP	C6-C5	4.75	1.49	1.41
61	y	703	GDP	C5-C4	2.62	1.47	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	y	703	GDP	C2-N3-C4	5.76	121.93	115.36
61	y	703	GDP	C5-C6-N1	-3.86	118.15	123.43
61	y	703	GDP	C6-N1-C2	3.43	121.37	115.93
61	y	703	GDP	C4-C5-N7	-3.36	105.90	109.40
61	y	703	GDP	C3'-C2'-C1'	3.28	105.91	100.98

There are no chirality outliers.

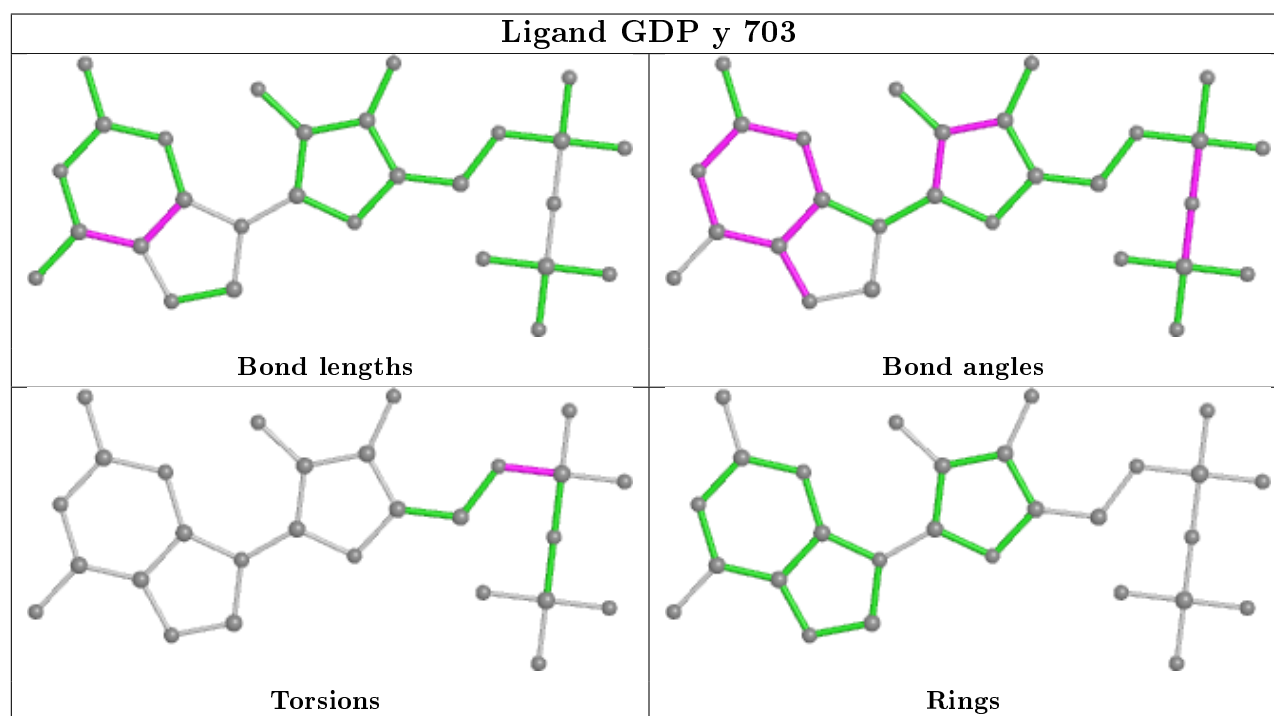
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	y	703	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2873/2915 (98%)	-0.06	101 (3%) 44 38	35, 61, 175, 394	0
2	B	120/122 (98%)	-0.11	0 100 100	65, 93, 121, 133	0
3	D	275/276 (99%)	-0.01	4 (1%) 73 73	35, 56, 75, 108	0
4	E	204/206 (99%)	-0.14	4 (1%) 65 63	34, 57, 77, 101	0
5	F	203/205 (99%)	0.03	1 (0%) 91 91	38, 70, 108, 135	0
6	G	181/182 (99%)	-0.06	5 (2%) 53 49	68, 84, 106, 128	0
7	H	174/180 (96%)	0.42	12 (6%) 16 13	62, 96, 131, 154	0
8	J	130/173 (75%)	2.10	50 (38%) 0 0	129, 161, 183, 197	0
9	K	139/147 (94%)	2.84	80 (57%) 0 0	192, 218, 229, 234	0
10	N	140/140 (100%)	-0.01	1 (0%) 87 87	47, 64, 93, 110	0
11	O	122/122 (100%)	-0.00	1 (0%) 86 86	37, 52, 68, 75	0
12	P	149/150 (99%)	0.68	22 (14%) 2 1	42, 81, 109, 116	0
13	Q	141/141 (100%)	-0.00	0 100 100	44, 64, 80, 97	0
14	R	118/118 (100%)	0.34	2 (1%) 70 69	46, 66, 86, 102	0
15	S	110/112 (98%)	0.27	5 (4%) 33 29	75, 90, 102, 113	0
16	T	131/146 (89%)	-0.04	1 (0%) 86 86	49, 61, 94, 113	0
17	U	116/118 (98%)	-0.09	0 100 100	42, 56, 75, 83	0
18	V	101/101 (100%)	0.04	0 100 100	41, 73, 93, 104	0
19	W	112/113 (99%)	0.28	4 (3%) 42 37	46, 62, 89, 128	0
20	X	95/96 (98%)	0.17	2 (2%) 63 61	56, 74, 95, 116	0
21	Y	107/110 (97%)	0.64	10 (9%) 8 6	66, 79, 116, 137	0
22	Z	185/206 (89%)	0.29	6 (3%) 47 43	68, 90, 114, 135	0
23	0	74/85 (87%)	0.51	5 (6%) 17 13	50, 67, 85, 105	0
24	1	97/98 (98%)	0.37	2 (2%) 63 61	48, 68, 104, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	2	70/72 (97%)	0.15	0 100 100	69, 86, 100, 109	0
26	3	59/60 (98%)	0.42	3 (5%) 28 24	52, 68, 101, 116	0
27	4	69/71 (97%)	0.13	3 (4%) 35 31	80, 107, 150, 158	0
28	5	59/60 (98%)	-0.24	1 (1%) 70 69	41, 63, 81, 100	0
29	6	53/54 (98%)	0.04	0 100 100	62, 71, 85, 87	0
30	7	49/49 (100%)	0.08	2 (4%) 37 32	40, 49, 73, 96	0
31	8	64/65 (98%)	0.10	0 100 100	51, 59, 65, 86	0
32	9	37/37 (100%)	0.76	4 (10%) 5 4	52, 63, 78, 88	0
33	x	67/76 (88%)	5.04	66 (98%) 0 0	94, 267, 283, 306	0
34	a	1496/1521 (98%)	-0.26	4 (0%) 94 94	37, 60, 119, 295	0
35	b	231/256 (90%)	-0.11	5 (2%) 62 59	53, 84, 134, 165	0
36	c	206/239 (86%)	-0.36	1 (0%) 91 91	50, 65, 88, 99	0
37	d	208/209 (99%)	0.03	2 (0%) 82 82	52, 68, 95, 109	0
38	e	148/162 (91%)	-0.25	1 (0%) 87 87	40, 55, 72, 107	0
39	f	100/101 (99%)	0.22	2 (2%) 65 63	74, 106, 138, 146	0
40	g	155/156 (99%)	-0.00	6 (3%) 39 35	54, 73, 124, 156	0
41	h	137/138 (99%)	0.03	0 100 100	47, 59, 72, 90	0
42	i	127/128 (99%)	0.07	0 100 100	45, 70, 91, 102	0
43	j	96/105 (91%)	-0.01	3 (3%) 49 44	42, 70, 119, 133	0
44	k	114/129 (88%)	0.05	3 (2%) 56 52	49, 77, 96, 104	0
45	l	122/132 (92%)	-0.17	1 (0%) 86 86	39, 53, 68, 80	0
46	m	119/126 (94%)	-0.03	2 (1%) 70 69	43, 72, 99, 111	0
47	n	60/61 (98%)	-0.27	0 100 100	42, 51, 66, 69	0
48	o	88/89 (98%)	0.19	3 (3%) 45 40	57, 74, 98, 107	0
49	p	82/88 (93%)	0.20	3 (3%) 41 37	45, 57, 69, 85	0
50	q	99/105 (94%)	0.12	5 (5%) 28 24	50, 62, 80, 93	0
51	r	68/88 (77%)	0.52	4 (5%) 22 18	67, 85, 107, 116	0
52	s	83/93 (89%)	-0.20	0 100 100	45, 57, 76, 89	0
53	t	96/106 (90%)	0.17	1 (1%) 82 82	51, 65, 88, 96	0
54	u	23/27 (85%)	0.43	1 (4%) 35 31	54, 62, 69, 79	0
55	w	68/76 (89%)	-0.31	0 100 100	43, 75, 96, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
56	v	7/18 (38%)	1.39	2 (28%) 0 0	49, 50, 130, 149	0
57	y	644/679 (94%)	1.55	202 (31%) 0 0	69, 151, 188, 213	0
All	All	11201/11638 (96%)	0.17	648 (5%) 23 19	34, 68, 168, 394	0

The worst 5 of 648 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	J	51	LEU	23.3
9	K	52	ILE	16.9
1	A	2178	C	15.9
1	A	2145	C	13.3
1	A	2165	G	13.2

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	5MU	x	54	21/22	0.20	0.65	275,282,283,285	0
33	4SU	x	8	20/21	0.32	0.42	263,275,277,277	0
33	PSU	x	55	20/21	0.33	0.83	274,285,289,293	0
33	7MG	x	46	24/25	0.34	0.36	275,282,285,287	0
33	PSU	x	32	20/21	0.41	0.63	188,202,216,216	0
33	MIA	x	37	22/30	0.50	0.78	204,221,237,241	0
33	PSU	x	39	20/21	0.73	0.33	175,193,200,201	0
55	F3O	w	76	33/34	0.92	0.26	50,60,79,81	0
55	7MG	w	46	24/25	0.92	0.18	59,76,103,118	0
55	PSU	w	55	20/21	0.93	0.17	75,83,85,86	0
55	4SU	w	8	20/21	0.95	0.14	56,58,64,64	0
55	MIA	w	37	29/30	0.95	0.17	46,55,61,64	0
55	PSU	w	39	20/21	0.96	0.14	41,50,55,56	0
55	5MU	w	54	21/22	0.96	0.14	67,77,82,84	0
55	PSU	w	32	20/21	0.97	0.12	40,46,49,51	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	A	3608	1/1	0.29	0.47	108,108,108,108	0
58	MG	A	3157	1/1	0.34	0.24	118,118,118,118	0
58	MG	A	3435	1/1	0.37	0.38	95,95,95,95	0
58	MG	a	3390	1/1	0.44	0.44	45,45,45,45	0
58	MG	x	3001	1/1	0.50	0.28	237,237,237,237	0
58	MG	U	203	1/1	0.54	0.47	67,67,67,67	0
58	MG	x	3003	1/1	0.55	1.33	215,215,215,215	0
58	MG	A	3282	1/1	0.56	0.44	66,66,66,66	0
58	MG	D	302	1/1	0.58	0.29	74,74,74,74	0
58	MG	A	3056	1/1	0.59	0.42	68,68,68,68	0
58	MG	A	3265	1/1	0.60	0.18	61,61,61,61	0
58	MG	B	215	1/1	0.61	0.12	114,114,114,114	0
58	MG	A	3011	1/1	0.61	0.47	79,79,79,79	0
58	MG	0	101	1/1	0.62	0.39	73,73,73,73	0
58	MG	a	3323	1/1	0.62	0.49	69,69,69,69	0
58	MG	B	214	1/1	0.62	1.50	83,83,83,83	0
58	MG	A	3253	1/1	0.63	0.30	66,66,66,66	0
