



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:10 PM UTC

PDB ID : 4W2E / pdb\_00004w2e  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

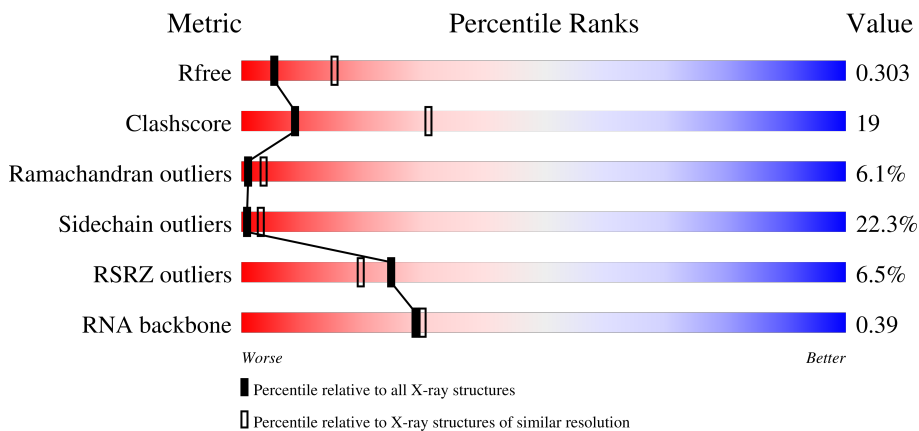
# 1 Overall quality at a glance i

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))
$R_{free}$	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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 of 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 style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 42%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-top: 5px;">2%      42%      45%      12%      .</p>
2	B	122	<div style="display: flex; align-items: center;"> <div style="width: 56%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-top: 5px;">56%      39%      . .</p>
3	D	276	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-top: 5px;">%      36%      48%      16%      .</p>
4	E	206	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-top: 5px;">2%      50%      36%      11%      . .</p>

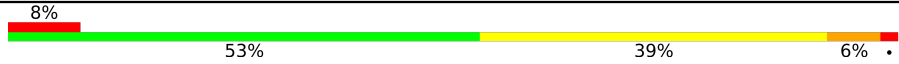

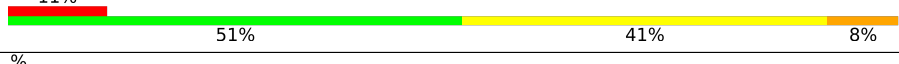
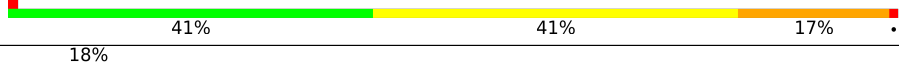
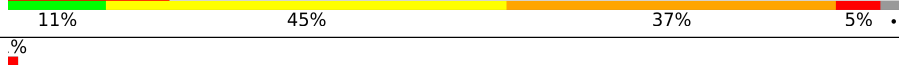
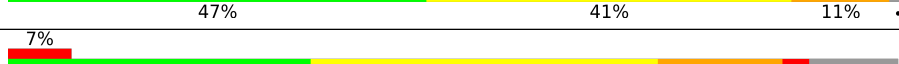
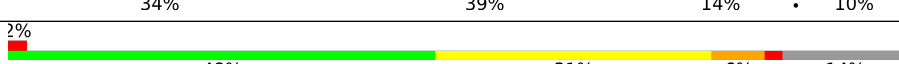
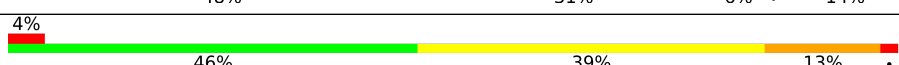
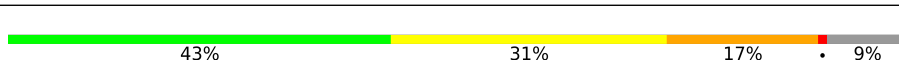






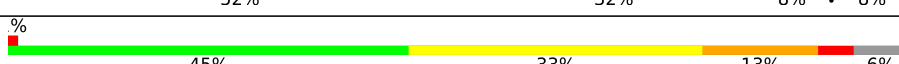
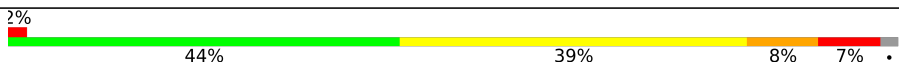



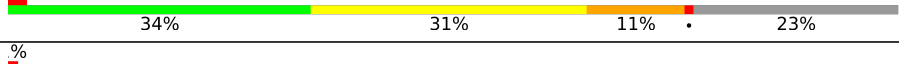
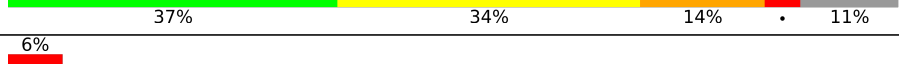



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Mol	Chain	Length	Quality of chain
5	F	205	4% 47% 41% 9% ..
6	G	182	3% 40% 44% 13% ..
7	H	180	6% 48% 34% 14% ..
8	J	173	33% 46% 21% 8% 25%
9	K	147	57% 39% 37% 16% 5%
10	N	140	3% 49% 34% 16% .
11	O	122	50% 41% 9%
12	P	150	6% 42% 45% 12% .
13	Q	141	59% 33% 8% .
14	R	118	3% 47% 42% 10% .
15	S	112	16% 43% 44% 10% ..
16	T	146	3% 38% 45% 6% 10%
17	U	118	% 36% 44% 17% ..
18	V	101	47% 40% 13% .
19	W	113	% 46% 39% 10% ..
20	X	96	6% 50% 36% 11% ..
21	Y	110	6% 39% 45% 13% ..
22	Z	206	8% 41% 32% 12% 5% 10%
23	0	85	4% 41% 39% 7% 13%
24	1	98	6% 41% 44% 14% .
25	2	72	44% 40% 12% .
26	3	60	47% 45% 5% ..
27	4	71	11% 25% 48% 20% . .
28	5	60	3% 38% 52% 7% ..
29	6	54	2% 44% 39% 15% .

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Mol	Chain	Length	Quality of chain
30	7	49	
31	8	65	
32	9	37	
33	w	76	
33	x	76	
34	a	1521	
35	b	256	
36	c	239	
37	d	209	
38	e	162	
39	f	101	
40	g	156	
41	h	138	
42	i	128	
43	j	105	
44	k	129	
45	l	132	
46	m	126	
47	n	61	
48	o	89	
49	p	88	
50	q	105	
51	r	88	
52	s	93	
53	t	106	

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Mol	Chain	Length	Quality of chain
54	u	27	
55	v	18	
56	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
59	SF4	d	501	-	-	X	-

## 2 Entry composition [i](#)

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
			Total	C	N	O	P			
1	A	2873	61879	27541	11577	19890	2871	0	0	0

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

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	204	1559	985	298	270	6	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	203	1584	1009	298	275	2	0	0	1

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	G	181	1425	914	256	251	4	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	H	174	1330	845	248	236	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	0
			1581	707	285	515	73	1			
33	w	76	Total	C	N	O	P	S	0	0	0
			1632	731	290	533	76	2			

- 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
			Total	C	N	O	S			
35	b	231	1850	1181	331	333	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called mRNA.

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

- Molecule 56 is a protein called 50S ribosomal protein L9, Elongation factor 4.

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	A	635	Total 635	Mg 635	0	0
57	B	18	Total 18	Mg 18	0	0
57	D	5	Total 5	Mg 5	0	0
57	E	4	Total 4	Mg 4	0	0
57	F	5	Total 5	Mg 5	0	0
57	G	3	Total 3	Mg 3	0	0
57	N	1	Total 1	Mg 1	0	0
57	O	1	Total 1	Mg 1	0	0
57	P	2	Total 2	Mg 2	0	0
57	Q	5	Total 5	Mg 5	0	0
57	R	3	Total 3	Mg 3	0	0
57	U	4	Total 4	Mg 4	0	0
57	V	2	Total 2	Mg 2	0	0
57	W	1	Total 1	Mg 1	0	0
57	X	1	Total 1	Mg 1	0	0
57	Z	1	Total 1	Mg 1	0	0
57	0	3	Total 3	Mg 3	0	0
57	5	1	Total 1	Mg 1	0	0
57	6	1	Total 1	Mg 1	0	0

*Continued on next page...*

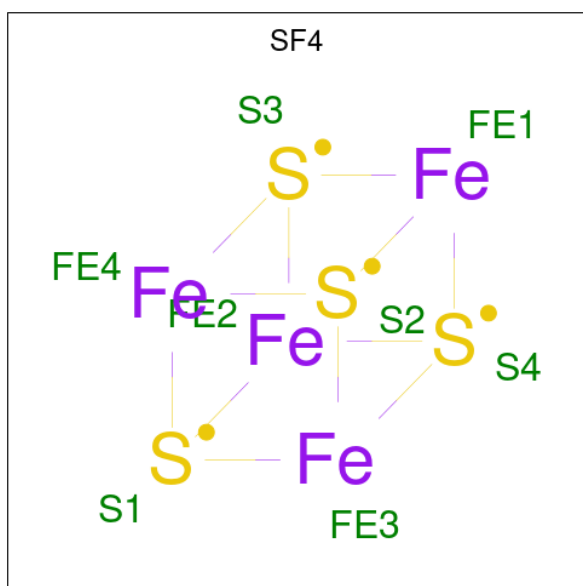
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	7	3	Total 3	Mg 3	0	0
57	8	1	Total 1	Mg 1	0	0
57	9	1	Total 1	Mg 1	0	0
57	x	3	Total 3	Mg 3	0	0
57	a	187	Total 187	Mg 187	0	0
57	e	1	Total 1	Mg 1	0	0
57	f	1	Total 1	Mg 1	0	0
57	l	2	Total 2	Mg 2	0	0
57	m	1	Total 1	Mg 1	0	0
57	n	1	Total 1	Mg 1	0	0
57	w	6	Total 6	Mg 6	0	0
57	v	1	Total 1	Mg 1	0	0
57	y	2	Total 2	Mg 2	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

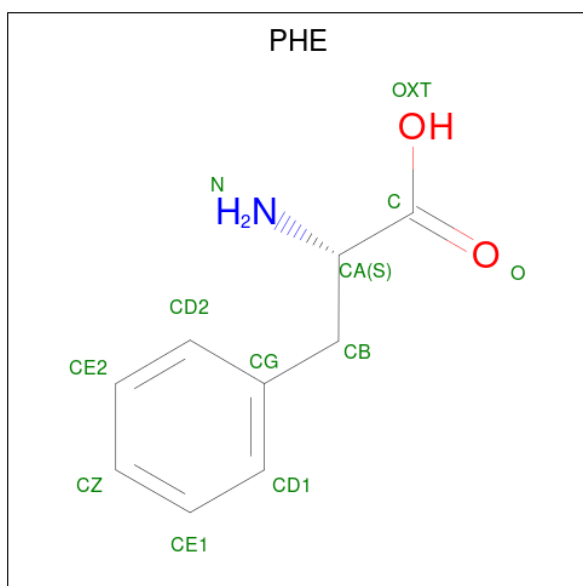
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y	1	Total 1	Zn 1	0	0
58	4	1	Total 1	Zn 1	0	0
58	5	1	Total 1	Zn 1	0	0
58	6	1	Total 1	Zn 1	0	0
58	9	1	Total 1	Zn 1	0	0
58	n	1	Total 1	Zn 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



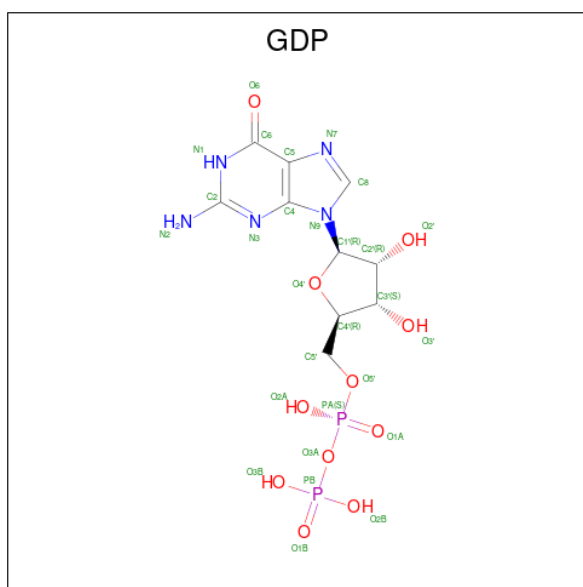
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is PHENYLALANINE (CCD ID: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	w	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

- Molecule 62 is water.