58	MG	B	216	1/1	0.63	0.12	86,86,86,86	0
58	MG	A	3161	1/1	0.63	0.45	67,67,67,67	0
58	MG	B	209	1/1	0.65	0.27	70,70,70,70	0
58	MG	A	3216	1/1	0.66	0.38	62,62,62,62	0
58	MG	A	3160	1/1	0.66	0.49	61,61,61,61	0
58	MG	A	3093	1/1	0.66	0.32	81,81,81,81	0
58	MG	A	3068	1/1	0.66	0.27	56,56,56,56	0
58	MG	A	3354	1/1	0.67	0.24	101,101,101,101	0
58	MG	A	3577	1/1	0.67	0.20	72,72,72,72	0
58	MG	B	213	1/1	0.67	0.11	81,81,81,81	0
58	MG	A	3334	1/1	0.67	0.13	84,84,84,84	0
58	MG	G	202	1/1	0.68	0.24	67,67,67,67	0
58	MG	A	3002	1/1	0.68	0.34	50,50,50,50	0
58	MG	A	3165	1/1	0.68	1.03	60,60,60,60	0
58	MG	A	3560	1/1	0.68	0.26	79,79,79,79	0
58	MG	A	3572	1/1	0.68	0.38	70,70,70,70	0
58	MG	A	3213	1/1	0.69	0.46	67,67,67,67	0
58	MG	a	3455	1/1	0.69	0.10	67,67,67,67	0
58	MG	a	3391	1/1	0.69	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3319	1/1	0.70	0.23	31,31,31,31	0
58	MG	A	3132	1/1	0.70	0.78	48,48,48,48	0
58	MG	A	3554	1/1	0.71	0.21	74,74,74,74	0
58	MG	A	3054	1/1	0.71	0.27	71,71,71,71	0
58	MG	A	3084	1/1	0.71	0.20	57,57,57,57	0
58	MG	A	3226	1/1	0.72	0.43	68,68,68,68	0
58	MG	B	208	1/1	0.72	0.11	74,74,74,74	0
58	MG	A	3044	1/1	0.72	0.38	72,72,72,72	0
58	MG	A	3408	1/1	0.72	0.12	98,98,98,98	0
58	MG	a	3388	1/1	0.73	0.23	59,59,59,59	0
58	MG	A	3603	1/1	0.74	0.35	82,82,82,82	0
58	MG	a	3316	1/1	0.74	0.24	54,54,54,54	0
58	MG	a	3392	1/1	0.74	0.14	65,65,65,65	0
58	MG	A	3254	1/1	0.74	0.37	67,67,67,67	0
58	MG	A	3152	1/1	0.74	0.43	68,68,68,68	0
58	MG	a	3472	1/1	0.75	0.17	61,61,61,61	0
58	MG	A	3410	1/1	0.75	0.20	51,51,51,51	0
58	MG	A	3058	1/1	0.75	0.51	57,57,57,57	0
58	MG	A	3619	1/1	0.76	0.28	78,78,78,78	0
58	MG	B	210	1/1	0.76	0.22	68,68,68,68	0
58	MG	A	3113	1/1	0.76	0.31	63,63,63,63	0
58	MG	A	3087	1/1	0.76	0.29	58,58,58,58	0
58	MG	A	3075	1/1	0.76	0.17	67,67,67,67	0
58	MG	N	201	1/1	0.76	0.39	57,57,57,57	0
58	MG	A	3220	1/1	0.76	0.22	49,49,49,49	0
58	MG	A	3231	1/1	0.76	0.39	48,48,48,48	0
58	MG	a	3369	1/1	0.76	0.24	60,60,60,60	0
58	MG	A	3025	1/1	0.77	0.20	60,60,60,60	0
58	MG	a	3440	1/1	0.77	0.14	69,69,69,69	0
58	MG	A	3108	1/1	0.77	0.35	54,54,54,54	0
58	MG	A	3284	1/1	0.77	0.29	67,67,67,67	0
58	MG	A	3052	1/1	0.78	0.38	59,59,59,59	0
58	MG	A	3066	1/1	0.78	0.19	56,56,56,56	0
58	MG	x	3002	1/1	0.78	1.22	101,101,101,101	0
58	MG	A	3564	1/1	0.78	0.21	75,75,75,75	0
58	MG	a	3480	1/1	0.78	0.27	77,77,77,77	0
58	MG	A	3182	1/1	0.78	0.32	53,53,53,53	0
58	MG	A	3263	1/1	0.78	0.33	55,55,55,55	0
58	MG	A	3095	1/1	0.78	0.40	63,63,63,63	0
58	MG	a	3352	1/1	0.79	0.25	59,59,59,59	0
58	MG	P	201	1/1	0.79	0.54	54,54,54,54	0
58	MG	A	3032	1/1	0.79	0.32	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3209	1/1	0.79	0.18	71,71,71,71	0
58	MG	A	3607	1/1	0.80	0.17	90,90,90,90	0
58	MG	A	3617	1/1	0.80	0.19	65,65,65,65	0
58	MG	6	101	1/1	0.80	0.32	64,64,64,64	0
58	MG	a	3436	1/1	0.80	0.26	66,66,66,66	0
58	MG	A	3294	1/1	0.80	0.37	44,44,44,44	0
58	MG	A	3240	1/1	0.80	0.24	79,79,79,79	0
58	MG	A	3297	1/1	0.80	0.24	67,67,67,67	0
58	MG	A	3073	1/1	0.80	0.45	56,56,56,56	0
58	MG	A	3339	1/1	0.80	0.17	68,68,68,68	0
58	MG	A	3375	1/1	0.80	0.12	55,55,55,55	0
58	MG	A	3293	1/1	0.80	0.33	51,51,51,51	0
58	MG	A	3245	1/1	0.80	0.29	56,56,56,56	0
58	MG	A	3040	1/1	0.80	0.28	58,58,58,58	0
58	MG	A	3570	1/1	0.80	0.17	57,57,57,57	0
58	MG	A	3270	1/1	0.80	0.25	61,61,61,61	0
58	MG	A	3305	1/1	0.80	0.29	70,70,70,70	0
58	MG	A	3059	1/1	0.80	0.34	66,66,66,66	0
58	MG	A	3101	1/1	0.80	0.32	74,74,74,74	0
58	MG	A	3568	1/1	0.81	0.20	83,83,83,83	0
58	MG	B	217	1/1	0.81	0.27	67,67,67,67	0
58	MG	A	3236	1/1	0.81	0.56	67,67,67,67	0
58	MG	A	3174	1/1	0.81	0.32	59,59,59,59	0
58	MG	a	3371	1/1	0.81	0.25	65,65,65,65	0
58	MG	A	3067	1/1	0.81	0.16	70,70,70,70	0
58	MG	B	207	1/1	0.81	0.26	103,103,103,103	0
58	MG	A	3287	1/1	0.81	0.26	54,54,54,54	0
58	MG	A	3259	1/1	0.81	0.09	74,74,74,74	0
58	MG	V	201	1/1	0.81	0.15	53,53,53,53	0
58	MG	A	3569	1/1	0.81	0.45	85,85,85,85	0
58	MG	A	3273	1/1	0.81	0.43	77,77,77,77	0
58	MG	A	3635	1/1	0.81	0.62	69,69,69,69	0
58	MG	A	3255	1/1	0.81	0.33	57,57,57,57	0
58	MG	A	3247	1/1	0.82	0.43	66,66,66,66	0
58	MG	A	3185	1/1	0.82	0.36	63,63,63,63	0
58	MG	A	3598	1/1	0.82	0.14	74,74,74,74	0
58	MG	A	3112	1/1	0.82	0.37	66,66,66,66	0
58	MG	B	206	1/1	0.82	0.18	75,75,75,75	0
58	MG	A	3003	1/1	0.82	0.29	59,59,59,59	0
58	MG	A	3357	1/1	0.82	0.24	69,69,69,69	0
58	MG	a	3348	1/1	0.82	0.50	53,53,53,53	0
58	MG	A	3057	1/1	0.82	0.25	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3288	1/1	0.82	0.32	60,60,60,60	0
58	MG	A	3352	1/1	0.82	0.32	47,47,47,47	0
58	MG	D	305	1/1	0.82	0.18	37,37,37,37	0
58	MG	A	3565	1/1	0.82	0.15	67,67,67,67	0
58	MG	A	3162	1/1	0.82	0.18	71,71,71,71	0
58	MG	A	3171	1/1	0.82	0.18	37,37,37,37	0
58	MG	A	3243	1/1	0.83	0.56	58,58,58,58	0
58	MG	a	3377	1/1	0.83	0.23	85,85,85,85	0
58	MG	f	201	1/1	0.83	0.25	92,92,92,92	0
58	MG	A	3576	1/1	0.83	0.33	89,89,89,89	0
58	MG	A	3596	1/1	0.83	0.20	45,45,45,45	0
58	MG	a	3484	1/1	0.83	0.24	67,67,67,67	0
58	MG	A	3426	1/1	0.83	0.28	55,55,55,55	0
58	MG	A	3029	1/1	0.83	0.18	52,52,52,52	0
58	MG	A	3122	1/1	0.83	0.20	35,35,35,35	0
58	MG	A	3114	1/1	0.83	1.03	57,57,57,57	0
58	MG	A	3045	1/1	0.83	0.22	68,68,68,68	0
58	MG	A	3405	1/1	0.83	0.15	61,61,61,61	0
58	MG	A	3563	1/1	0.83	0.19	73,73,73,73	0
58	MG	A	3434	1/1	0.83	0.23	56,56,56,56	0
58	MG	A	3175	1/1	0.83	0.38	46,46,46,46	0
58	MG	A	3117	1/1	0.83	1.10	50,50,50,50	0
58	MG	A	3034	1/1	0.83	0.20	71,71,71,71	0
58	MG	A	3124	1/1	0.83	0.14	54,54,54,54	0
58	MG	a	3393	1/1	0.83	0.52	69,69,69,69	0