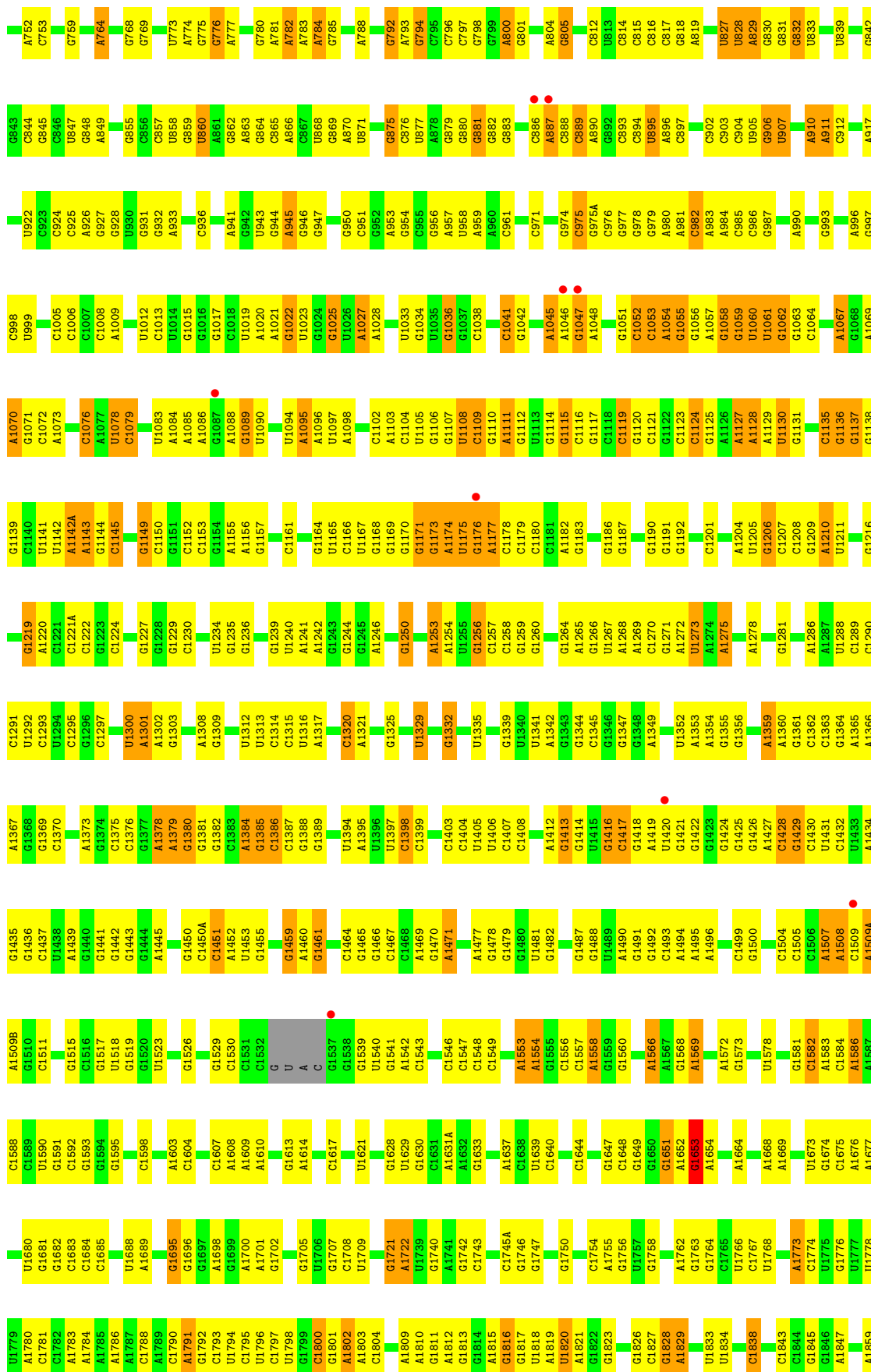
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	A	710	Total	O	0	2
			710	710		
62	B	34	Total	O	0	0
			34	34		
62	D	4	Total	O	0	0
			4	4		
62	E	7	Total	O	0	0
			7	7		
62	F	5	Total	O	0	0
			5	5		
62	G	1	Total	O	0	0
			1	1		
62	H	1	Total	O	0	0
			1	1		
62	N	1	Total	O	0	0
			1	1		
62	O	3	Total	O	0	0
			3	3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

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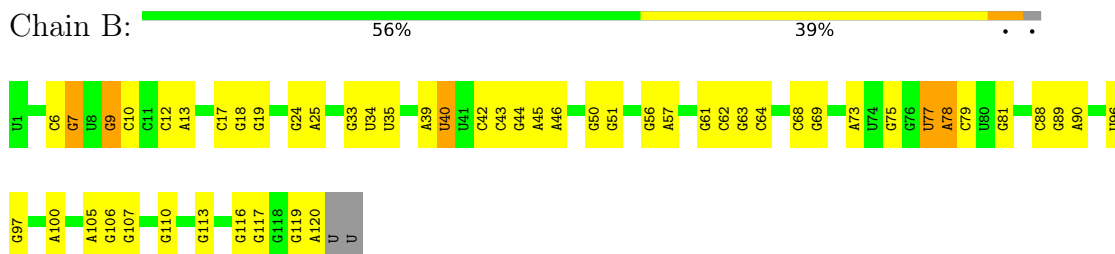
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	R	2	Total O 2 2	0	0
62	T	1	Total O 1 1	0	0
62	U	2	Total O 2 2	0	0
62	V	1	Total O 1 1	0	0
62	W	2	Total O 2 2	0	0
62	Y	1	Total O 1 1	0	0
62	0	4	Total O 4 4	0	0
62	1	2	Total O 2 2	0	0
62	3	1	Total O 1 1	0	0
62	5	1	Total O 1 1	0	0
62	7	2	Total O 2 2	0	0
62	8	4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



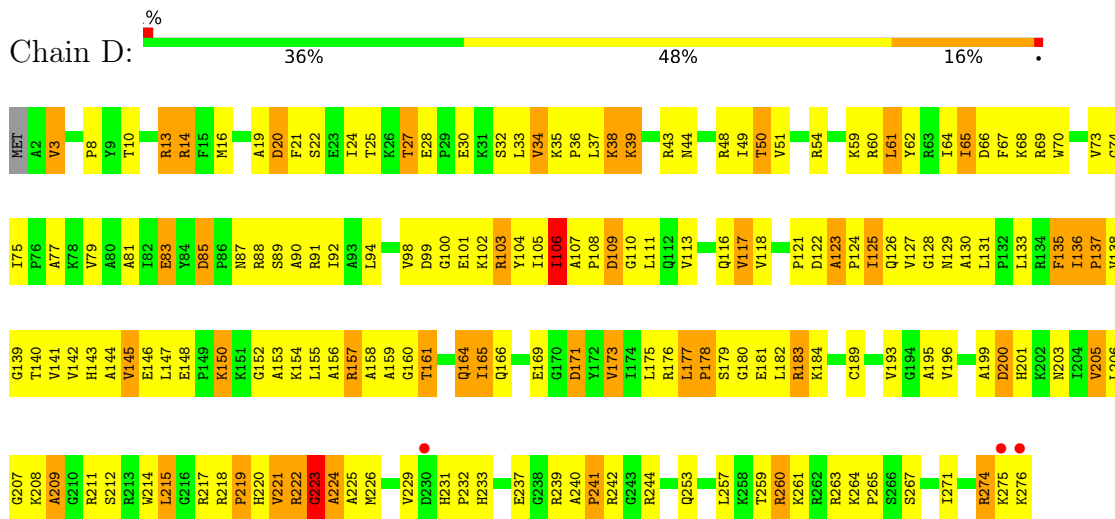




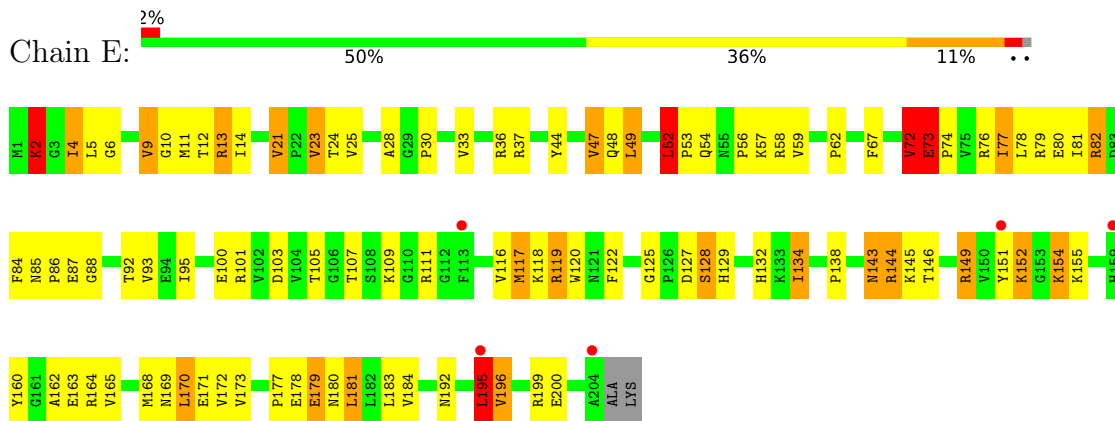
- Molecule 2: 5S Ribosomal RNA



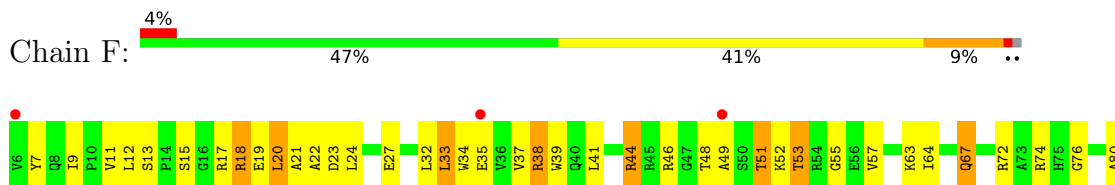
- Molecule 3: 50S ribosomal protein L2

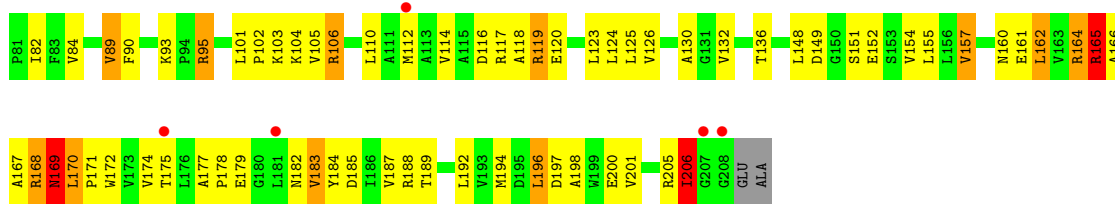


- Molecule 4: 50S ribosomal protein L3

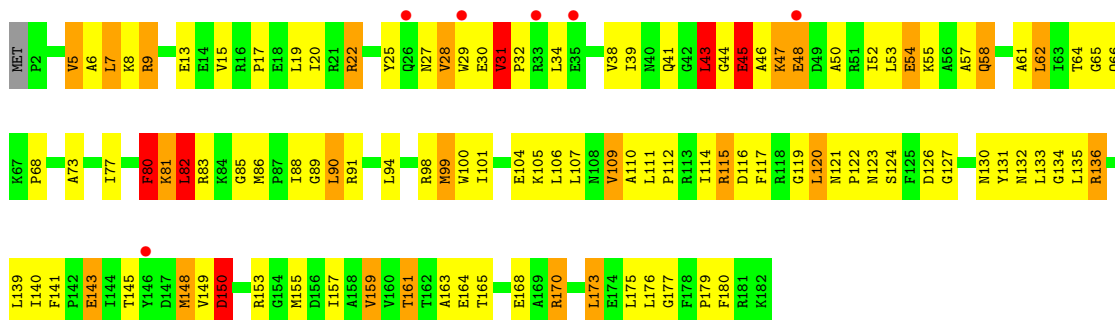
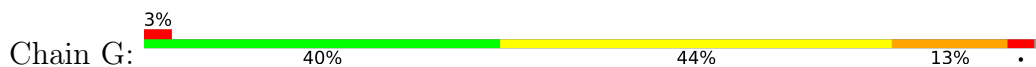


- Molecule 5: 50S ribosomal protein L4

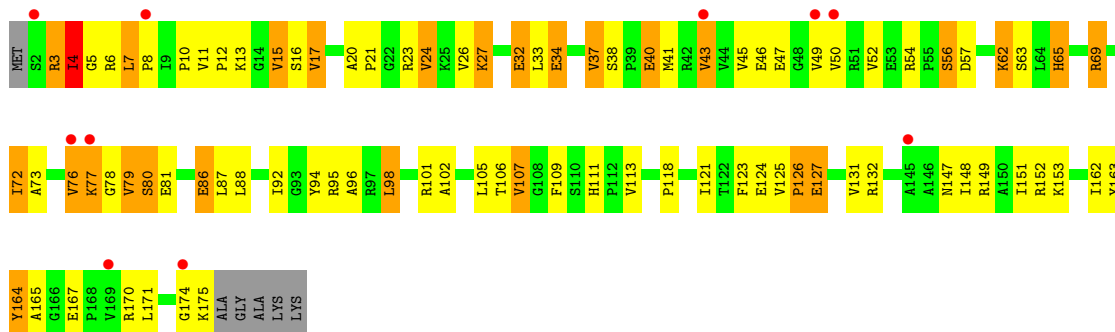




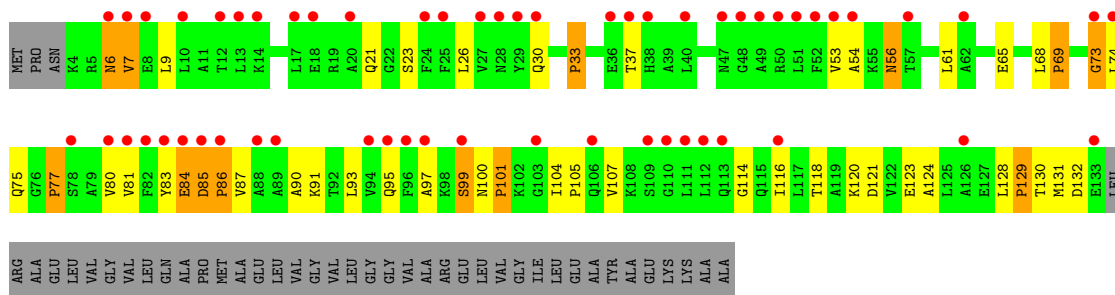
• Molecule 6: 50S ribosomal protein L5



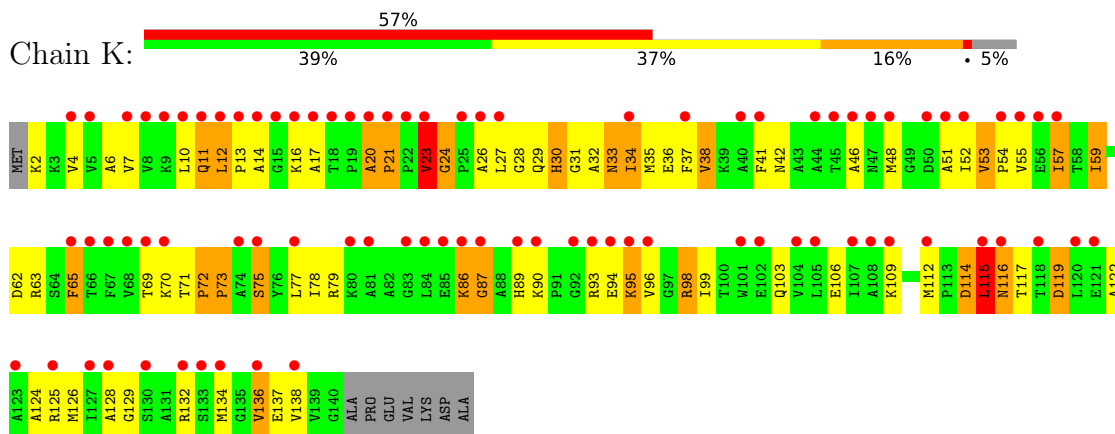
• Molecule 7: 50S ribosomal protein L6



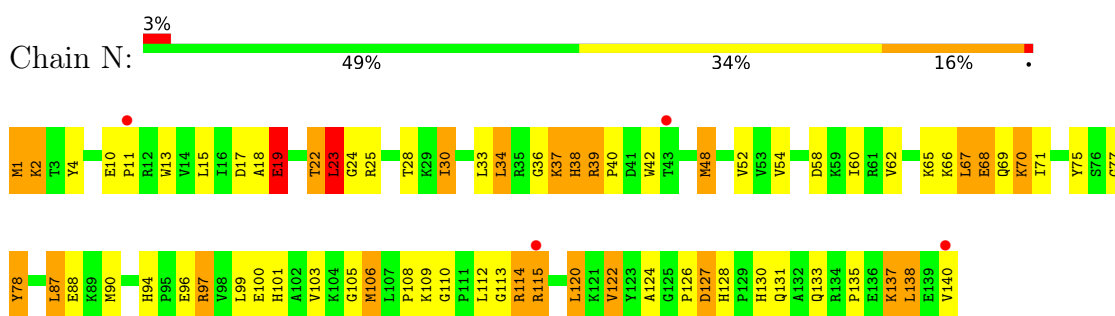
• Molecule 8: 50S ribosomal protein L10



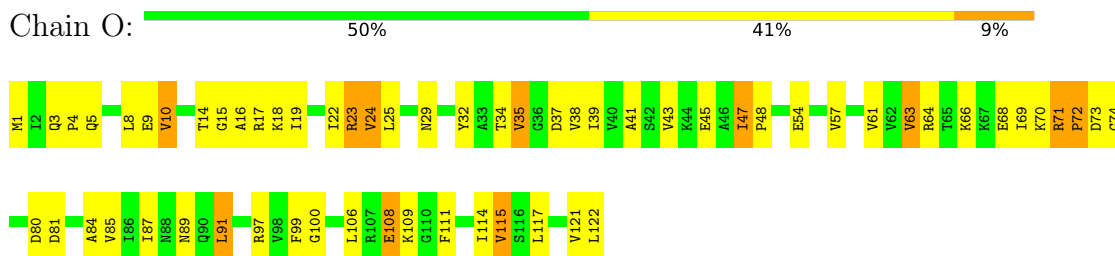
• Molecule 9: 50S ribosomal protein L11



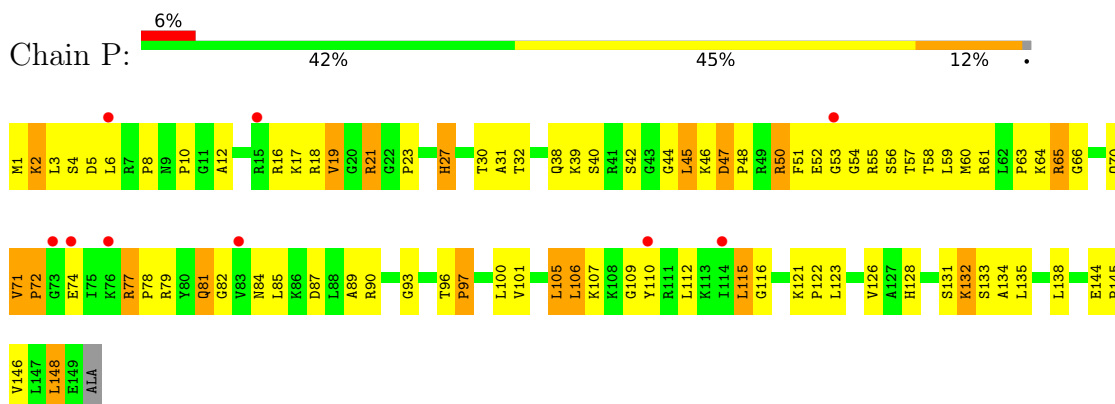
- Molecule 10: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L14

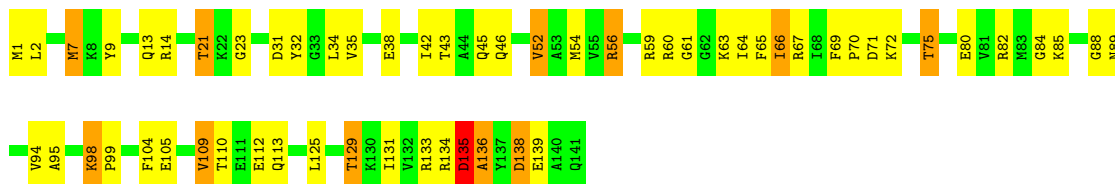


- Molecule 12: 50S ribosomal protein L15



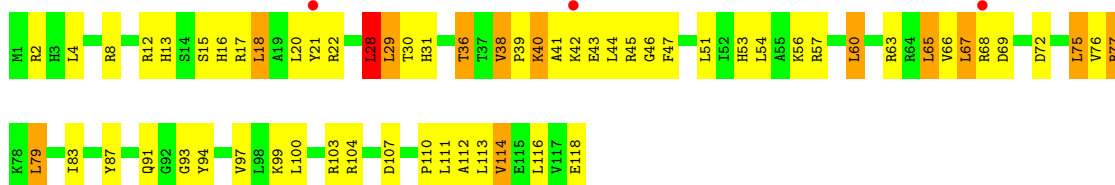
- Molecule 13: 50S ribosomal protein L16

Chain Q:  59% 33% 8%



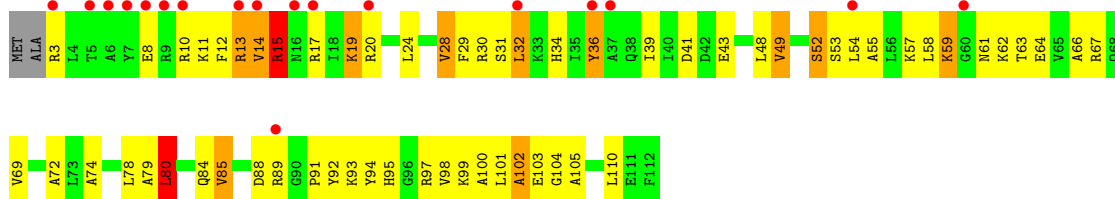
• Molecule 14: 50S ribosomal protein L17

Chain R:  3% 47% 42% 10%



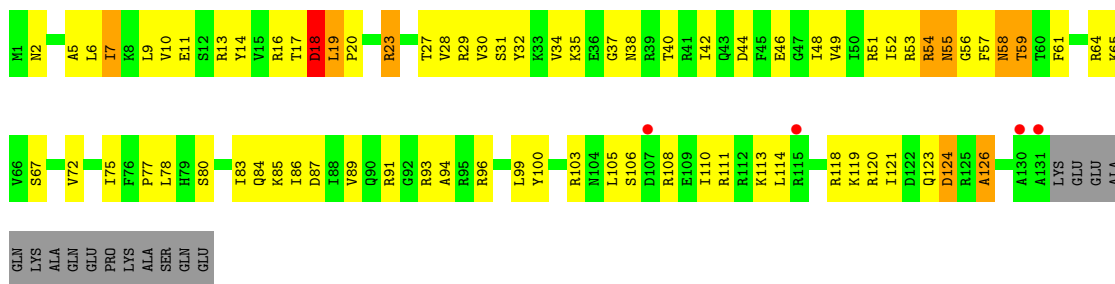
• Molecule 15: 50S ribosomal protein L18

Chain S:  16% 43% 44% 10%



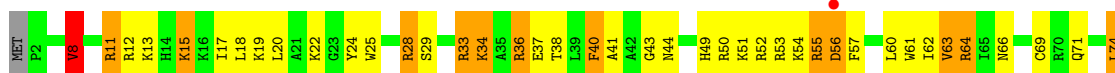
• Molecule 16: 50S ribosomal protein L19

Chain T:  3% 38% 45% 6% 10%



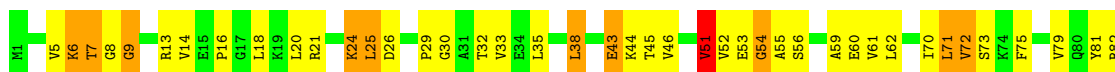
• Molecule 17: 50S ribosomal protein L20

Chain U:  36% 44% 17%





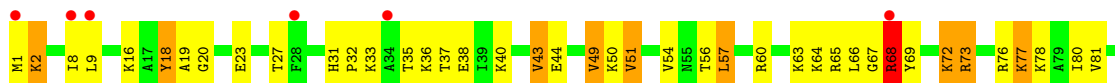
- Molecule 18: 50S ribosomal protein L21



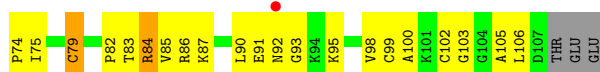
- Molecule 19: 50S ribosomal protein L22



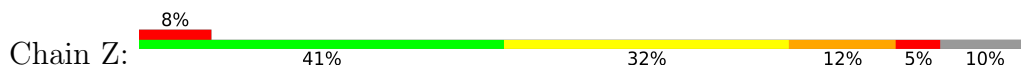
- Molecule 20: 50S ribosomal protein L23

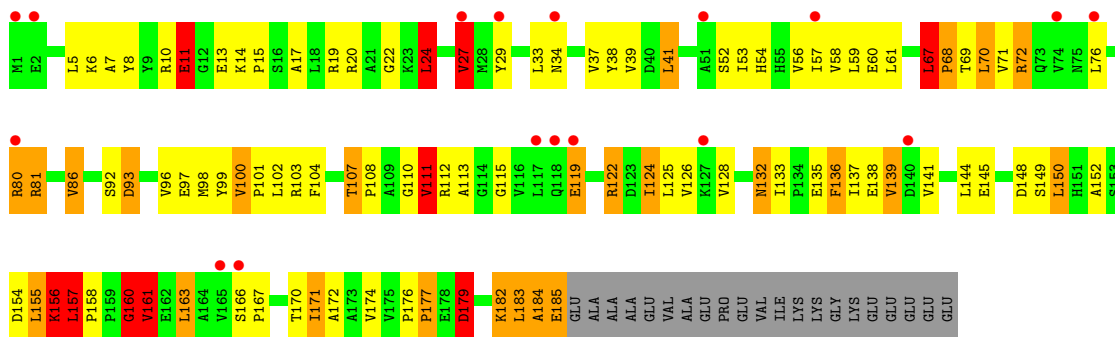


- Molecule 21: 50S ribosomal protein L24

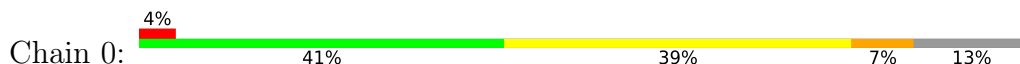


- Molecule 22: 50S ribosomal protein L25

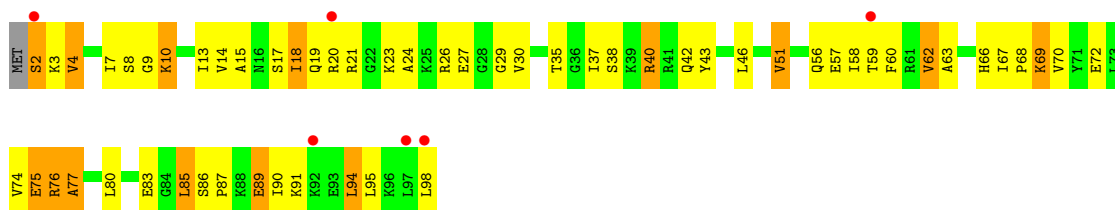




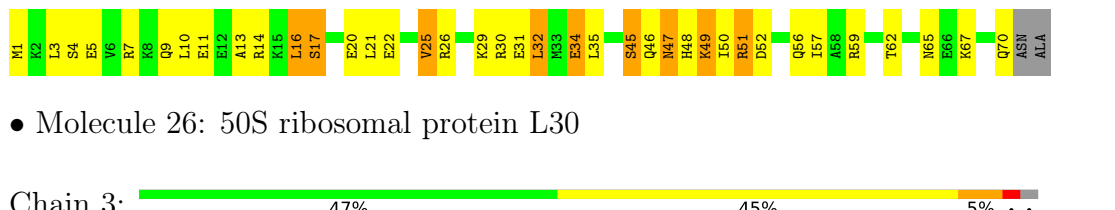
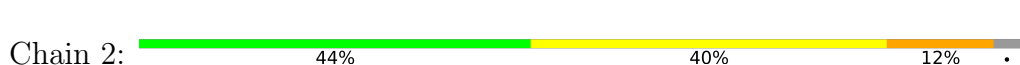
• Molecule 23: 50S ribosomal protein L27