58	MG	A	3481	1/1	0.83	0.32	65,65,65,65	0
58	MG	A	3120	1/1	0.83	0.76	52,52,52,52	0
58	MG	a	3327	1/1	0.84	0.12	62,62,62,62	0
58	MG	A	3573	1/1	0.84	0.20	70,70,70,70	0
58	MG	A	3121	1/1	0.84	0.18	62,62,62,62	0
58	MG	A	3360	1/1	0.84	0.21	60,60,60,60	0
58	MG	a	3329	1/1	0.84	0.16	46,46,46,46	0
58	MG	7	102	1/1	0.84	1.31	66,66,66,66	0
58	MG	A	3388	1/1	0.84	0.15	47,47,47,47	0
58	MG	R	201	1/1	0.84	0.54	67,67,67,67	0
58	MG	a	3425	1/1	0.84	0.26	47,47,47,47	0
58	MG	A	3102	1/1	0.84	0.13	59,59,59,59	0
58	MG	A	3328	1/1	0.84	0.20	62,62,62,62	0
58	MG	a	3332	1/1	0.84	0.16	45,45,45,45	0
58	MG	A	3246	1/1	0.84	0.24	49,49,49,49	0
58	MG	A	3181	1/1	0.84	0.10	35,35,35,35	0
58	MG	v	101	1/1	0.84	0.53	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3001	1/1	0.85	0.34	70,70,70,70	0
58	MG	A	3601	1/1	0.85	0.20	45,45,45,45	0
58	MG	A	3514	1/1	0.85	0.14	34,34,34,34	0
58	MG	0	102	1/1	0.85	0.10	61,61,61,61	0
58	MG	A	3085	1/1	0.85	0.34	52,52,52,52	0
58	MG	a	3400	1/1	0.85	0.31	61,61,61,61	0
58	MG	A	3383	1/1	0.85	0.24	55,55,55,55	0
58	MG	a	3403	1/1	0.85	0.16	61,61,61,61	0
58	MG	P	202	1/1	0.85	0.27	86,86,86,86	0
58	MG	A	3615	1/1	0.85	0.24	50,50,50,50	0
58	MG	A	3549	1/1	0.85	0.47	75,75,75,75	0
58	MG	A	3589	1/1	0.85	0.25	46,46,46,46	0
58	MG	a	3434	1/1	0.85	0.24	54,54,54,54	0
58	MG	F	305	1/1	0.85	0.25	59,59,59,59	0
58	MG	A	3009	1/1	0.85	0.30	50,50,50,50	0
58	MG	A	3244	1/1	0.85	0.20	59,59,59,59	0
58	MG	A	3376	1/1	0.85	0.12	67,67,67,67	0
58	MG	y	701	1/1	0.85	0.26	68,68,68,68	0
58	MG	a	3426	1/1	0.85	0.13	69,69,69,69	0
58	MG	A	3276	1/1	0.85	0.07	73,73,73,73	0
58	MG	a	3450	1/1	0.85	0.08	55,55,55,55	0
58	MG	A	3451	1/1	0.85	0.18	82,82,82,82	0
58	MG	A	3298	1/1	0.85	0.17	58,58,58,58	0
58	MG	a	3428	1/1	0.85	0.27	46,46,46,46	0
58	MG	A	3614	1/1	0.85	0.16	75,75,75,75	0
58	MG	A	3039	1/1	0.85	0.82	59,59,59,59	0
58	MG	A	3081	1/1	0.85	0.28	61,61,61,61	0
58	MG	A	3135	1/1	0.85	0.46	54,54,54,54	0
58	MG	A	3436	1/1	0.85	0.18	87,87,87,87	0
58	MG	A	3239	1/1	0.85	0.33	56,56,56,56	0
58	MG	A	3018	1/1	0.85	0.24	49,49,49,49	0
58	MG	A	3110	1/1	0.86	0.26	42,42,42,42	0
58	MG	a	3306	1/1	0.86	0.68	55,55,55,55	0
58	MG	A	3109	1/1	0.86	0.26	52,52,52,52	0
58	MG	A	3520	1/1	0.86	0.21	80,80,80,80	0
58	MG	a	3373	1/1	0.86	0.24	63,63,63,63	0
58	MG	a	3328	1/1	0.86	0.25	60,60,60,60	0
58	MG	a	3419	1/1	0.86	0.24	72,72,72,72	0
58	MG	a	3458	1/1	0.86	0.26	62,62,62,62	0
58	MG	a	3396	1/1	0.86	0.11	42,42,42,42	0
58	MG	A	3275	1/1	0.86	0.16	63,63,63,63	0
58	MG	A	3600	1/1	0.86	0.26	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3141	1/1	0.86	0.23	55,55,55,55	0
58	MG	A	3461	1/1	0.86	0.51	59,59,59,59	0
58	MG	7	103	1/1	0.86	0.26	57,57,57,57	0
58	MG	A	3353	1/1	0.86	0.18	79,79,79,79	0
58	MG	A	3370	1/1	0.86	0.16	64,64,64,64	0
58	MG	A	3148	1/1	0.86	0.38	60,60,60,60	0
58	MG	A	3498	1/1	0.86	0.18	76,76,76,76	0
58	MG	a	3451	1/1	0.86	0.13	49,49,49,49	0
58	MG	A	3532	1/1	0.86	0.42	66,66,66,66	0
58	MG	a	3360	1/1	0.86	0.35	40,40,40,40	0
58	MG	5	101	1/1	0.86	0.58	69,69,69,69	0
58	MG	Q	203	1/1	0.86	0.21	45,45,45,45	0
58	MG	V	202	1/1	0.87	0.74	51,51,51,51	0
58	MG	a	3410	1/1	0.87	0.37	45,45,45,45	0
58	MG	A	3309	1/1	0.87	0.25	52,52,52,52	0
58	MG	A	3042	1/1	0.87	0.16	92,92,92,92	0
58	MG	a	3358	1/1	0.87	0.36	70,70,70,70	0
58	MG	A	3278	1/1	0.87	0.46	64,64,64,64	0
58	MG	A	3606	1/1	0.87	0.19	55,55,55,55	0
58	MG	A	3197	1/1	0.87	0.29	40,40,40,40	0
58	MG	A	3272	1/1	0.87	0.33	62,62,62,62	0
58	MG	A	3072	1/1	0.87	0.33	43,43,43,43	0
58	MG	A	3119	1/1	0.87	0.27	50,50,50,50	0
58	MG	A	3145	1/1	0.87	0.09	48,48,48,48	0
58	MG	A	3097	1/1	0.87	0.13	60,60,60,60	0
58	MG	a	3341	1/1	0.87	0.28	60,60,60,60	0
58	MG	A	3212	1/1	0.87	0.15	55,55,55,55	0
58	MG	A	3104	1/1	0.87	0.21	64,64,64,64	0
58	MG	A	3350	1/1	0.87	0.10	63,63,63,63	0
58	MG	A	3544	1/1	0.87	0.17	55,55,55,55	0
58	MG	a	3362	1/1	0.87	0.15	73,73,73,73	0
58	MG	a	3418	1/1	0.87	0.12	67,67,67,67	0
58	MG	A	3373	1/1	0.87	0.08	64,64,64,64	0
58	MG	A	3014	1/1	0.87	0.14	39,39,39,39	0
58	MG	A	3237	1/1	0.87	0.17	51,51,51,51	0
58	MG	a	3409	1/1	0.87	0.10	74,74,74,74	0
58	MG	A	3490	1/1	0.87	0.25	47,47,47,47	0
58	MG	a	3368	1/1	0.87	0.23	44,44,44,44	0
58	MG	A	3092	1/1	0.87	0.38	67,67,67,67	0
58	MG	w	101	1/1	0.87	0.79	60,60,60,60	0
58	MG	A	3586	1/1	0.87	0.28	55,55,55,55	0
58	MG	A	3215	1/1	0.88	0.19	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3562	1/1	0.88	0.18	59,59,59,59	0
58	MG	Z	301	1/1	0.88	0.17	66,66,66,66	0
58	MG	a	3314	1/1	0.88	0.20	60,60,60,60	0
58	MG	a	3468	1/1	0.88	0.18	69,69,69,69	0
58	MG	A	3574	1/1	0.88	0.16	57,57,57,57	0
58	MG	A	3624	1/1	0.88	0.15	52,52,52,52	0
58	MG	a	3340	1/1	0.88	0.43	81,81,81,81	0
58	MG	A	3419	1/1	0.88	0.13	74,74,74,74	0
58	MG	A	3089	1/1	0.88	0.19	47,47,47,47	0
58	MG	A	3285	1/1	0.88	0.24	50,50,50,50	0
58	MG	A	3126	1/1	0.88	0.21	60,60,60,60	0
58	MG	A	3464	1/1	0.88	0.25	49,49,49,49	0
58	MG	A	3129	1/1	0.88	0.24	48,48,48,48	0
58	MG	A	3502	1/1	0.88	0.25	56,56,56,56	0
58	MG	A	3118	1/1	0.88	0.87	52,52,52,52	0
58	MG	A	3103	1/1	0.88	0.29	56,56,56,56	0
58	MG	a	3321	1/1	0.88	0.18	48,48,48,48	0
58	MG	A	3064	1/1	0.88	0.38	50,50,50,50	0
58	MG	A	3430	1/1	0.88	0.14	44,44,44,44	0
58	MG	A	3030	1/1	0.88	0.36	64,64,64,64	0
58	MG	a	3413	1/1	0.88	0.14	54,54,54,54	0
58	MG	a	3359	1/1	0.88	0.14	65,65,65,65	0
58	MG	A	3286	1/1	0.88	0.16	62,62,62,62	0
58	MG	A	3086	1/1	0.88	0.19	50,50,50,50	0
58	MG	A	3223	1/1	0.88	0.30	61,61,61,61	0
58	MG	A	3516	1/1	0.88	0.21	55,55,55,55	0
58	MG	A	3013	1/1	0.88	0.22	52,52,52,52	0
58	MG	A	3355	1/1	0.88	0.13	84,84,84,84	0