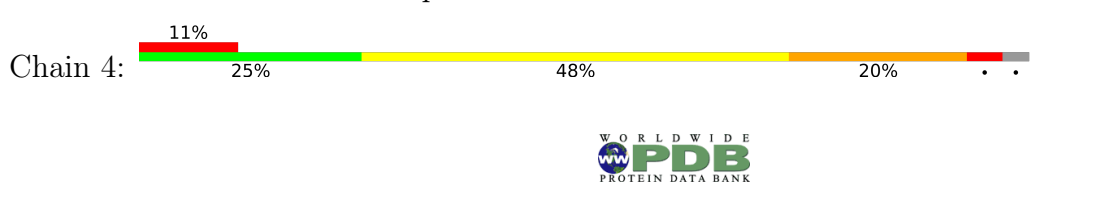
• Molecule 24: 50S ribosomal protein L28



• Molecule 25: 50S ribosomal protein L29

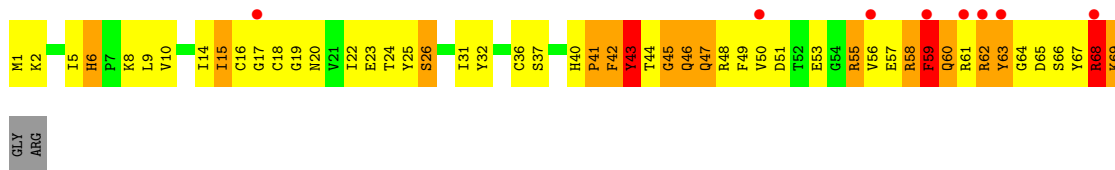


• Molecule 26: 50S ribosomal protein L30



• Molecule 27: 50S ribosomal protein L31

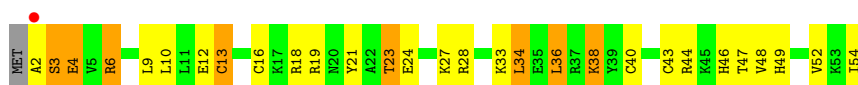
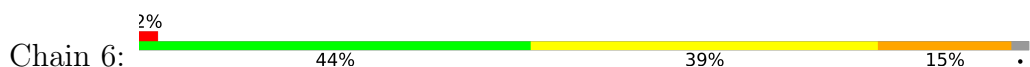




● Molecule 28: 50S ribosomal protein L32



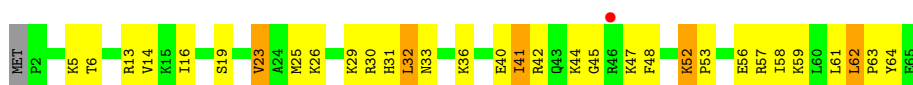
● Molecule 29: 50S ribosomal protein L33



● Molecule 30: 50S ribosomal protein L34



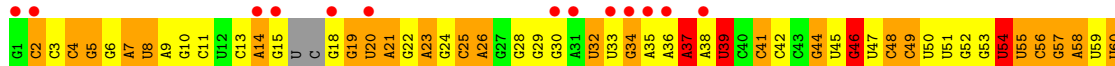
● Molecule 31: 50S ribosomal protein L35



● Molecule 32: 50S ribosomal protein L36

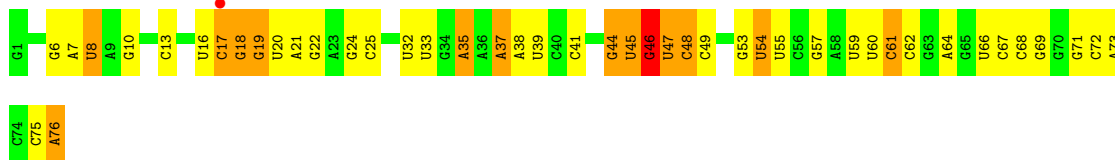


● Molecule 33: E-site tRNA

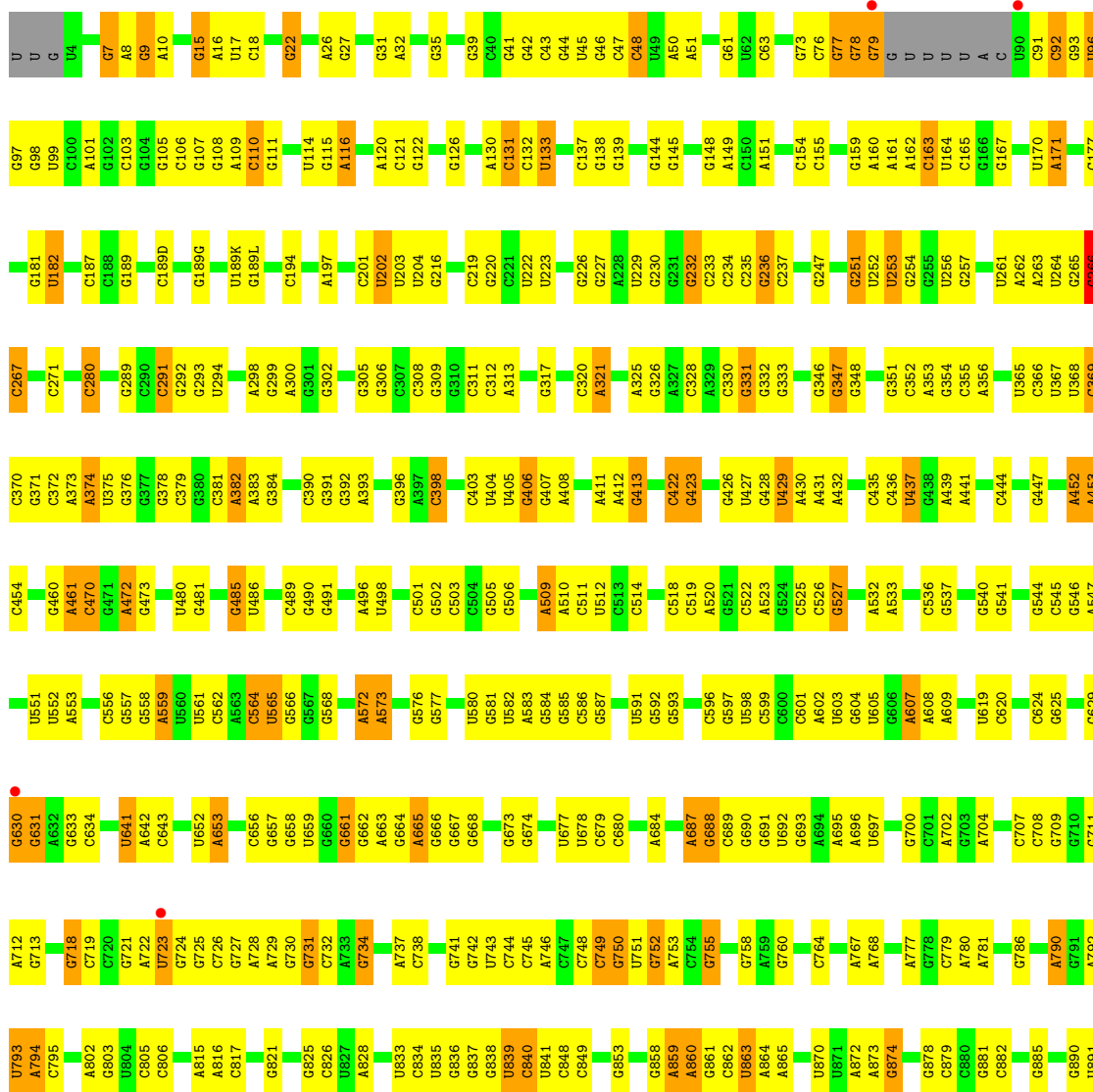


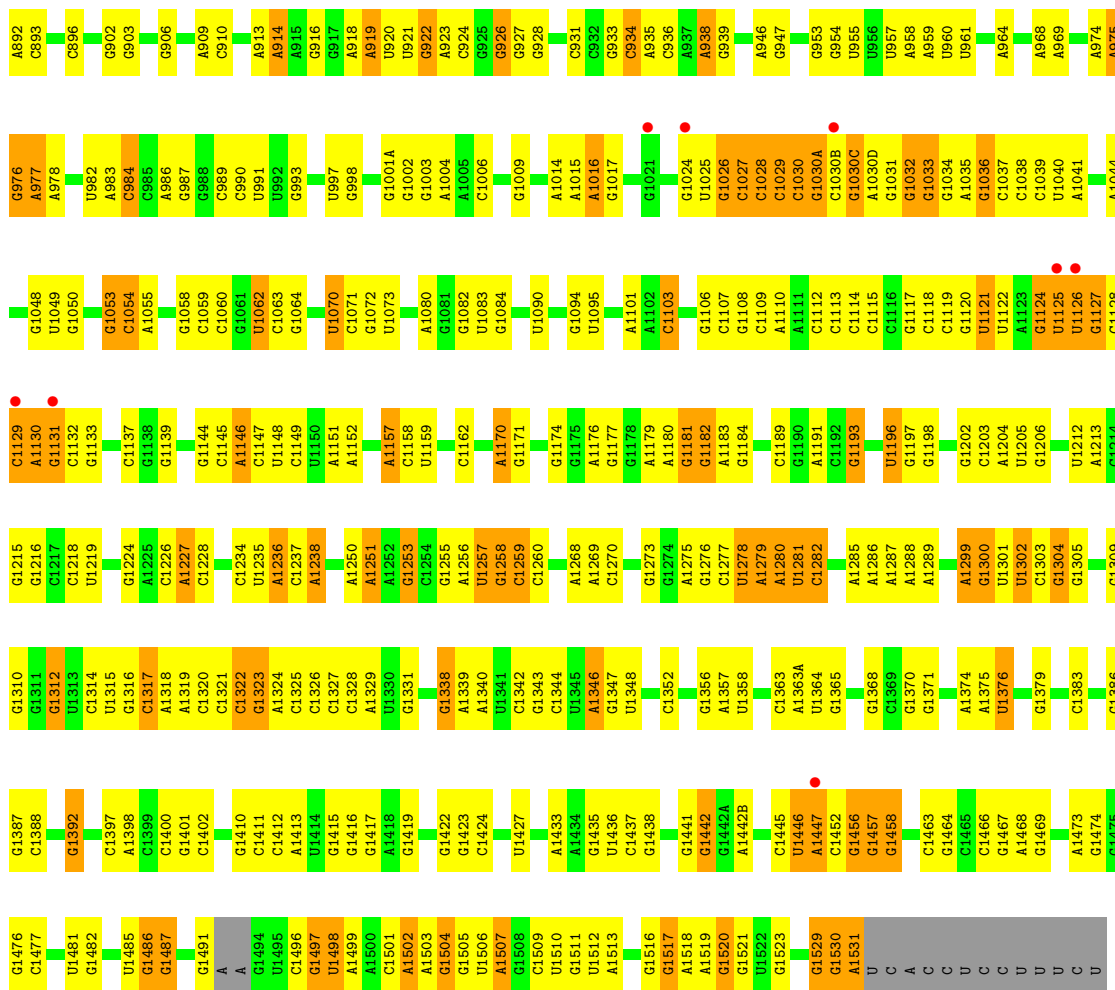


• Molecule 33: E-site tRNA

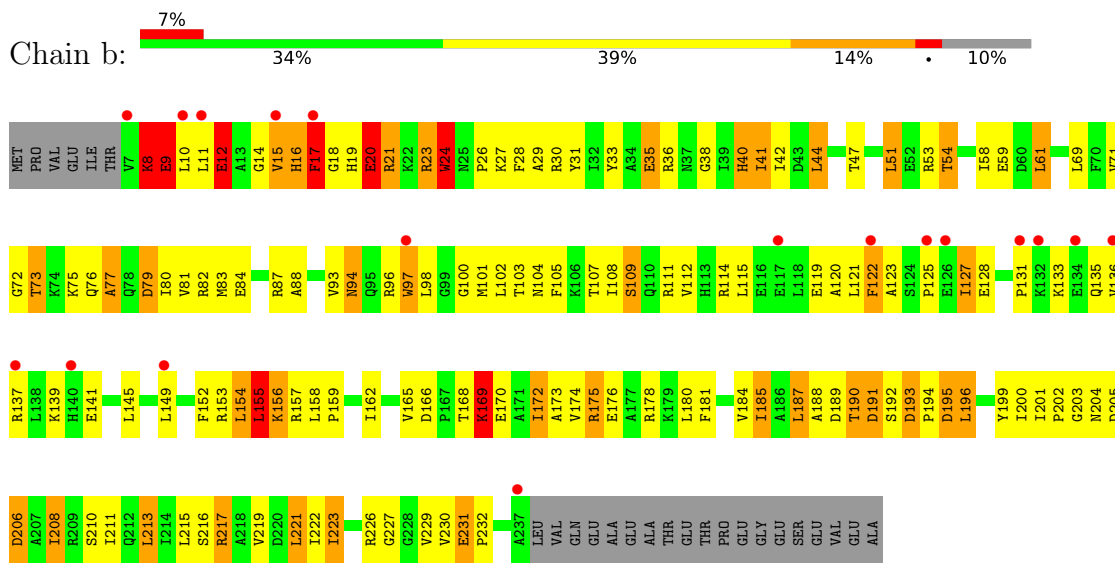


• Molecule 34: 16S Ribosomal RNA





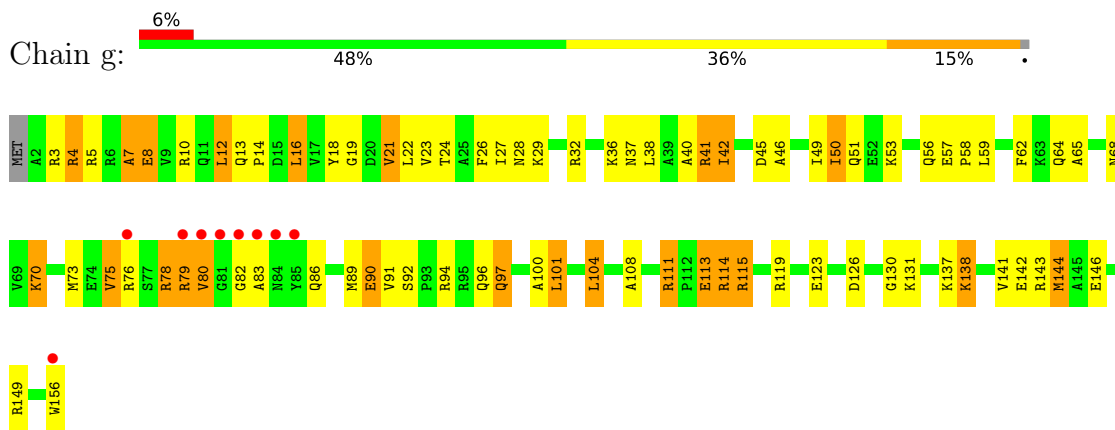
• Molecule 35: 30S ribosomal protein S2



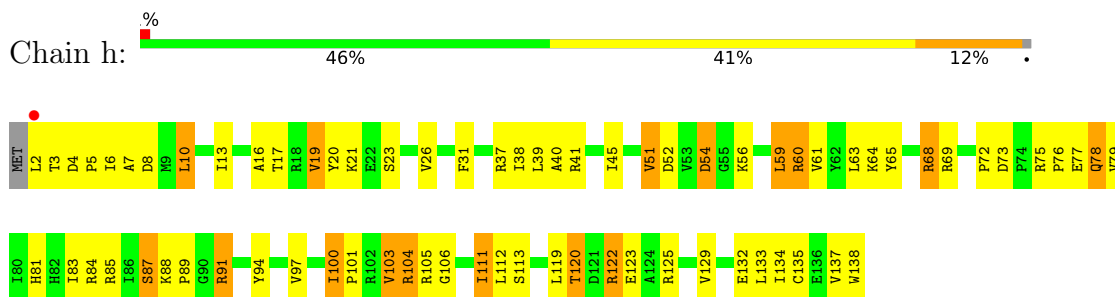
• Molecule 36: 30S ribosomal protein S3



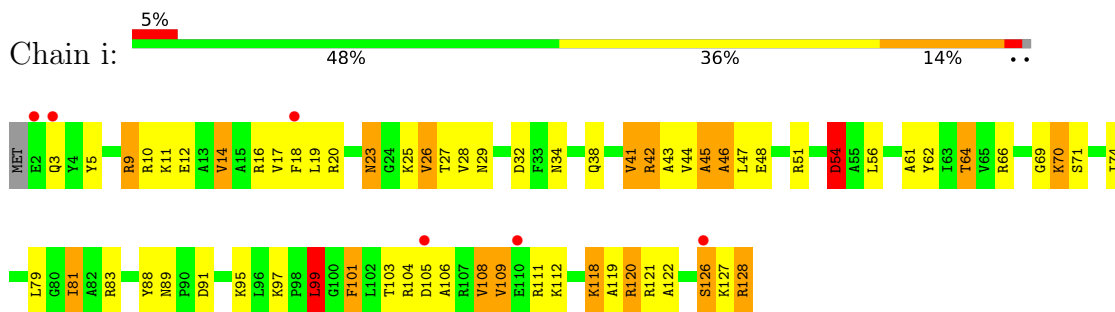




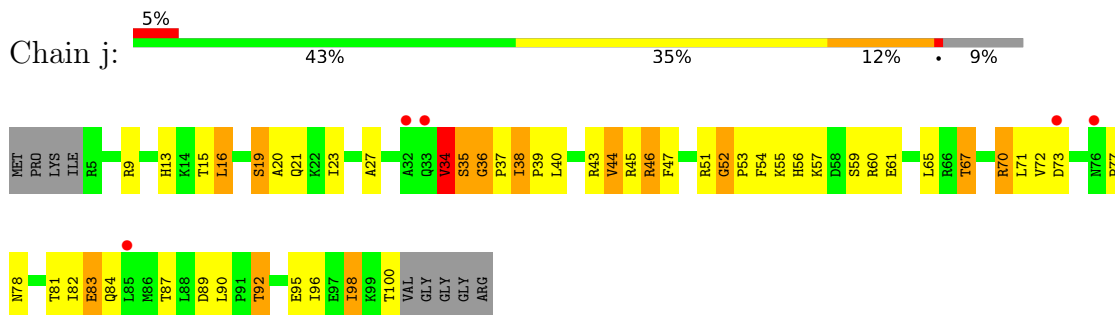
• Molecule 41: 30S ribosomal protein S8



• Molecule 42: 30S ribosomal protein S9

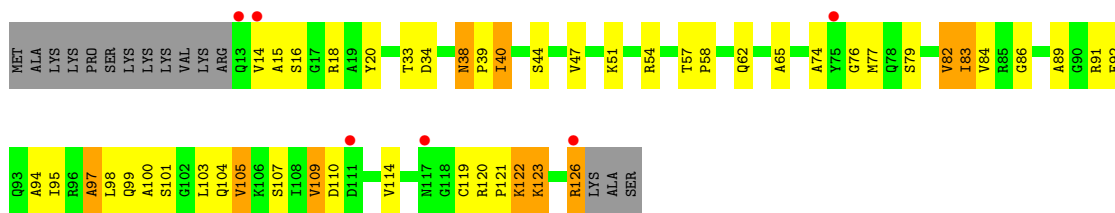


• Molecule 43: 30S ribosomal protein S10

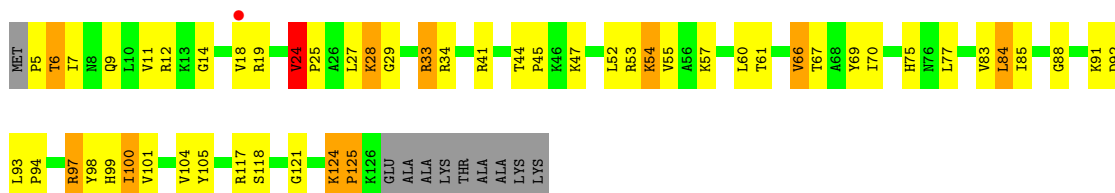


• Molecule 44: 30S ribosomal protein S11

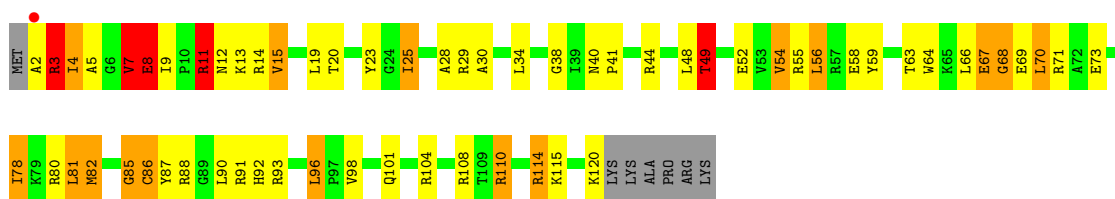
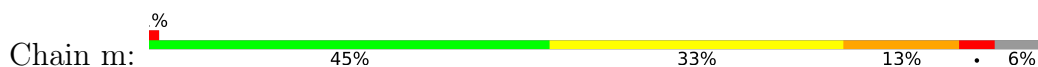




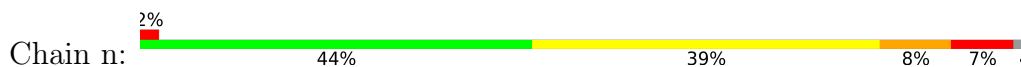
• Molecule 45: 30S ribosomal protein S12



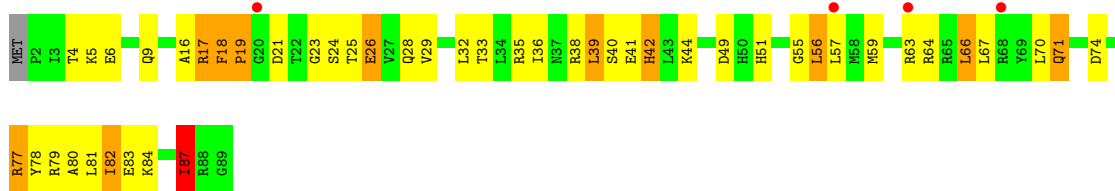
• Molecule 46: 30S ribosomal protein S13



• Molecule 47: 30S ribosomal protein S14 type Z

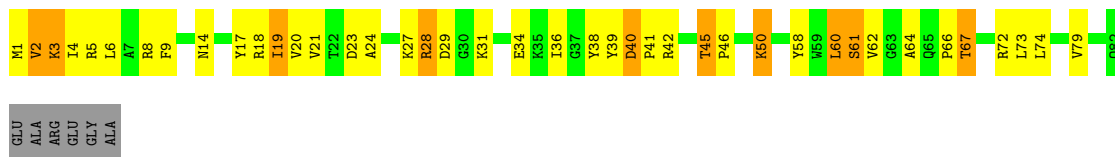


• Molecule 48: 30S ribosomal protein S15

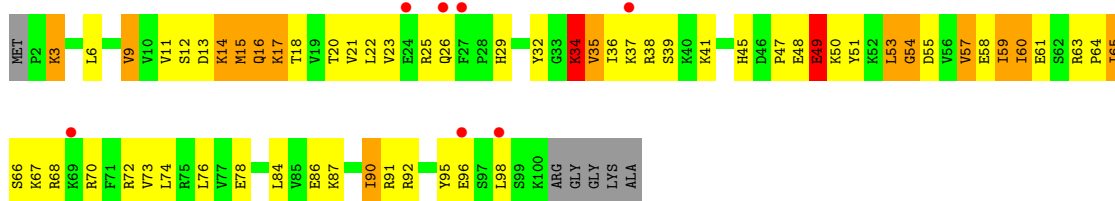


• Molecule 49: 30S ribosomal protein S16

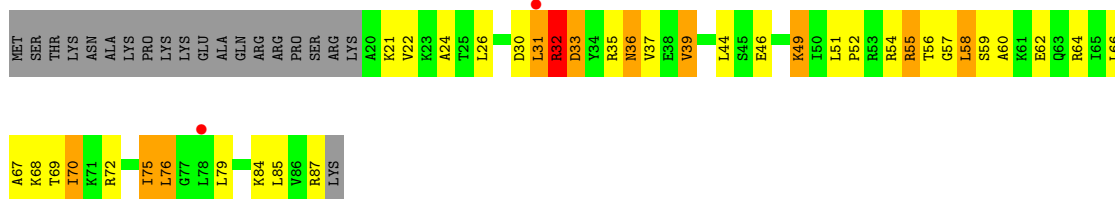
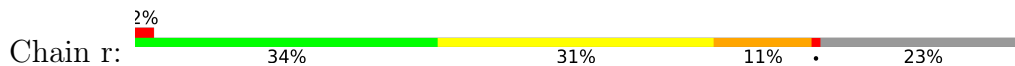