58	MG	A	3433	1/1	0.88	0.09	64,64,64,64	0
58	MG	A	3134	1/1	0.88	0.43	67,67,67,67	0
58	MG	a	3423	1/1	0.88	0.40	66,66,66,66	0
58	MG	a	3421	1/1	0.88	0.11	61,61,61,61	0
58	MG	A	3347	1/1	0.88	0.18	75,75,75,75	0
58	MG	A	3264	1/1	0.88	0.33	65,65,65,65	0
58	MG	A	3551	1/1	0.88	0.20	63,63,63,63	0
58	MG	a	3474	1/1	0.88	0.16	64,64,64,64	0
58	MG	A	3543	1/1	0.88	0.14	71,71,71,71	0
58	MG	A	3326	1/1	0.88	0.17	69,69,69,69	0
58	MG	A	3268	1/1	0.88	0.26	58,58,58,58	0
58	MG	A	3010	1/1	0.89	0.20	41,41,41,41	0
58	MG	A	3611	1/1	0.89	0.20	52,52,52,52	0
58	MG	A	3173	1/1	0.89	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3525	1/1	0.89	0.14	54,54,54,54	0
58	MG	A	3507	1/1	0.89	0.17	46,46,46,46	0
58	MG	A	3079	1/1	0.89	0.46	63,63,63,63	0
58	MG	a	3303	1/1	0.89	0.17	58,58,58,58	0
58	MG	A	3060	1/1	0.89	0.26	81,81,81,81	0
58	MG	A	3465	1/1	0.89	0.15	68,68,68,68	0
58	MG	a	3346	1/1	0.89	0.14	50,50,50,50	0
58	MG	A	3602	1/1	0.89	0.11	73,73,73,73	0
58	MG	A	3585	1/1	0.89	0.18	47,47,47,47	0
58	MG	A	3367	1/1	0.89	0.48	51,51,51,51	0
58	MG	a	3313	1/1	0.89	0.20	61,61,61,61	0
58	MG	A	3020	1/1	0.89	0.16	50,50,50,50	0
58	MG	A	3616	1/1	0.89	0.32	59,59,59,59	0
58	MG	A	3555	1/1	0.89	0.17	69,69,69,69	0
58	MG	A	3005	1/1	0.89	0.37	40,40,40,40	0
58	MG	A	3346	1/1	0.89	0.24	68,68,68,68	0
58	MG	A	3605	1/1	0.89	0.24	70,70,70,70	0
58	MG	A	3423	1/1	0.89	0.21	59,59,59,59	0
58	MG	A	3374	1/1	0.89	0.15	58,58,58,58	0
58	MG	A	3250	1/1	0.89	0.21	58,58,58,58	0
58	MG	A	3335	1/1	0.89	0.09	56,56,56,56	0
58	MG	A	3281	1/1	0.89	0.14	57,57,57,57	0
58	MG	a	3310	1/1	0.89	0.10	52,52,52,52	0
58	MG	a	3385	1/1	0.89	0.12	33,33,33,33	0
58	MG	A	3252	1/1	0.89	0.27	58,58,58,58	0
58	MG	A	3397	1/1	0.89	0.16	36,36,36,36	0
58	MG	A	3366	1/1	0.89	0.11	58,58,58,58	0
58	MG	A	3478	1/1	0.89	0.11	65,65,65,65	0
58	MG	A	3198	1/1	0.89	0.22	55,55,55,55	0
58	MG	a	3334	1/1	0.89	0.35	43,43,43,43	0
58	MG	A	3186	1/1	0.89	0.16	90,90,90,90	0
58	MG	a	3330	1/1	0.89	0.57	63,63,63,63	0
58	MG	A	3224	1/1	0.89	0.45	51,51,51,51	0
58	MG	A	3343	1/1	0.89	0.14	69,69,69,69	0
58	MG	A	3467	1/1	0.89	0.35	52,52,52,52	0
58	MG	l	201	1/1	0.89	0.48	61,61,61,61	0
58	MG	A	3330	1/1	0.89	0.34	55,55,55,55	0
58	MG	E	304	1/1	0.89	0.21	55,55,55,55	0
58	MG	a	3315	1/1	0.89	0.21	60,60,60,60	0
58	MG	A	3053	1/1	0.89	0.45	61,61,61,61	0
58	MG	a	3361	1/1	0.89	0.15	73,73,73,73	0
58	MG	a	3335	1/1	0.89	0.37	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	a	3366	1/1	0.89	0.24	38,38,38,38	0
58	MG	a	3350	1/1	0.89	0.12	73,73,73,73	0
58	MG	A	3050	1/1	0.89	0.12	39,39,39,39	0
58	MG	D	303	1/1	0.89	0.93	49,49,49,49	0
58	MG	A	3322	1/1	0.90	0.24	61,61,61,61	0
58	MG	A	3511	1/1	0.90	0.17	99,99,99,99	0
58	MG	a	3459	1/1	0.90	0.26	91,91,91,91	0
58	MG	A	3312	1/1	0.90	0.23	59,59,59,59	0
58	MG	X	101	1/1	0.90	0.22	72,72,72,72	0
58	MG	A	3023	1/1	0.90	0.30	48,48,48,48	0
58	MG	A	3150	1/1	0.90	0.14	74,74,74,74	0
58	MG	A	3571	1/1	0.90	0.38	89,89,89,89	0
58	MG	A	3062	1/1	0.90	0.26	42,42,42,42	0
58	MG	A	3242	1/1	0.90	0.11	63,63,63,63	0
58	MG	A	3479	1/1	0.90	0.18	43,43,43,43	0
58	MG	A	3139	1/1	0.90	0.59	62,62,62,62	0
58	MG	A	3533	1/1	0.90	0.18	47,47,47,47	0
58	MG	a	3325	1/1	0.90	0.83	55,55,55,55	0
58	MG	A	3063	1/1	0.90	0.16	62,62,62,62	0
58	MG	G	201	1/1	0.90	0.17	71,71,71,71	0
58	MG	A	3308	1/1	0.90	0.13	56,56,56,56	0
58	MG	A	3512	1/1	0.90	0.15	51,51,51,51	0
58	MG	E	301	1/1	0.90	0.79	56,56,56,56	0
58	MG	A	3078	1/1	0.90	0.35	47,47,47,47	0
58	MG	A	3207	1/1	0.90	0.17	40,40,40,40	0
58	MG	A	3046	1/1	0.90	0.18	55,55,55,55	0
58	MG	A	3235	1/1	0.90	0.14	48,48,48,48	0
58	MG	Q	202	1/1	0.90	0.98	51,51,51,51	0
58	MG	A	3431	1/1	0.90	0.35	69,69,69,69	0
58	MG	A	3199	1/1	0.90	0.15	42,42,42,42	0
58	MG	A	3074	1/1	0.90	0.16	42,42,42,42	0
58	MG	A	3107	1/1	0.90	1.43	75,75,75,75	0
58	MG	A	3037	1/1	0.90	0.27	61,61,61,61	0
58	MG	A	3304	1/1	0.90	0.18	39,39,39,39	0
58	MG	a	3324	1/1	0.90	0.47	40,40,40,40	0
58	MG	A	3008	1/1	0.90	0.98	80,80,80,80	0
58	MG	F	301	1/1	0.90	0.31	71,71,71,71	0
58	MG	A	3269	1/1	0.90	0.23	54,54,54,54	0
58	MG	A	3386	1/1	0.90	0.17	59,59,59,59	0
58	MG	A	3251	1/1	0.90	0.14	35,35,35,35	0
58	MG	A	3106	1/1	0.90	0.40	57,57,57,57	0
58	MG	A	3493	1/1	0.90	0.37	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	a	3383	1/1	0.90	0.21	56,56,56,56	0
58	MG	a	3380	1/1	0.90	0.22	57,57,57,57	0
58	MG	a	3357	1/1	0.90	0.12	48,48,48,48	0
58	MG	Q	205	1/1	0.90	0.18	55,55,55,55	0
58	MG	A	3260	1/1	0.90	0.10	68,68,68,68	0
58	MG	B	211	1/1	0.90	0.34	61,61,61,61	0
58	MG	A	3143	1/1	0.90	0.27	60,60,60,60	0
58	MG	A	3463	1/1	0.90	0.25	46,46,46,46	0
58	MG	A	3131	1/1	0.90	0.29	53,53,53,53	0
58	MG	A	3277	1/1	0.90	0.52	71,71,71,71	0
58	MG	A	3291	1/1	0.90	0.12	60,60,60,60	0
58	MG	A	3299	1/1	0.90	0.19	64,64,64,64	0
58	MG	A	3448	1/1	0.90	0.45	48,48,48,48	0
58	MG	A	3517	1/1	0.90	0.25	51,51,51,51	0
58	MG	A	3262	1/1	0.91	0.08	63,63,63,63	0
58	MG	a	3353	1/1	0.91	0.16	48,48,48,48	0
58	MG	A	3261	1/1	0.91	0.23	61,61,61,61	0
58	MG	A	3177	1/1	0.91	0.18	65,65,65,65	0
58	MG	A	3578	1/1	0.91	0.24	64,64,64,64	0
58	MG	A	3069	1/1	0.91	0.23	46,46,46,46	0
58	MG	A	3491	1/1	0.91	0.26	72,72,72,72	0
58	MG	A	3142	1/1	0.91	0.10	84,84,84,84	0
58	MG	A	3406	1/1	0.91	0.14	56,56,56,56	0
58	MG	A	3248	1/1	0.91	0.61	57,57,57,57	0
58	MG	F	304	1/1	0.91	0.27	60,60,60,60	0
58	MG	A	3290	1/1	0.91	0.23	49,49,49,49	0
58	MG	a	3336	1/1	0.91	0.29	62,62,62,62	0
58	MG	A	3414	1/1	0.91	0.28	31,31,31,31	0
58	MG	Q	204	1/1	0.91	0.62	56,56,56,56	0
58	MG	a	3454	1/1	0.91	0.24	39,39,39,39	0
58	MG	A	3515	1/1	0.91	0.29	48,48,48,48	0