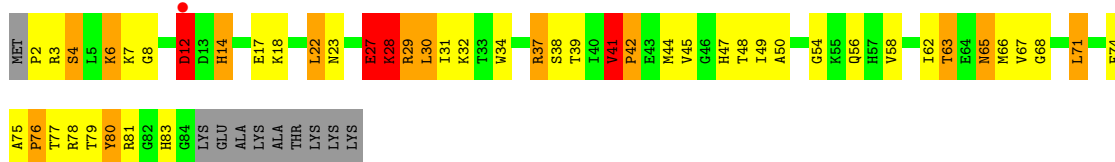
- Molecule 50: 30S ribosomal protein S17



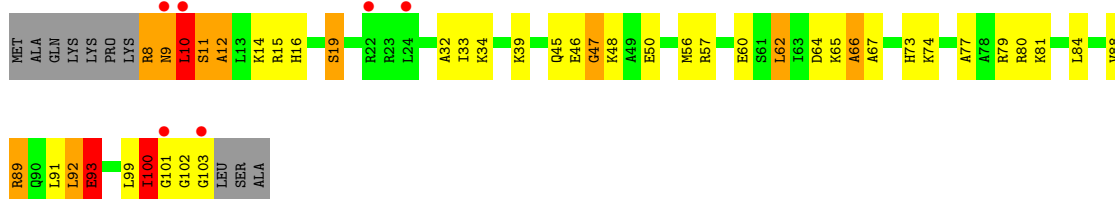
- Molecule 51: 30S ribosomal protein S18



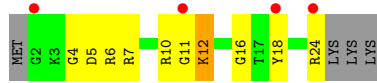
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



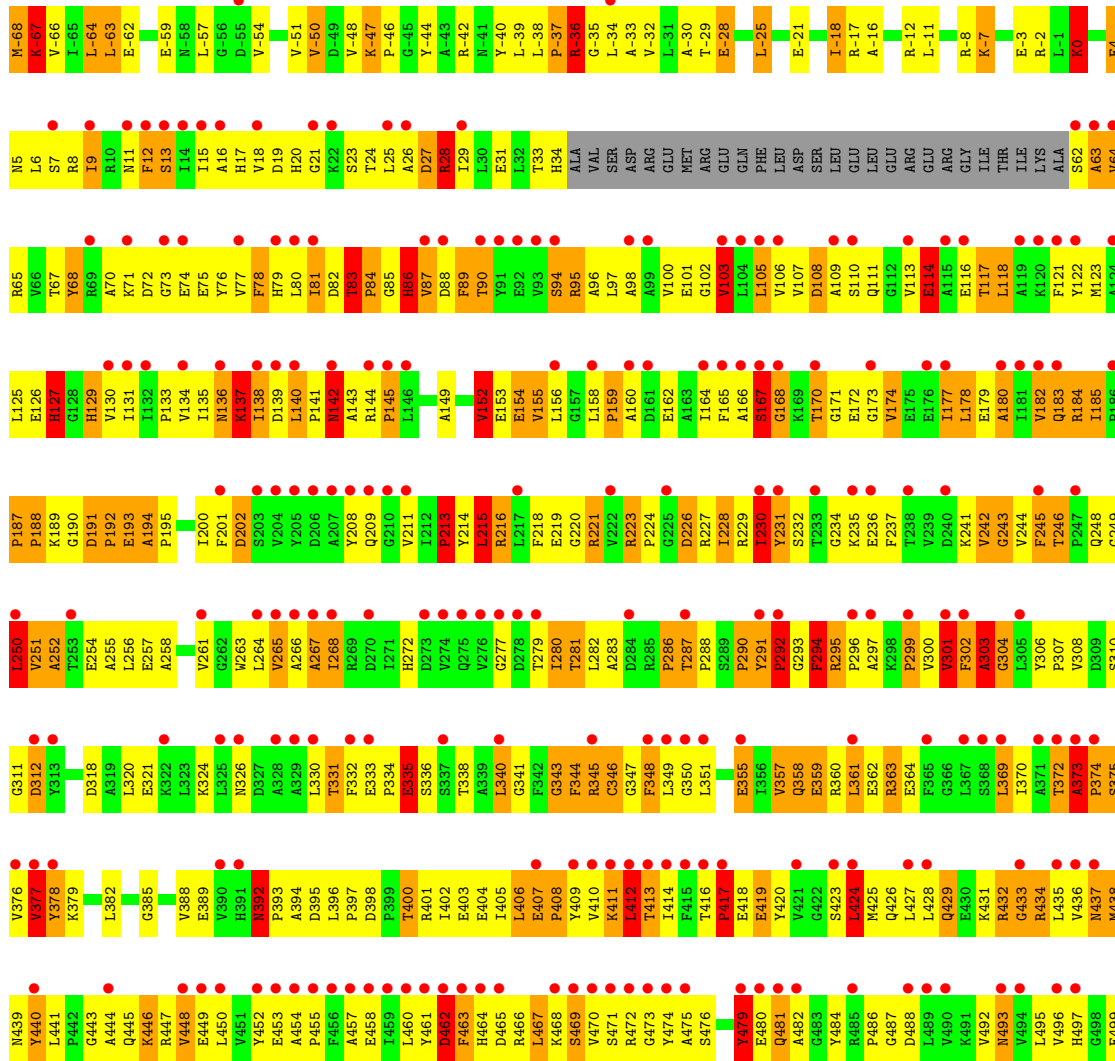
- Molecule 54: 30S ribosomal protein Thx

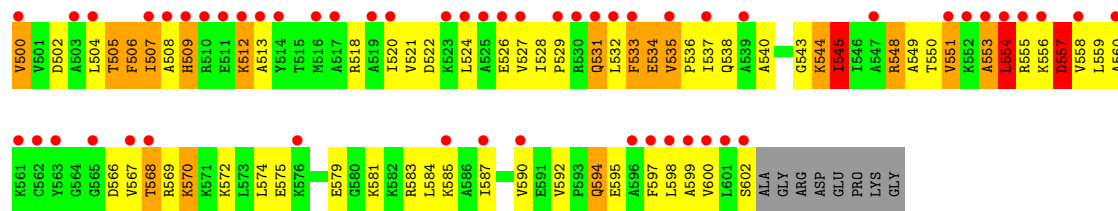


• Molecule 55: mRNA



• Molecule 56: 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 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.76-2.90) 93.8 (49.76-2.90)	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)	Xtrriage
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 (4.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	152111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtrriage'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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU, SF4, MIA, MG, 7MG, ZN, 4SU, GDP

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	0.46	0/69298	0.69	8/108168 (0.0%)
2	B	0.34	0/2878	0.54	0/4490
3	D	0.82	2/2186 (0.1%)	1.25	18/2944 (0.6%)
4	E	0.80	0/1592	1.28	10/2149 (0.5%)
5	F	0.73	0/1619	1.16	13/2193 (0.6%)
6	G	0.58	0/1450	1.12	14/1959 (0.7%)
7	H	0.59	0/1356	1.13	10/1834 (0.5%)
8	J	0.65	0/640	1.40	11/889 (1.2%)
9	K	0.46	0/1044	1.12	13/1416 (0.9%)
10	N	0.71	0/1144	1.09	8/1543 (0.5%)
11	O	0.91	0/943	1.35	7/1269 (0.6%)
12	P	0.62	0/1152	1.25	8/1533 (0.5%)
13	Q	0.75	0/1143	1.10	7/1527 (0.5%)
14	R	0.69	0/982	1.02	0/1312
15	S	0.55	0/887	1.02	2/1180 (0.2%)
16	T	0.72	0/1105	1.14	4/1477 (0.3%)
17	U	0.75	0/977	1.11	6/1301 (0.5%)
18	V	0.70	0/782	1.19	3/1049 (0.3%)
19	W	0.79	0/897	1.19	5/1205 (0.4%)
20	X	0.68	0/764	1.07	2/1025 (0.2%)
21	Y	0.70	0/819	1.11	3/1095 (0.3%)
22	Z	0.65	0/1483	1.16	14/2017 (0.7%)
23	0	0.63	0/599	0.99	1/798 (0.1%)
24	1	0.73	0/762	1.15	3/1014 (0.3%)
25	2	0.59	0/590	1.05	4/781 (0.5%)
26	3	0.74	0/474	1.28	4/635 (0.6%)
27	4	0.60	0/570	1.23	7/768 (0.9%)
28	5	0.69	0/473	1.15	2/639 (0.3%)
29	6	0.67	0/460	0.98	0/613
30	7	0.83	0/438	1.16	1/575 (0.2%)
31	8	0.74	0/519	1.06	2/684 (0.3%)
32	9	0.70	0/310	1.15	2/407 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	w	0.49	0/1651	0.74	2/2569 (0.1%)
33	x	0.34	1/1602 (0.1%)	0.59	0/2493
34	a	0.46	2/36002 (0.0%)	0.68	3/56188 (0.0%)
35	b	0.69	0/1885	1.22	15/2547 (0.6%)
36	c	0.74	0/1574	1.09	7/2127 (0.3%)
37	d	0.71	0/1685	1.14	8/2262 (0.4%)
38	e	0.86	0/1145	1.25	7/1543 (0.5%)
39	f	0.57	0/819	1.12	5/1111 (0.5%)
40	g	0.67	0/1246	1.12	8/1674 (0.5%)
41	h	0.76	0/1108	1.12	5/1494 (0.3%)
42	i	0.70	0/1002	1.18	6/1346 (0.4%)
43	j	0.73	0/711	1.26	6/968 (0.6%)
44	k	0.69	0/844	1.12	6/1145 (0.5%)
45	l	0.79	0/946	1.33	5/1274 (0.4%)
46	m	0.72	0/934	1.23	5/1256 (0.4%)
47	n	0.81	0/501	1.12	1/664 (0.2%)
48	o	0.67	0/739	1.08	5/985 (0.5%)
49	p	0.82	0/697	1.19	5/939 (0.5%)
50	q	0.77	0/836	1.15	4/1117 (0.4%)
51	r	0.61	0/560	0.97	1/746 (0.1%)
52	s	0.77	0/665	1.25	5/897 (0.6%)
53	t	0.71	0/726	1.13	4/961 (0.4%)
54	u	0.58	0/203	1.00	1/266 (0.4%)
55	v	0.46	0/165	0.61	0/254
56	y	1.14	30/4067 (0.7%)	1.86	169/5503 (3.1%)
All	All	0.57	35/162649 (0.0%)	0.88	475/242818 (0.2%)

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

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

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	y	191	ASP	C-N	8.27	1.40	1.33
56	y	460	LEU	C-O	7.74	1.32	1.24
56	y	188	PRO	C-N	-7.53	1.24	1.33
56	y	302	PHE	CA-C	-7.11	1.46	1.53
56	y	528	ILE	C-N	6.30	1.41	1.33

The worst 5 of 475 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	y	463	PHE	N-CA-C	21.14	134.32	111.28
56	y	527	VAL	N-CA-C	12.72	123.57	110.72
56	y	388	VAL	N-CA-C	12.44	123.29	110.72
56	y	282	LEU	N-CA-C	-11.73	94.71	110.55
56	y	142	ASN	N-CA-C	-11.67	98.42	112.89