58	MG	A	3471	1/1	0.91	0.33	56,56,56,56	0
58	MG	A	3444	1/1	0.91	0.34	48,48,48,48	0
58	MG	a	3486	1/1	0.91	0.19	38,38,38,38	0
58	MG	A	3043	1/1	0.91	0.16	59,59,59,59	0
58	MG	D	304	1/1	0.91	0.36	74,74,74,74	0
58	MG	A	3048	1/1	0.91	0.20	43,43,43,43	0
58	MG	A	3356	1/1	0.91	0.24	57,57,57,57	0
58	MG	A	3168	1/1	0.91	0.41	48,48,48,48	0
58	MG	A	3051	1/1	0.91	0.24	43,43,43,43	0
58	MG	a	3370	1/1	0.91	0.18	66,66,66,66	0
58	MG	A	3061	1/1	0.91	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3580	1/1	0.91	0.24	67,67,67,67	0
58	MG	a	3407	1/1	0.91	0.35	82,82,82,82	0
58	MG	A	3031	1/1	0.91	0.18	70,70,70,70	0
58	MG	A	3403	1/1	0.91	0.15	40,40,40,40	0
58	MG	A	3411	1/1	0.91	0.23	47,47,47,47	0
58	MG	A	3432	1/1	0.91	0.20	58,58,58,58	0
58	MG	a	3405	1/1	0.91	0.19	70,70,70,70	0
58	MG	A	3631	1/1	0.91	0.24	87,87,87,87	0
58	MG	A	3266	1/1	0.91	0.39	61,61,61,61	0
58	MG	W	201	1/1	0.91	1.28	77,77,77,77	0
58	MG	a	3433	1/1	0.91	0.12	32,32,32,32	0
58	MG	A	3452	1/1	0.91	0.27	53,53,53,53	0
58	MG	a	3376	1/1	0.91	0.20	46,46,46,46	0
58	MG	a	3308	1/1	0.91	0.21	41,41,41,41	0
58	MG	A	3546	1/1	0.91	0.32	53,53,53,53	0
58	MG	a	3319	1/1	0.91	0.38	39,39,39,39	0
58	MG	A	3019	1/1	0.92	0.28	49,49,49,49	0
58	MG	A	3036	1/1	0.92	0.11	74,74,74,74	0
58	MG	A	3581	1/1	0.92	0.14	55,55,55,55	0
58	MG	a	3424	1/1	0.92	0.11	43,43,43,43	0
58	MG	a	3339	1/1	0.92	0.24	50,50,50,50	0
58	MG	A	3591	1/1	0.92	0.13	66,66,66,66	0
58	MG	a	3326	1/1	0.92	0.21	48,48,48,48	0
58	MG	A	3590	1/1	0.92	0.13	59,59,59,59	0
58	MG	A	3159	1/1	0.92	0.13	78,78,78,78	0
58	MG	A	3398	1/1	0.92	0.26	43,43,43,43	0
58	MG	A	3613	1/1	0.92	0.17	52,52,52,52	0
58	MG	A	3341	1/1	0.92	0.33	57,57,57,57	0
58	MG	A	3487	1/1	0.92	0.23	60,60,60,60	0
58	MG	a	3364	1/1	0.92	0.43	56,56,56,56	0
58	MG	A	3441	1/1	0.92	0.14	73,73,73,73	0
58	MG	A	3504	1/1	0.92	0.37	38,38,38,38	0
58	MG	A	3227	1/1	0.92	0.44	43,43,43,43	0
58	MG	A	3365	1/1	0.92	0.14	51,51,51,51	0
58	MG	A	3136	1/1	0.92	0.39	49,49,49,49	0
58	MG	A	3004	1/1	0.92	0.22	55,55,55,55	0
58	MG	A	3497	1/1	0.92	0.26	50,50,50,50	0
58	MG	A	3505	1/1	0.92	0.18	68,68,68,68	0
58	MG	A	3204	1/1	0.92	0.25	43,43,43,43	0
58	MG	A	3201	1/1	0.92	0.20	63,63,63,63	0
58	MG	a	3461	1/1	0.92	0.15	44,44,44,44	0
58	MG	A	3575	1/1	0.92	0.09	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3508	1/1	0.92	0.13	46,46,46,46	0
58	MG	A	3323	1/1	0.92	0.15	42,42,42,42	0
58	MG	A	3567	1/1	0.92	0.17	47,47,47,47	0
58	MG	A	3099	1/1	0.92	0.20	34,34,34,34	0
58	MG	A	3146	1/1	0.92	0.27	56,56,56,56	0
58	MG	A	3076	1/1	0.92	0.19	41,41,41,41	0
58	MG	A	3345	1/1	0.92	0.19	44,44,44,44	0
58	MG	e	201	1/1	0.92	0.15	69,69,69,69	0
58	MG	A	3407	1/1	0.92	0.10	38,38,38,38	0
58	MG	A	3006	1/1	0.92	0.60	57,57,57,57	0
58	MG	A	3425	1/1	0.92	0.23	62,62,62,62	0
58	MG	A	3594	1/1	0.92	0.19	37,37,37,37	0
58	MG	A	3232	1/1	0.92	0.30	36,36,36,36	0
58	MG	A	3625	1/1	0.92	0.19	84,84,84,84	0
58	MG	A	3466	1/1	0.92	0.08	67,67,67,67	0
58	MG	A	3196	1/1	0.92	0.18	44,44,44,44	0
58	MG	A	3415	1/1	0.92	0.27	42,42,42,42	0
58	MG	A	3138	1/1	0.92	0.21	77,77,77,77	0
58	MG	A	3393	1/1	0.92	0.32	57,57,57,57	0
58	MG	A	3627	1/1	0.92	0.14	91,91,91,91	0
58	MG	E	303	1/1	0.92	0.19	41,41,41,41	0
58	MG	a	3462	1/1	0.92	0.13	74,74,74,74	0
58	MG	A	3217	1/1	0.92	0.39	50,50,50,50	0
58	MG	a	3420	1/1	0.92	0.17	62,62,62,62	0
58	MG	F	302	1/1	0.92	0.81	52,52,52,52	0
58	MG	A	3130	1/1	0.92	0.47	43,43,43,43	0
58	MG	A	3336	1/1	0.92	0.22	36,36,36,36	0
58	MG	A	3214	1/1	0.92	0.41	52,52,52,52	0
58	MG	A	3482	1/1	0.92	0.09	67,67,67,67	0
58	MG	A	3361	1/1	0.92	0.12	84,84,84,84	0
58	MG	A	3158	1/1	0.93	0.50	97,97,97,97	0
58	MG	A	3111	1/1	0.93	0.51	61,61,61,61	0
58	MG	a	3437	1/1	0.93	0.15	54,54,54,54	0
58	MG	a	3345	1/1	0.93	0.22	47,47,47,47	0
58	MG	a	3331	1/1	0.93	0.24	55,55,55,55	0
58	MG	a	3356	1/1	0.93	0.22	49,49,49,49	0
58	MG	A	3016	1/1	0.93	0.14	49,49,49,49	0
58	MG	A	3313	1/1	0.93	0.17	44,44,44,44	0
58	MG	A	3595	1/1	0.93	0.15	63,63,63,63	0
58	MG	A	3621	1/1	0.93	0.30	59,59,59,59	0
58	MG	a	3349	1/1	0.93	0.37	47,47,47,47	0
58	MG	a	3354	1/1	0.93	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3428	1/1	0.93	0.15	36,36,36,36	0
58	MG	A	3325	1/1	0.93	0.28	52,52,52,52	0
58	MG	A	3271	1/1	0.93	0.16	57,57,57,57	0
61	GDP	y	703	28/28	0.93	0.15	91,120,142,146	0
58	MG	a	3401	1/1	0.93	0.38	44,44,44,44	0
58	MG	a	3481	1/1	0.93	0.27	46,46,46,46	0
58	MG	A	3392	1/1	0.93	0.22	47,47,47,47	0
58	MG	A	3610	1/1	0.93	0.22	61,61,61,61	0
58	MG	A	3221	1/1	0.93	0.49	58,58,58,58	0
58	MG	A	3584	1/1	0.93	0.25	62,62,62,62	0
58	MG	a	3470	1/1	0.93	0.15	56,56,56,56	0
58	MG	F	303	1/1	0.93	0.11	36,36,36,36	0
58	MG	A	3542	1/1	0.93	0.66	60,60,60,60	0
58	MG	A	3080	1/1	0.93	0.31	54,54,54,54	0
58	MG	a	3445	1/1	0.93	0.20	66,66,66,66	0
58	MG	A	3449	1/1	0.93	0.23	51,51,51,51	0
58	MG	w	105	1/1	0.93	0.23	29,29,29,29	0
58	MG	A	3442	1/1	0.93	0.19	56,56,56,56	0
58	MG	A	3301	1/1	0.93	0.17	57,57,57,57	0
58	MG	9	101	1/1	0.93	0.30	57,57,57,57	0
58	MG	A	3082	1/1	0.93	0.64	53,53,53,53	0
58	MG	A	3024	1/1	0.93	0.15	63,63,63,63	0
58	MG	a	3463	1/1	0.93	0.21	45,45,45,45	0
58	MG	A	3327	1/1	0.93	0.14	49,49,49,49	0
58	MG	U	201	1/1	0.93	0.38	72,72,72,72	0
58	MG	A	3125	1/1	0.93	0.29	31,31,31,31	0
58	MG	A	3091	1/1	0.93	0.21	63,63,63,63	0
58	MG	a	3435	1/1	0.93	0.19	57,57,57,57	0
58	MG	A	3203	1/1	0.93	0.19	53,53,53,53	0
58	MG	A	3137	1/1	0.93	0.48	59,59,59,59	0
58	MG	a	3429	1/1	0.93	0.14	49,49,49,49	0
58	MG	a	3427	1/1	0.93	0.26	50,50,50,50	0
58	MG	A	3202	1/1	0.93	0.37	50,50,50,50	0
58	MG	A	3211	1/1	0.93	0.47	55,55,55,55	0
58	MG	a	3333	1/1	0.93	0.16	51,51,51,51	0
58	MG	A	3506	1/1	0.93	0.13	49,49,49,49	0
58	MG	A	3484	1/1	0.93	0.14	50,50,50,50	0
58	MG	A	3007	1/1	0.93	0.27	46,46,46,46	0
58	MG	0	103	1/1	0.93	0.19	61,61,61,61	0
58	MG	A	3154	1/1	0.93	0.18	60,60,60,60	0
58	MG	A	3404	1/1	0.93	0.20	57,57,57,57	0
58	MG	a	3408	1/1	0.93	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3027	1/1	0.93	0.24	44,44,44,44	0
58	MG	A	3469	1/1	0.93	0.12	54,54,54,54	0
58	MG	A	3140	1/1	0.93	0.16	57,57,57,57	0
58	MG	A	3153	1/1	0.93	0.22	82,82,82,82	0
58	MG	a	3431	1/1	0.93	0.10	41,41,41,41	0
58	MG	A	3096	1/1	0.93	0.23	58,58,58,58	0
58	MG	A	3439	1/1	0.93	0.18	58,58,58,58	0
58	MG	a	3301	1/1	0.93	0.23	49,49,49,49	0
58	MG	a	3411	1/1	0.93	0.16	53,53,53,53	0
58	MG	8	101	1/1	0.93	0.12	66,66,66,66	0
58	MG	A	3454	1/1	0.93	0.50	51,51,51,51	0
58	MG	A	3172	1/1	0.93	0.32	31,31,31,31	0
58	MG	A	3022	1/1	0.93	0.28	33,33,33,33	0
58	MG	a	3384	1/1	0.94	0.14	49,49,49,49	0
58	MG	A	3427	1/1	0.94	0.16	62,62,62,62	0
58	MG	A	3342	1/1	0.94	0.16	61,61,61,61	0
58	MG	B	204	1/1	0.94	0.15	85,85,85,85	0
58	MG	A	3552	1/1	0.94	0.18	64,64,64,64	0
58	MG	a	3422	1/1	0.94	0.32	50,50,50,50	0
58	MG	a	3337	1/1	0.94	0.26	50,50,50,50	0
58	MG	A	3315	1/1	0.94	0.27	56,56,56,56	0
58	MG	A	3210	1/1	0.94	0.20	56,56,56,56	0
58	MG	a	3477	1/1	0.94	0.12	68,68,68,68	0
58	MG	a	3342	1/1	0.94	0.46	50,50,50,50	0
58	MG	U	202	1/1	0.94	0.35	62,62,62,62	0
58	MG	a	3469	1/1	0.94	0.38	42,42,42,42	0
58	MG	Q	201	1/1	0.94	0.50	51,51,51,51	0
58	MG	A	3401	1/1	0.94	0.11	37,37,37,37	0
58	MG	A	3382	1/1	0.94	0.24	36,36,36,36	0
58	MG	A	3311	1/1	0.94	0.28	52,52,52,52	0
58	MG	A	3065	1/1	0.94	0.25	74,74,74,74	0
59	ZN	5	102	1/1	0.94	0.08	70,70,70,70	0
58	MG	A	3289	1/1	0.94	0.15	43,43,43,43	0
58	MG	A	3316	1/1	0.94	0.30	47,47,47,47	0
58	MG	A	3167	1/1	0.94	0.54	65,65,65,65	0
58	MG	a	3442	1/1	0.94	0.08	45,45,45,45	0
58	MG	A	3545	1/1	0.94	0.23	64,64,64,64	0
58	MG	A	3333	1/1	0.94	0.08	62,62,62,62	0
58	MG	a	3304	1/1	0.94	0.10	55,55,55,55	0
58	MG	A	3026	1/1	0.94	0.09	55,55,55,55	0
58	MG	A	3629	1/1	0.94	0.20	70,70,70,70	0
58	MG	A	3450	1/1	0.94	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	w	103	1/1	0.94	0.18	38,38,38,38	0
58	MG	A	3524	1/1	0.94	0.12	53,53,53,53	0
58	MG	A	3456	1/1	0.94	0.29	47,47,47,47	0
58	MG	A	3295	1/1	0.94	0.27	30,30,30,30	0
58	MG	A	3402	1/1	0.94	0.09	50,50,50,50	0
58	MG	A	3363	1/1	0.94	0.18	30,30,30,30	0
58	MG	A	3446	1/1	0.94	0.29	39,39,39,39	0
58	MG	a	3320	1/1	0.94	0.14	39,39,39,39	0
58	MG	A	3486	1/1	0.94	0.23	40,40,40,40	0
58	MG	a	3351	1/1	0.94	0.18	36,36,36,36	0
58	MG	R	202	1/1	0.94	0.29	53,53,53,53	0
58	MG	G	203	1/1	0.94	0.09	69,69,69,69	0
58	MG	a	3302	1/1	0.94	0.25	58,58,58,58	0
58	MG	A	3047	1/1	0.94	0.19	39,39,39,39	0
58	MG	a	3467	1/1	0.94	0.16	62,62,62,62	0
58	MG	A	3331	1/1	0.94	0.12	54,54,54,54	0
58	MG	a	3441	1/1	0.94	0.19	62,62,62,62	0
58	MG	A	3149	1/1	0.94	0.18	53,53,53,53	0
58	MG	A	3472	1/1	0.94	0.17	53,53,53,53	0
58	MG	A	3462	1/1	0.94	0.12	53,53,53,53	0
58	MG	A	3302	1/1	0.94	0.34	59,59,59,59	0
58	MG	E	302	1/1	0.94	0.13	35,35,35,35	0
58	MG	A	3033	1/1	0.94	0.18	39,39,39,39	0
58	MG	A	3622	1/1	0.94	0.24	49,49,49,49	0
58	MG	A	3310	1/1	0.94	0.14	45,45,45,45	0
58	MG	a	3363	1/1	0.94	0.24	43,43,43,43	0
58	MG	A	3147	1/1	0.94	0.22	64,64,64,64	0
58	MG	A	3241	1/1	0.94	0.15	42,42,42,42	0
58	MG	A	3531	1/1	0.94	0.07	91,91,91,91	0
58	MG	A	3476	1/1	0.94	0.30	50,50,50,50	0
58	MG	a	3387	1/1	0.94	0.08	55,55,55,55	0
58	MG	A	3028	1/1	0.94	0.27	66,66,66,66	0
58	MG	a	3457	1/1	0.94	0.33	41,41,41,41	0
58	MG	a	3476	1/1	0.94	0.10	50,50,50,50	0
58	MG	A	3279	1/1	0.94	0.14	55,55,55,55	0
58	MG	A	3379	1/1	0.94	0.25	50,50,50,50	0
58	MG	A	3558	1/1	0.94	0.15	73,73,73,73	0
58	MG	A	3371	1/1	0.94	0.11	53,53,53,53	0
58	MG	A	3380	1/1	0.94	0.20	52,52,52,52	0
58	MG	A	3489	1/1	0.94	0.12	55,55,55,55	0
58	MG	A	3628	1/1	0.94	0.16	87,87,87,87	0
58	MG	a	3446	1/1	0.94	0.18	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3529	1/1	0.94	0.25	56,56,56,56	0
58	MG	A	3041	1/1	0.94	0.24	42,42,42,42	0
58	MG	a	3466	1/1	0.94	0.18	60,60,60,60	0
58	MG	m	201	1/1	0.94	0.20	35,35,35,35	0
58	MG	A	3258	1/1	0.94	0.21	43,43,43,43	0
58	MG	a	3372	1/1	0.94	0.30	47,47,47,47	0
58	MG	a	3485	1/1	0.94	0.25	51,51,51,51	0
58	MG	A	3620	1/1	0.94	0.31	49,49,49,49	0
58	MG	A	3477	1/1	0.95	0.14	65,65,65,65	0
58	MG	A	3359	1/1	0.95	0.13	45,45,45,45	0
58	MG	A	3453	1/1	0.95	0.15	44,44,44,44	0
58	MG	A	3618	1/1	0.95	0.29	45,45,45,45	0
58	MG	A	3180	1/1	0.95	0.65	44,44,44,44	0
58	MG	A	3098	1/1	0.95	0.16	48,48,48,48	0
58	MG	a	3389	1/1	0.95	0.11	38,38,38,38	0
58	MG	A	3133	1/1	0.95	0.49	44,44,44,44	0
58	MG	A	3035	1/1	0.95	0.09	47,47,47,47	0
59	ZN	4	501	1/1	0.95	0.06	117,117,117,117	0
58	MG	A	3475	1/1	0.95	0.07	55,55,55,55	0
58	MG	A	3539	1/1	0.95	0.14	52,52,52,52	0
58	MG	A	3559	1/1	0.95	0.22	46,46,46,46	0
58	MG	A	3228	1/1	0.95	0.19	62,62,62,62	0
58	MG	A	3300	1/1	0.95	0.17	60,60,60,60	0
58	MG	A	3105	1/1	0.95	0.11	35,35,35,35	0
58	MG	A	3344	1/1	0.95	0.07	53,53,53,53	0
58	MG	a	3386	1/1	0.95	0.47	41,41,41,41	0
58	MG	A	3550	1/1	0.95	0.13	58,58,58,58	0
58	MG	A	3200	1/1	0.95	0.18	44,44,44,44	0
58	MG	A	3088	1/1	0.95	0.15	63,63,63,63	0
58	MG	A	3623	1/1	0.95	0.20	52,52,52,52	0
58	MG	A	3280	1/1	0.95	0.28	32,32,32,32	0
58	MG	A	3206	1/1	0.95	0.14	65,65,65,65	0
58	MG	A	3218	1/1	0.95	0.45	32,32,32,32	0
58	MG	A	3189	1/1	0.95	0.31	37,37,37,37	0
58	MG	a	3416	1/1	0.95	0.25	61,61,61,61	0
58	MG	A	3351	1/1	0.95	0.20	38,38,38,38	0
58	MG	A	3222	1/1	0.95	0.20	33,33,33,33	0