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](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61879	0	31203	1296	0
2	B	2573	0	1306	33	0
3	D	2136	0	2217	147	0
4	E	1559	0	1618	77	0
5	F	1584	0	1625	73	0
6	G	1425	0	1443	68	0
7	H	1330	0	1407	59	0
8	J	641	0	309	13	0
9	K	1025	0	1066	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	N	1117	0	1184	59	0
11	O	933	0	996	40	0
12	P	1135	0	1212	73	0
13	Q	1122	0	1179	39	0
14	R	968	0	1033	40	0
15	S	877	0	938	40	0
16	T	1091	0	1151	54	0
17	U	959	0	1019	64	0
18	V	771	0	830	29	0
19	W	886	0	940	39	0
20	X	750	0	814	42	0
21	Y	806	0	881	37	0
22	Z	1451	0	1457	75	0
23	0	591	0	607	36	0
24	1	755	0	826	39	0
25	2	588	0	643	23	0
26	3	469	0	518	15	0
27	4	557	0	537	46	0
28	5	459	0	476	29	0
29	6	453	0	473	17	0
30	7	430	0	480	18	0
31	8	511	0	571	31	0
32	9	307	0	335	12	0
33	w	1632	0	838	26	0
33	x	1581	0	805	88	0
34	a	32163	0	16234	615	0
35	b	1850	0	1871	99	0
36	c	1550	0	1539	67	0
37	d	1655	0	1673	84	0
38	e	1129	0	1185	48	0
39	f	806	0	793	44	0
40	g	1227	0	1232	55	0
41	h	1088	0	1126	48	0
42	i	983	0	986	54	0
43	j	698	0	637	31	0
44	k	829	0	825	26	0
45	l	930	0	980	40	0
46	m	924	0	960	45	0
47	n	492	0	528	27	0
48	o	728	0	760	37	0
49	p	681	0	697	25	0
50	q	823	0	891	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	r	555	0	618	32	0
52	s	650	0	655	44	0
53	t	724	0	787	29	0
54	u	199	0	208	6	0
55	v	148	0	76	1	0
56	y	4000	0	3218	694	0
57	0	3	0	0	0	0
57	5	1	0	0	0	0
57	6	1	0	0	0	0
57	7	3	0	0	0	0
57	8	1	0	0	0	0
57	9	1	0	0	0	0
57	A	635	0	0	0	0
57	B	18	0	0	0	0
57	D	5	0	0	0	0
57	E	4	0	0	0	0
57	F	5	0	0	0	0
57	G	3	0	0	0	0
57	N	1	0	0	0	0
57	O	1	0	0	0	0
57	P	2	0	0	0	0
57	Q	5	0	0	0	0
57	R	3	0	0	0	0
57	U	4	0	0	0	0
57	V	2	0	0	0	0
57	W	1	0	0	0	0
57	X	1	0	0	0	0
57	Z	1	0	0	0	0
57	a	187	0	0	0	0
57	e	1	0	0	0	0
57	f	1	0	0	0	0
57	l	2	0	0	0	0
57	m	1	0	0	0	0
57	n	1	0	0	0	0
57	v	1	0	0	0	0
57	w	6	0	0	0	0
57	x	3	0	0	0	0
57	y	2	0	0	0	0
58	4	1	0	0	0	0
58	5	1	0	0	0	0
58	6	1	0	0	0	0
58	9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	Y	1	0	0	0	0
58	n	1	0	0	0	0
59	d	8	0	0	2	0
60	w	11	0	8	0	0
61	y	28	0	12	8	0
62	0	4	0	0	0	0
62	1	2	0	0	0	0
62	3	1	0	0	0	0
62	5	1	0	0	0	0
62	7	2	0	0	0	0
62	8	4	0	0	0	0
62	9	1	0	0	0	0
62	A	710	0	0	109	0
62	B	34	0	0	2	0
62	D	4	0	0	2	0
62	E	7	0	0	1	0
62	F	5	0	0	0	0
62	G	1	0	0	0	0
62	H	1	0	0	0	0
62	N	1	0	0	0	0
62	O	3	0	0	0	0
62	P	3	0	0	0	0
62	Q	4	0	0	1	0
62	R	2	0	0	0	0
62	T	1	0	0	0	0
62	U	2	0	0	1	0
62	V	1	0	0	1	0
62	W	2	0	0	0	0
62	Y	1	0	0	0	0
62	a	167	0	0	17	0
62	l	1	0	0	0	0
62	v	3	0	0	0	0
62	x	1	0	0	0	0
All	All	152111	0	101436	4546	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 4546 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:200:ILE:CA	56:y:215:LEU:HB3	1.30	1.57
56:y:245:PHE:CB	56:y:250:LEU:HA	1.37	1.50
56:y:306:TYR:HD2	56:y:343:GLY:CA	1.25	1.48
56:y:87:VAL:HG13	56:y:88:ASP:C	1.43	1.43
56:y:200:ILE:CA	56:y:215:LEU:CB	1.97	1.43

There are no symmetry-related clashes.

## 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%)	1	6
4	E	202/206 (98%)	165 (82%)	27 (13%)	10 (5%)	1	6
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	4
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	2
10	N	138/140 (99%)	106 (77%)	24 (17%)	8 (6%)	1	4
11	O	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	3	13
12	P	147/150 (98%)	108 (74%)	29 (20%)	10 (7%)	1	2
13	Q	139/141 (99%)	122 (88%)	12 (9%)	5 (4%)	2	11
14	R	116/118 (98%)	92 (79%)	21 (18%)	3 (3%)	4	17
15	S	108/112 (96%)	77 (71%)	20 (18%)	11 (10%)	0	1
16	T	129/146 (88%)	113 (88%)	15 (12%)	1 (1%)	16	44
17	U	114/118 (97%)	92 (81%)	16 (14%)	6 (5%)	1	5
18	V	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	W	110/113 (97%)	86 (78%)	14 (13%)	10 (9%)	0	1
20	X	93/96 (97%)	73 (78%)	12 (13%)	8 (9%)	0	1
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%)	9	30
24	1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	3
25	2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	8	28
26	3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	12
27	4	67/71 (94%)	42 (63%)	14 (21%)	11 (16%)	0	0
28	5	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	0	1
29	6	51/54 (94%)	43 (84%)	6 (12%)	2 (4%)	2	10
30	7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	5	21
31	8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
32	9	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	3	15
35	b	229/256 (90%)	167 (73%)	41 (18%)	21 (9%)	0	1
36	c	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	2	10
37	d	206/209 (99%)	163 (79%)	33 (16%)	10 (5%)	1	6
38	e	146/162 (90%)	108 (74%)	30 (20%)	8 (6%)	1	4
39	f	98/101 (97%)	70 (71%)	20 (20%)	8 (8%)	0	2
40	g	153/156 (98%)	123 (80%)	26 (17%)	4 (3%)	4	17
41	h	135/138 (98%)	115 (85%)	18 (13%)	2 (2%)	8	28
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%)	2	11
45	l	120/132 (91%)	106 (88%)	9 (8%)	5 (4%)	2	9
46	m	117/126 (93%)	91 (78%)	16 (14%)	10 (8%)	0	1
47	n	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	1	5
48	o	86/89 (97%)	69 (80%)	15 (17%)	2 (2%)	5	19
49	p	80/88 (91%)	61 (76%)	17 (21%)	2 (2%)	4	17
50	q	97/105 (92%)	78 (80%)	13 (13%)	6 (6%)	1	3
51	r	66/88 (75%)	57 (86%)	6 (9%)	3 (4%)	2	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
56	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 [i](#)

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%)	164 (76%)	51 (24%)	1	2
4	E	164/166 (99%)	134 (82%)	30 (18%)	2	6
5	F	160/162 (99%)	128 (80%)	32 (20%)	1	4
6	G	143/156 (92%)	106 (74%)	37 (26%)	0	2
7	H	144/148 (97%)	111 (77%)	33 (23%)	1	3
9	K	104/111 (94%)	81 (78%)	23 (22%)	1	3
10	N	118/119 (99%)	90 (76%)	28 (24%)	1	2
11	O	100/100 (100%)	85 (85%)	15 (15%)	3	10
12	P	115/116 (99%)	93 (81%)	22 (19%)	1	5
13	Q	111/111 (100%)	92 (83%)	19 (17%)	2	7
14	R	101/101 (100%)	79 (78%)	22 (22%)	1	3
15	S	87/88 (99%)	71 (82%)	16 (18%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	T	115/127 (91%)	94 (82%)	21 (18%)	2	6
17	U	93/94 (99%)	72 (77%)	21 (23%)	1	3
18	V	80/82 (98%)	62 (78%)	18 (22%)	1	3
19	W	90/92 (98%)	70 (78%)	20 (22%)	1	3
20	X	77/78 (99%)	63 (82%)	14 (18%)	2	6
21	Y	85/91 (93%)	68 (80%)	17 (20%)	1	4
22	Z	156/179 (87%)	118 (76%)	38 (24%)	1	2
23	0	59/67 (88%)	50 (85%)	9 (15%)	3	9
24	1	80/83 (96%)	60 (75%)	20 (25%)	0	2
25	2	65/67 (97%)	51 (78%)	14 (22%)	1	3
26	3	51/52 (98%)	39 (76%)	12 (24%)	1	3
27	4	60/63 (95%)	46 (77%)	14 (23%)	1	3
28	5	51/52 (98%)	40 (78%)	11 (22%)	1	3
29	6	51/52 (98%)	38 (74%)	13 (26%)	0	2
30	7	42/42 (100%)	33 (79%)	9 (21%)	1	4
31	8	53/55 (96%)	46 (87%)	7 (13%)	4	13
32	9	34/34 (100%)	30 (88%)	4 (12%)	5	17
35	b	193/220 (88%)	142 (74%)	51 (26%)	0	2
36	c	142/188 (76%)	120 (84%)	22 (16%)	2	9
37	d	169/181 (93%)	126 (75%)	43 (25%)	0	2
38	e	113/123 (92%)	80 (71%)	33 (29%)	0	1
39	f	83/90 (92%)	65 (78%)	18 (22%)	1	3
40	g	118/127 (93%)	91 (77%)	27 (23%)	1	3
41	h	114/119 (96%)	90 (79%)	24 (21%)	1	4
42	i	90/99 (91%)	72 (80%)	18 (20%)	1	4
43	j	65/92 (71%)	46 (71%)	19 (29%)	0	1
44	k	82/99 (83%)	70 (85%)	12 (15%)	3	10
45	l	97/109 (89%)	82 (84%)	15 (16%)	2	9
46	m	89/101 (88%)	70 (79%)	19 (21%)	1	4
47	n	49/50 (98%)	32 (65%)	17 (35%)	0	0
48	o	78/80 (98%)	64 (82%)	14 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	p	69/74 (93%)	55 (80%)	14 (20%)	1	4
50	q	94/97 (97%)	73 (78%)	21 (22%)	1	3
51	r	59/77 (77%)	44 (75%)	15 (25%)	0	2
52	s	68/80 (85%)	50 (74%)	18 (26%)	0	2
53	t	69/82 (84%)	57 (83%)	12 (17%)	2	7
54	u	18/22 (82%)	15 (83%)	3 (17%)	2	7
56	y	289/560 (52%)	189 (65%)	100 (35%)	0	0
All	All	4952/5576 (89%)	3847 (78%)	1105 (22%)	1	3

5 of 1105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	p	20	VAL
50	q	78	GLU
49	p	19	ILE
56	y	142	ASN
19	W	8	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
36	c	136	GLN
40	g	28	ASN
56	y	142	ASN
36	c	181	ASN
38	e	38	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2865/2915 (98%)	643 (22%)	38 (1%)
2	B	119/122 (97%)	18 (15%)	0
33	w	75/76 (98%)	23 (30%)	0
33	x	72/76 (94%)	38 (52%)	0
34	a	1493/1521 (98%)	311 (20%)	0
55	v	6/18 (33%)	1 (16%)	0
All	All	4630/4728 (97%)	1034 (22%)	38 (0%)

5 of 1034 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	2110	G
1	A	2611	U
1	A	2132	U
1	A	2318	G
1	A	2873	A

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

14 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
33	MIA	x	37	33	21,24,32	1.64	4 (19%)	30,35,47	1.99	7 (23%)
33	PSU	x	32	33	18,21,22	1.41	2 (11%)	21,30,33	1.93	4 (19%)
33	4SU	w	8	33	18,21,22	1.60	4 (22%)	25,30,33	2.15	5 (20%)
33	PSU	w	32	33	18,21,22	1.39	1 (5%)	21,30,33	1.89	5 (23%)
33	PSU	w	39	33	18,21,22	1.42	2 (11%)	21,30,33	2.38	4 (19%)
33	MIA	w	37	33	28,31,32	2.81	8 (28%)	38,44,47	3.21	11 (28%)
33	5MU	w	54	33	19,22,23	1.36	5 (26%)	27,32,35	2.03	6 (22%)
33	4SU	x	8	33	18,21,22	1.77	3 (16%)	25,30,33	2.33	6 (24%)
33	5MU	x	54	33	19,22,23	1.56	5 (26%)	27,32,35	2.04	6 (22%)
33	PSU	x	55	33	18,21,22	1.32	2 (11%)	21,30,33	2.10	5 (23%)
33	PSU	x	39	33	18,21,22	1.43	2 (11%)	21,30,33	1.87	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	7MG	w	46	33	23,26,27	1.33	4 (17%)	27,39,42	2.72	8 (29%)
33	PSU	w	55	33	18,21,22	1.47	3 (16%)	21,30,33	2.23	5 (23%)
33	7MG	x	46	33	23,26,27	1.26	2 (8%)	27,39,42	3.06	9 (33%)

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
33	MIA	x	37	33	-	3/7/25/34	0/3/3/3
33	PSU	x	32	33	-	2/7/25/26	0/2/2/2
33	4SU	w	8	33	-	0/7/25/26	0/2/2/2
33	PSU	w	32	33	-	0/7/25/26	0/2/2/2
33	PSU	w	39	33	-	0/7/25/26	0/2/2/2
33	MIA	w	37	33	-	4/15/33/34	0/3/3/3
33	5MU	w	54	33	-	0/7/25/26	0/2/2/2
33	4SU	x	8	33	-	0/7/25/26	0/2/2/2
33	5MU	x	54	33	-	4/7/25/26	0/2/2/2
33	PSU	x	55	33	-	1/7/25/26	0/2/2/2
33	PSU	x	39	33	-	2/7/25/26	0/2/2/2
33	7MG	w	46	33	-	1/7/37/38	0/3/3/3
33	PSU	w	55	33	-	0/7/25/26	0/2/2/2
33	7MG	x	46	33	-	4/7/37/38	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	w	37	MIA	C2-S10	-9.46	1.67	1.75
33	w	37	MIA	C13-C14	7.43	1.54	1.32
33	x	37	MIA	C5-C4	5.21	1.48	1.39
33	w	37	MIA	C5-C4	5.08	1.48	1.39
33	x	8	4SU	C4-S4	-4.90	1.60	1.68

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	w	37	MIA	C11-S10-C2	-15.04	90.96	102.25
33	x	46	7MG	N9-C4-N3	10.87	141.39	125.46
33	w	46	7MG	N9-C4-N3	8.16	137.42	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	w	39	PSU	N1-C2-N3	6.98	122.53	115.17
33	x	8	4SU	C4-N3-C2	-6.96	120.64	127.31