58	MG	A	3274	1/1	0.95	0.47	45,45,45,45	0
58	MG	A	3420	1/1	0.95	0.20	31,31,31,31	0
58	MG	A	3384	1/1	0.95	0.23	51,51,51,51	0
58	MG	7	101	1/1	0.95	0.72	48,48,48,48	0
58	MG	A	3314	1/1	0.95	0.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	a	3365	1/1	0.95	0.74	45,45,45,45	0
58	MG	a	3430	1/1	0.95	0.08	65,65,65,65	0
58	MG	A	3205	1/1	0.95	0.12	43,43,43,43	0
58	MG	A	3303	1/1	0.95	0.07	55,55,55,55	0
58	MG	a	3464	1/1	0.95	0.07	44,44,44,44	0
58	MG	A	3394	1/1	0.95	0.20	30,30,30,30	0
58	MG	B	212	1/1	0.95	0.18	75,75,75,75	0
58	MG	A	3208	1/1	0.95	0.27	40,40,40,40	0
58	MG	B	201	1/1	0.95	0.33	51,51,51,51	0
58	MG	a	3456	1/1	0.95	0.19	59,59,59,59	0
58	MG	a	3311	1/1	0.95	0.20	51,51,51,51	0
58	MG	A	3368	1/1	0.95	0.23	47,47,47,47	0
58	MG	A	3474	1/1	0.95	0.13	51,51,51,51	0
58	MG	w	106	1/1	0.95	0.17	45,45,45,45	0
58	MG	A	3083	1/1	0.95	0.07	37,37,37,37	0
58	MG	A	3390	1/1	0.95	0.24	46,46,46,46	0
58	MG	A	3348	1/1	0.95	0.19	71,71,71,71	0
58	MG	B	218	1/1	0.95	0.22	74,74,74,74	0
58	MG	A	3582	1/1	0.95	0.14	63,63,63,63	0
58	MG	a	3444	1/1	0.95	0.16	53,53,53,53	0
58	MG	l	202	1/1	0.95	0.33	61,61,61,61	0
58	MG	A	3455	1/1	0.95	0.22	73,73,73,73	0
58	MG	A	3604	1/1	0.95	0.35	64,64,64,64	0
58	MG	a	3414	1/1	0.95	0.20	50,50,50,50	0
58	MG	A	3257	1/1	0.95	0.18	50,50,50,50	0
58	MG	A	3151	1/1	0.95	0.29	43,43,43,43	0
58	MG	A	3553	1/1	0.95	0.08	40,40,40,40	0
58	MG	A	3123	1/1	0.95	0.17	51,51,51,51	0
58	MG	A	3634	1/1	0.95	0.14	56,56,56,56	0
58	MG	A	3164	1/1	0.95	0.19	51,51,51,51	0
58	MG	a	3375	1/1	0.96	0.57	41,41,41,41	0
58	MG	A	3534	1/1	0.96	0.36	45,45,45,45	0
58	MG	A	3527	1/1	0.96	0.20	63,63,63,63	0
58	MG	A	3155	1/1	0.96	0.28	44,44,44,44	0
58	MG	A	3307	1/1	0.96	0.21	45,45,45,45	0
58	MG	A	3412	1/1	0.96	0.22	45,45,45,45	0
58	MG	A	3566	1/1	0.96	0.11	40,40,40,40	0
58	MG	a	3404	1/1	0.96	0.44	38,38,38,38	0
58	MG	A	3548	1/1	0.96	0.14	40,40,40,40	0
58	MG	A	3561	1/1	0.96	0.14	54,54,54,54	0
58	MG	A	3501	1/1	0.96	0.26	46,46,46,46	0
58	MG	A	3540	1/1	0.96	0.22	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3267	1/1	0.96	0.28	59,59,59,59	0
58	MG	A	3385	1/1	0.96	0.19	57,57,57,57	0
58	MG	A	3422	1/1	0.96	0.18	52,52,52,52	0
58	MG	A	3381	1/1	0.96	0.24	43,43,43,43	0
58	MG	a	3399	1/1	0.96	0.18	36,36,36,36	0
58	MG	A	3166	1/1	0.96	0.30	57,57,57,57	0
58	MG	A	3557	1/1	0.96	0.33	60,60,60,60	0
58	MG	A	3156	1/1	0.96	0.08	86,86,86,86	0
58	MG	A	3234	1/1	0.96	0.36	48,48,48,48	0
58	MG	A	3163	1/1	0.96	0.16	34,34,34,34	0
58	MG	A	3522	1/1	0.96	0.17	51,51,51,51	0
58	MG	A	3473	1/1	0.96	0.15	46,46,46,46	0
58	MG	A	3128	1/1	0.96	0.19	45,45,45,45	0
58	MG	a	3452	1/1	0.96	0.11	52,52,52,52	0
58	MG	a	3367	1/1	0.96	0.25	30,30,30,30	0
58	MG	A	3115	1/1	0.96	0.12	48,48,48,48	0
58	MG	A	3071	1/1	0.96	0.22	41,41,41,41	0
58	MG	A	3070	1/1	0.96	0.11	57,57,57,57	0
58	MG	a	3378	1/1	0.96	0.24	39,39,39,39	0
58	MG	A	3324	1/1	0.96	0.21	43,43,43,43	0
58	MG	w	104	1/1	0.96	0.09	38,38,38,38	0
58	MG	A	3597	1/1	0.96	0.28	65,65,65,65	0
58	MG	a	3347	1/1	0.96	0.23	41,41,41,41	0
58	MG	A	3492	1/1	0.96	0.10	62,62,62,62	0
58	MG	A	3187	1/1	0.96	0.44	47,47,47,47	0
58	MG	A	3219	1/1	0.96	0.11	61,61,61,61	0
58	MG	A	3499	1/1	0.96	0.10	60,60,60,60	0
58	MG	B	203	1/1	0.96	0.07	56,56,56,56	0
58	MG	A	3587	1/1	0.96	0.25	48,48,48,48	0
58	MG	A	3468	1/1	0.96	0.13	48,48,48,48	0
58	MG	A	3190	1/1	0.96	0.30	38,38,38,38	0
58	MG	A	3445	1/1	0.96	0.08	51,51,51,51	0
58	MG	A	3500	1/1	0.96	0.29	40,40,40,40	0
58	MG	A	3318	1/1	0.96	0.32	60,60,60,60	0
58	MG	A	3541	1/1	0.96	0.26	56,56,56,56	0
58	MG	a	3309	1/1	0.96	0.81	37,37,37,37	0
58	MG	A	3292	1/1	0.96	0.24	54,54,54,54	0
58	MG	A	3496	1/1	0.96	0.17	47,47,47,47	0
58	MG	B	205	1/1	0.96	0.21	81,81,81,81	0
58	MG	A	3349	1/1	0.96	0.27	39,39,39,39	0
58	MG	A	3536	1/1	0.96	0.21	39,39,39,39	0
58	MG	A	3503	1/1	0.96	0.21	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	a	3432	1/1	0.96	0.09	46,46,46,46	0
58	MG	A	3510	1/1	0.96	0.15	60,60,60,60	0
58	MG	A	3547	1/1	0.96	0.20	60,60,60,60	0
58	MG	A	3077	1/1	0.96	0.13	48,48,48,48	0
58	MG	A	3090	1/1	0.96	0.39	38,38,38,38	0
58	MG	a	3338	1/1	0.96	0.17	66,66,66,66	0
58	MG	A	3317	1/1	0.96	0.20	31,31,31,31	0
58	MG	A	3387	1/1	0.96	0.18	53,53,53,53	0
58	MG	A	3012	1/1	0.96	0.16	37,37,37,37	0
58	MG	a	3417	1/1	0.96	0.31	37,37,37,37	0
58	MG	A	3417	1/1	0.96	0.20	30,30,30,30	0
58	MG	A	3440	1/1	0.96	0.20	74,74,74,74	0
58	MG	R	203	1/1	0.96	0.25	44,44,44,44	0
58	MG	a	3475	1/1	0.96	0.38	38,38,38,38	0
58	MG	A	3556	1/1	0.96	0.15	55,55,55,55	0
58	MG	A	3116	1/1	0.96	0.34	50,50,50,50	0
58	MG	A	3321	1/1	0.96	0.09	41,41,41,41	0
58	MG	A	3599	1/1	0.96	0.22	57,57,57,57	0
58	MG	a	3344	1/1	0.96	0.12	51,51,51,51	0
58	MG	A	3358	1/1	0.96	0.18	63,63,63,63	0
58	MG	A	3632	1/1	0.96	0.27	63,63,63,63	0
58	MG	A	3470	1/1	0.97	0.17	43,43,43,43	0
58	MG	A	3593	1/1	0.97	0.30	41,41,41,41	0
58	MG	A	3169	1/1	0.97	0.30	57,57,57,57	0
58	MG	a	3465	1/1	0.97	0.07	57,57,57,57	0
58	MG	A	3372	1/1	0.97	0.17	59,59,59,59	0
58	MG	A	3229	1/1	0.97	0.13	46,46,46,46	0
58	MG	A	3535	1/1	0.97	0.22	49,49,49,49	0
58	MG	A	3364	1/1	0.97	0.16	61,61,61,61	0
59	ZN	Y	501	1/1	0.97	0.08	92,92,92,92	0
58	MG	A	3049	1/1	0.97	0.19	41,41,41,41	0
58	MG	A	3362	1/1	0.97	0.18	50,50,50,50	0
58	MG	A	3579	1/1	0.97	0.19	53,53,53,53	0
58	MG	a	3412	1/1	0.97	0.11	48,48,48,48	0
58	MG	A	3633	1/1	0.97	0.30	64,64,64,64	0
58	MG	a	3482	1/1	0.97	0.14	37,37,37,37	0
58	MG	A	3457	1/1	0.97	0.20	41,41,41,41	0
58	MG	a	3448	1/1	0.97	0.07	42,42,42,42	0
58	MG	a	3415	1/1	0.97	0.20	62,62,62,62	0
58	MG	A	3369	1/1	0.97	0.16	54,54,54,54	0
58	MG	A	3338	1/1	0.97	0.28	30,30,30,30	0
58	MG	a	3473	1/1	0.97	0.45	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3459	1/1	0.97	0.18	36,36,36,36	0
58	MG	A	3283	1/1	0.97	0.12	55,55,55,55	0
58	MG	A	3225	1/1	0.97	0.26	36,36,36,36	0
58	MG	a	3307	1/1	0.97	0.14	35,35,35,35	0
59	ZN	9	102	1/1	0.97	0.10	72,72,72,72	0
58	MG	a	3453	1/1	0.97	0.07	41,41,41,41	0
58	MG	a	3460	1/1	0.97	0.14	52,52,52,52	0
58	MG	A	3396	1/1	0.97	0.24	38,38,38,38	0
58	MG	A	3296	1/1	0.97	0.36	52,52,52,52	0
58	MG	A	3526	1/1	0.97	0.10	41,41,41,41	0
58	MG	A	3409	1/1	0.97	0.25	60,60,60,60	0
58	MG	A	3438	1/1	0.97	0.12	53,53,53,53	0
58	MG	A	3306	1/1	0.97	0.18	50,50,50,50	0
58	MG	a	3382	1/1	0.97	0.21	31,31,31,31	0
58	MG	D	301	1/1	0.97	0.29	41,41,41,41	0
58	MG	a	3355	1/1	0.97	0.20	39,39,39,39	0
58	MG	A	3538	1/1	0.97	0.16	40,40,40,40	0
58	MG	A	3519	1/1	0.97	0.30	30,30,30,30	0
58	MG	A	3100	1/1	0.97	0.13	45,45,45,45	0
58	MG	A	3458	1/1	0.97	0.32	27,27,27,27	0
58	MG	A	3389	1/1	0.97	0.25	30,30,30,30	0
58	MG	a	3439	1/1	0.97	0.21	48,48,48,48	0
58	MG	a	3381	1/1	0.97	0.18	55,55,55,55	0
58	MG	A	3612	1/1	0.97	0.05	53,53,53,53	0
58	MG	A	3485	1/1	0.97	0.22	38,38,38,38	0
58	MG	A	3178	1/1	0.97	0.23	31,31,31,31	0
58	MG	a	3478	1/1	0.97	0.14	48,48,48,48	0
58	MG	A	3055	1/1	0.97	0.12	45,45,45,45	0
58	MG	A	3340	1/1	0.97	0.23	65,65,65,65	0
58	MG	A	3509	1/1	0.97	0.25	51,51,51,51	0
58	MG	A	3337	1/1	0.97	0.27	44,44,44,44	0
58	MG	A	3144	1/1	0.97	0.32	38,38,38,38	0
58	MG	A	3400	1/1	0.97	0.09	35,35,35,35	0
58	MG	A	3630	1/1	0.97	0.18	43,43,43,43	0
58	MG	a	3449	1/1	0.97	0.21	50,50,50,50	0
58	MG	a	3443	1/1	0.97	0.06	46,46,46,46	0
58	MG	a	3398	1/1	0.97	0.39	27,27,27,27	0
58	MG	a	3317	1/1	0.97	0.31	26,26,26,26	0
58	MG	U	204	1/1	0.97	0.14	37,37,37,37	0
58	MG	A	3230	1/1	0.97	0.24	46,46,46,46	0
58	MG	A	3320	1/1	0.97	0.12	49,49,49,49	0
58	MG	a	3479	1/1	0.97	0.18	47,47,47,47	0

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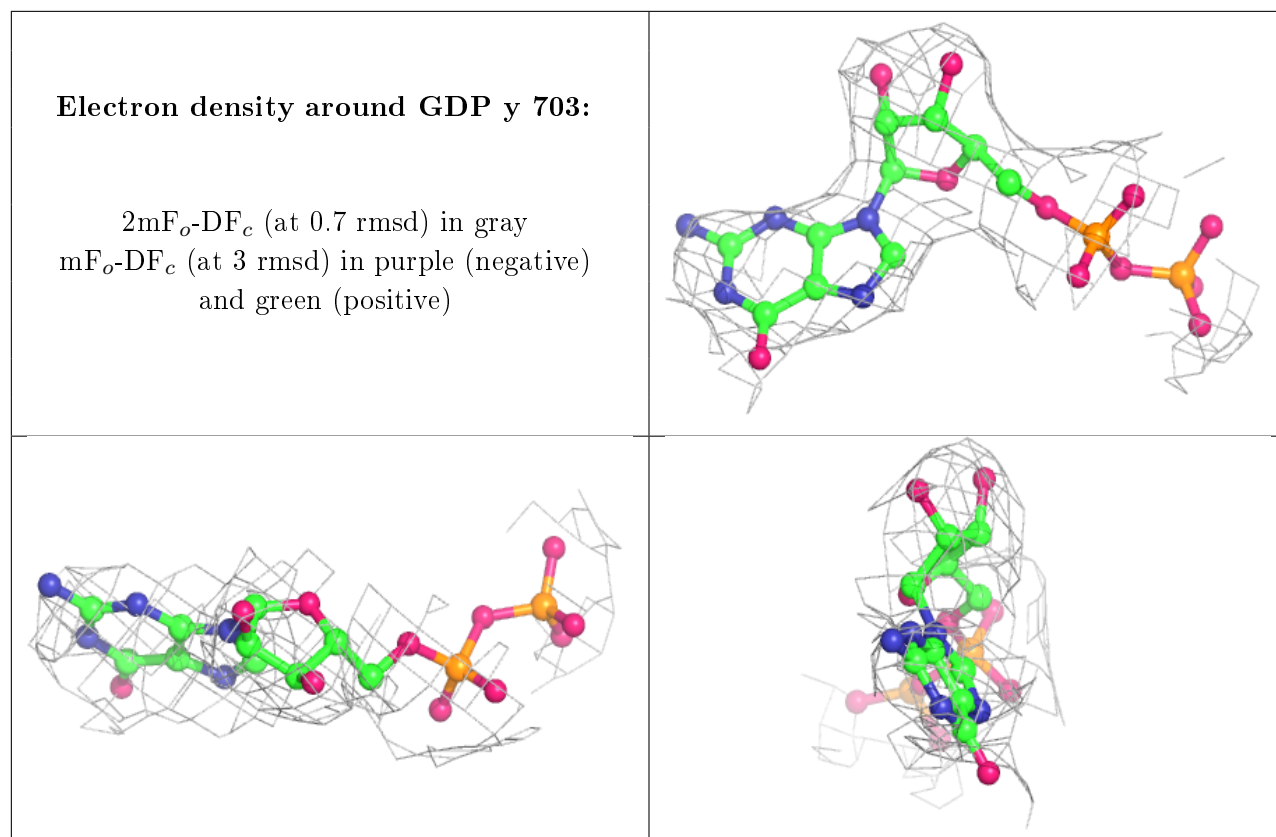
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	a	3397	1/1	0.97	0.39	27,27,27,27	0
58	MG	A	3447	1/1	0.97	0.21	67,67,67,67	0
58	MG	a	3312	1/1	0.97	0.07	26,26,26,26	0
58	MG	O	201	1/1	0.97	0.09	38,38,38,38	0
59	ZN	6	102	1/1	0.97	0.09	70,70,70,70	0
58	MG	A	3583	1/1	0.97	0.10	55,55,55,55	0
58	MG	A	3609	1/1	0.97	0.14	39,39,39,39	0
58	MG	A	3424	1/1	0.97	0.27	57,57,57,57	0
58	MG	A	3437	1/1	0.97	0.20	28,28,28,28	0
58	MG	A	3494	1/1	0.97	0.17	42,42,42,42	0
58	MG	A	3391	1/1	0.97	0.21	30,30,30,30	0
58	MG	A	3592	1/1	0.97	0.09	67,67,67,67	0
58	MG	a	3322	1/1	0.97	0.09	50,50,50,50	0
58	MG	A	3488	1/1	0.97	0.31	50,50,50,50	0
58	MG	A	3626	1/1	0.97	0.14	51,51,51,51	0
58	MG	a	3471	1/1	0.97	0.27	49,49,49,49	0
58	MG	a	3447	1/1	0.98	0.41	36,36,36,36	0
58	MG	a	3487	1/1	0.98	0.32	35,35,35,35	0
58	MG	a	3379	1/1	0.98	0.21	30,30,30,30	0
58	MG	n	101	1/1	0.98	0.25	42,42,42,42	0
58	MG	A	3537	1/1	0.98	0.18	32,32,32,32	0
59	ZN	n	102	1/1	0.98	0.15	61,61,61,61	0
58	MG	a	3343	1/1	0.98	0.16	29,29,29,29	0
58	MG	A	3179	1/1	0.98	0.18	43,43,43,43	0
58	MG	A	3191	1/1	0.98	0.36	33,33,33,33	0
58	MG	A	3170	1/1	0.98	0.23	43,43,43,43	0
58	MG	A	3523	1/1	0.98	0.23	36,36,36,36	0
58	MG	y	702	1/1	0.98	0.18	75,75,75,75	0
58	MG	a	3395	1/1	0.98	0.30	32,32,32,32	0
58	MG	A	3413	1/1	0.98	0.25	51,51,51,51	0
58	MG	A	3483	1/1	0.98	0.18	55,55,55,55	0
58	MG	A	3176	1/1	0.98	0.10	35,35,35,35	0
58	MG	A	3233	1/1	0.98	0.17	53,53,53,53	0
58	MG	A	3249	1/1	0.98	0.11	31,31,31,31	0
58	MG	A	3443	1/1	0.98	0.14	39,39,39,39	0
58	MG	A	3518	1/1	0.98	0.04	65,65,65,65	0
58	MG	A	3377	1/1	0.98	0.17	44,44,44,44	0
58	MG	A	3015	1/1	0.98	0.20	43,43,43,43	0
58	MG	A	3184	1/1	0.98	0.39	40,40,40,40	0
58	MG	A	3418	1/1	0.98	0.38	32,32,32,32	0
58	MG	a	3318	1/1	0.98	0.24	41,41,41,41	0
58	MG	A	3399	1/1	0.98	0.28	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3528	1/1	0.98	0.09	51,51,51,51	0
58	MG	A	3421	1/1	0.98	0.18	40,40,40,40	0
58	MG	A	3183	1/1	0.98	0.19	54,54,54,54	0
58	MG	A	3188	1/1	0.98	0.32	44,44,44,44	0
58	MG	A	3256	1/1	0.98	0.15	55,55,55,55	0
58	MG	A	3460	1/1	0.98	0.20	44,44,44,44	0
58	MG	A	3238	1/1	0.98	0.27	45,45,45,45	0
58	MG	A	3429	1/1	0.98	0.24	30,30,30,30	0
58	MG	A	3332	1/1	0.98	0.20	39,39,39,39	0
58	MG	A	3195	1/1	0.98	0.23	41,41,41,41	0
58	MG	A	3480	1/1	0.98	0.15	35,35,35,35	0
58	MG	A	3416	1/1	0.98	0.21	41,41,41,41	0
58	MG	A	3495	1/1	0.98	0.25	40,40,40,40	0
58	MG	A	3021	1/1	0.98	0.18	34,34,34,34	0
58	MG	A	3329	1/1	0.98	0.14	40,40,40,40	0
58	MG	a	3374	1/1	0.98	0.41	30,30,30,30	0
58	MG	a	3394	1/1	0.98	0.19	32,32,32,32	0
58	MG	A	3127	1/1	0.98	0.14	73,73,73,73	0
58	MG	A	3194	1/1	0.98	0.34	34,34,34,34	0
58	MG	A	3588	1/1	0.98	0.17	40,40,40,40	0
58	MG	A	3530	1/1	0.99	0.25	38,38,38,38	0
58	MG	a	3305	1/1	0.99	0.19	46,46,46,46	0
58	MG	a	3402	1/1	0.99	0.19	43,43,43,43	0
58	MG	A	3017	1/1	0.99	0.11	63,63,63,63	0
58	MG	A	3193	1/1	0.99	0.22	38,38,38,38	0
58	MG	A	3521	1/1	0.99	0.22	60,60,60,60	0
58	MG	a	3483	1/1	0.99	0.18	39,39,39,39	0
58	MG	A	3378	1/1	0.99	0.19	31,31,31,31	0
58	MG	A	3192	1/1	0.99	0.28	39,39,39,39	0
58	MG	A	3395	1/1	0.99	0.12	31,31,31,31	0
58	MG	a	3406	1/1	0.99	0.21	52,52,52,52	0
60	SF4	d	501	8/8	0.99	0.16	48,60,64,65	0
58	MG	A	3094	1/1	0.99	0.27	31,31,31,31	0
58	MG	A	3513	1/1	0.99	0.29	41,41,41,41	0
58	MG	a	3438	1/1	0.99	0.16	34,34,34,34	0
58	MG	w	102	1/1	0.99	0.30	49,49,49,49	0
58	MG	B	202	1/1	0.99	0.27	66,66,66,66	0
58	MG	A	3038	1/1	0.99	0.15	55,55,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.