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	x	32	PSU	O4'-C4'-C5'-O5'
33	x	46	7MG	C4'-C5'-O5'-P
33	w	37	MIA	C5-C6-N6-C12
33	w	37	MIA	N1-C6-N6-C12
33	w	37	MIA	C12-C13-C14-C16

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	x	37	MIA	1	0
33	w	8	4SU	1	0
33	w	54	5MU	2	0
33	x	8	4SU	1	0
33	x	54	5MU	1	0
33	x	55	PSU	2	0
33	x	39	PSU	2	0
33	w	46	7MG	1	0
33	x	46	7MG	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 915 ligands modelled in this entry, 912 are monoatomic - leaving 3 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	PHE	w	107	33	10,11,12	1.37	0	8,13,15	1.11	0
59	SF4	d	501	37	0,12,12	-	-	-		
61	GDP	y	703	57	29,30,30	1.31	4 (13%)	45,47,47	1.96	7 (15%)

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	PHE	w	107	33	-	2/5/6/8	0/1/1/1
61	GDP	y	703	57	-	1/16/32/32	0/3/3/3
59	SF4	d	501	37	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	y	703	GDP	C5-C4	3.32	1.47	1.38
61	y	703	GDP	PA-O3A	2.57	1.62	1.59
61	y	703	GDP	C6-N1	-2.55	1.34	1.38
61	y	703	GDP	C5-N7	-2.41	1.34	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	y	703	GDP	C5-C4-N3	-7.44	116.55	128.39
61	y	703	GDP	C2-N3-C4	5.59	121.93	112.30
61	y	703	GDP	N9-C4-N3	5.25	136.44	125.95
61	y	703	GDP	C4-C5-N7	-3.01	105.90	110.67
61	y	703	GDP	C6-C5-N7	2.91	135.58	130.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

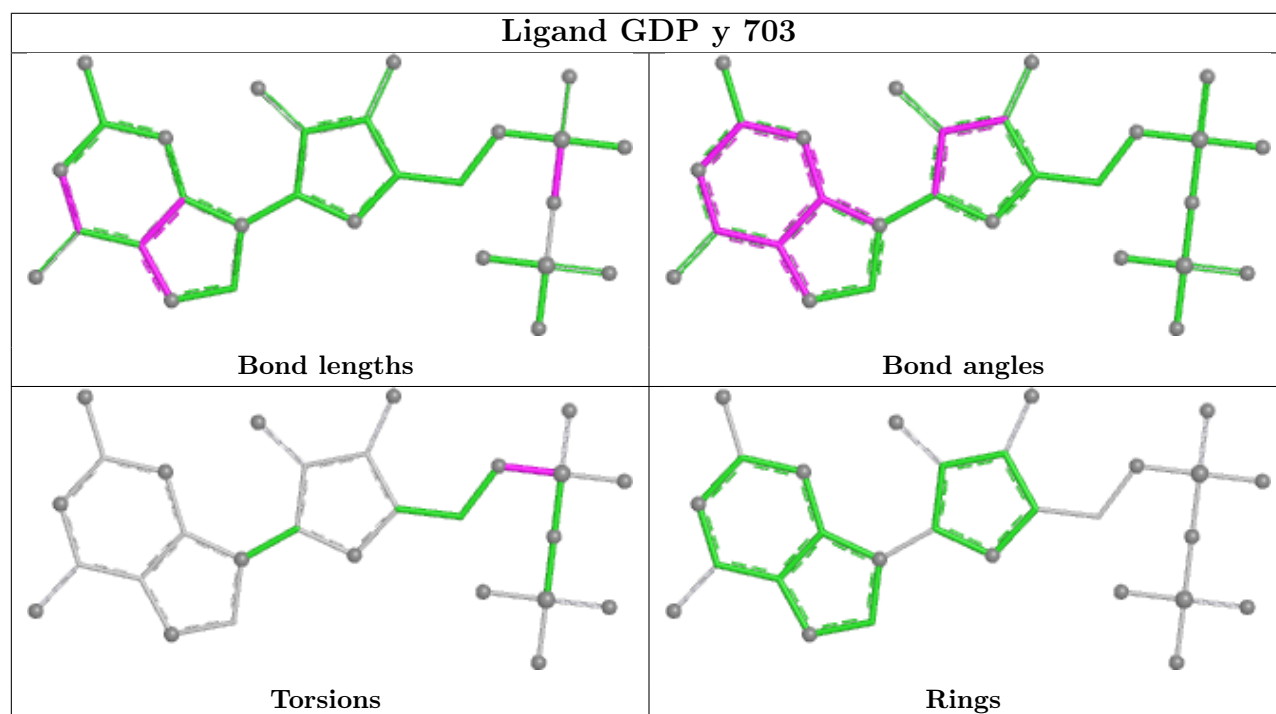
Mol	Chain	Res	Type	Atoms
60	w	107	PHE	CA-CB-CG-CD2
60	w	107	PHE	CA-CB-CG-CD1
61	y	703	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	d	501	SF4	2	0
61	y	703	GDP	8	0

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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%)	-0.10	58 (2%) 65 56	35, 61, 175, 394	0
2	B	120/122 (98%)	0.18	0 100 100	65, 93, 121, 133	0
3	D	275/276 (99%)	0.27	3 (1%) 78 71	35, 56, 75, 108	0
4	E	204/206 (99%)	0.15	5 (2%) 58 48	34, 57, 77, 101	0
5	F	203/205 (99%)	0.43	8 (3%) 43 35	38, 70, 108, 135	0
6	G	181/182 (99%)	0.55	6 (3%) 49 40	68, 84, 106, 128	0
7	H	174/180 (96%)	0.76	10 (5%) 29 23	62, 96, 131, 154	0
8	J	130/173 (75%)	2.06	57 (43%) 0 0	129, 161, 183, 197	0
9	K	139/147 (94%)	2.46	84 (60%) 0 0	192, 218, 229, 234	0
10	N	140/140 (100%)	0.30	4 (2%) 53 45	47, 64, 93, 110	0
11	O	122/122 (100%)	0.02	0 100 100	37, 52, 68, 75	0
12	P	149/150 (99%)	0.71	9 (6%) 27 21	42, 81, 109, 116	0
13	Q	141/141 (100%)	0.40	0 100 100	44, 64, 80, 97	0
14	R	118/118 (100%)	0.45	3 (2%) 58 48	46, 66, 86, 102	0
15	S	110/112 (98%)	0.98	18 (16%) 4 3	75, 90, 102, 113	0
16	T	131/146 (89%)	0.20	4 (3%) 51 42	49, 61, 94, 113	0
17	U	116/118 (98%)	0.32	1 (0%) 81 75	42, 56, 75, 83	0
18	V	101/101 (100%)	0.34	0 100 100	41, 73, 93, 104	0
19	W	112/113 (99%)	0.37	1 (0%) 81 75	46, 62, 89, 128	0
20	X	95/96 (98%)	0.56	6 (6%) 26 20	56, 74, 95, 116	0
21	Y	107/110 (97%)	0.66	7 (6%) 25 20	66, 79, 116, 137	0
22	Z	185/206 (89%)	0.86	17 (9%) 14 12	68, 90, 114, 135	0
23	0	74/85 (87%)	0.58	3 (4%) 41 33	50, 67, 85, 105	0
24	1	97/98 (98%)	0.80	6 (6%) 26 21	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%)	0.50	0 100 100	69, 86, 100, 109	0
26	3	59/60 (98%)	0.44	0 100 100	52, 68, 101, 116	0
27	4	69/71 (97%)	0.95	8 (11%) 9 8	80, 107, 150, 158	0
28	5	59/60 (98%)	0.17	2 (3%) 48 39	41, 63, 81, 100	0
29	6	53/54 (98%)	0.40	1 (1%) 66 58	62, 71, 85, 87	0
30	7	49/49 (100%)	0.45	4 (8%) 17 14	40, 49, 73, 96	0
31	8	64/65 (98%)	0.71	1 (1%) 70 62	51, 59, 65, 86	0
32	9	37/37 (100%)	0.88	4 (10%) 11 9	52, 63, 78, 88	0
33	w	69/76 (90%)	-0.41	1 (1%) 73 65	43, 73, 96, 137	0
33	x	67/76 (88%)	1.52	14 (20%) 2 2	94, 267, 283, 306	0
34	a	1496/1521 (98%)	-0.23	12 (0%) 82 77	37, 60, 119, 295	0
35	b	231/256 (90%)	0.61	18 (7%) 19 16	53, 84, 134, 165	0
36	c	206/239 (86%)	0.13	4 (1%) 66 58	50, 65, 88, 99	0
37	d	208/209 (99%)	0.42	8 (3%) 44 36	52, 68, 95, 109	0
38	e	148/162 (91%)	-0.03	0 100 100	40, 55, 72, 107	0
39	f	100/101 (99%)	1.04	10 (10%) 12 10	74, 106, 138, 146	0
40	g	155/156 (99%)	0.30	9 (5%) 29 22	54, 73, 124, 156	0
41	h	137/138 (99%)	0.07	1 (0%) 84 79	47, 59, 72, 90	0
42	i	127/128 (99%)	0.48	6 (4%) 36 28	45, 70, 91, 102	0
43	j	96/105 (91%)	0.68	5 (5%) 33 26	42, 70, 119, 133	0
44	k	114/129 (88%)	0.47	6 (5%) 32 25	49, 77, 96, 104	0
45	l	122/132 (92%)	-0.04	1 (0%) 82 77	39, 53, 68, 80	0
46	m	119/126 (94%)	0.28	1 (0%) 82 77	43, 72, 99, 111	0
47	n	60/61 (98%)	0.14	1 (1%) 69 61	42, 51, 66, 69	0
48	o	88/89 (98%)	0.51	4 (4%) 38 30	57, 74, 98, 107	0
49	p	82/88 (93%)	0.25	0 100 100	45, 57, 69, 85	0
50	q	99/105 (94%)	0.45	7 (7%) 22 17	50, 62, 80, 93	0
51	r	68/88 (77%)	0.54	2 (2%) 53 45	67, 85, 107, 116	0
52	s	83/93 (89%)	0.13	1 (1%) 76 69	45, 57, 76, 89	0
53	t	96/106 (90%)	0.59	6 (6%) 26 20	51, 65, 88, 96	0
54	u	23/27 (85%)	1.04	4 (17%) 4 3	54, 62, 69, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
55	v	7/18 (38%)	0.87	1 (14%) 6 5	49, 50, 130, 149	0
56	y	644/679 (94%)	1.93	272 (42%) 0 0	69, 151, 188, 213	0
All	All	11202/11638 (96%)	0.34	724 (6%) 25 20	34, 68, 168, 394	0

The worst 5 of 724 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	K	52	ILE	8.1
56	y	13	SER	7.9
56	y	209	GLN	7.9
9	K	22	PRO	6.9
8	J	51	LEU	6.7

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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	7MG	x	46	24/25	0.18	0.17	275,282,285,287	0
33	5MU	x	54	21/22	0.29	0.14	275,282,283,285	0
33	PSU	x	55	20/21	0.37	0.15	274,285,289,293	0
33	PSU	x	32	20/21	0.47	0.18	188,202,216,216	0
33	MIA	x	37	22/30	0.51	0.20	204,221,237,241	0
33	4SU	x	8	20/21	0.58	0.12	263,275,277,277	0
33	PSU	x	39	20/21	0.65	0.14	175,193,200,201	0
33	7MG	w	46	24/25	0.85	0.10	59,76,103,118	0
33	MIA	w	37	29/30	0.92	0.11	46,55,61,64	0
33	4SU	w	8	20/21	0.92	0.07	56,58,64,64	0
33	PSU	w	55	20/21	0.92	0.07	75,83,85,86	0
33	5MU	w	54	21/22	0.94	0.08	67,77,82,84	0
33	PSU	w	39	20/21	0.96	0.07	41,50,55,56	0
33	PSU	w	32	20/21	0.96	0.09	40,46,49,51	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands i

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
57	MG	A	3157	1/1	0.15	0.28	118,118,118,118	0
57	MG	x	3001	1/1	0.16	0.18	237,237,237,237	0
57	MG	x	3003	1/1	0.25	0.17	215,215,215,215	0
57	MG	A	3435	1/1	0.26	0.20	95,95,95,95	0
57	MG	A	3608	1/1	0.32	0.21	108,108,108,108	0
57	MG	0	101	1/1	0.48	0.20	73,73,73,73	0
57	MG	A	3576	1/1	0.50	0.20	89,89,89,89	0
57	MG	A	3186	1/1	0.51	0.26	90,90,90,90	0
57	MG	A	3057	1/1	0.52	0.15	56,56,56,56	0
57	MG	A	3282	1/1	0.54	0.15	66,66,66,66	0
57	MG	A	3408	1/1	0.55	0.20	98,98,98,98	0
57	MG	A	3607	1/1	0.58	0.23	90,90,90,90	0
57	MG	B	207	1/1	0.59	0.21	103,103,103,103	0
57	MG	A	3554	1/1	0.59	0.21	74,74,74,74	0
57	MG	A	3265	1/1	0.59	0.12	61,61,61,61	0
57	MG	A	3625	1/1	0.59	0.24	84,84,84,84	0
57	MG	A	3354	1/1	0.61	0.20	101,101,101,101	0
57	MG	A	3564	1/1	0.62	0.20	75,75,75,75	0
57	MG	A	3569	1/1	0.64	0.12	85,85,85,85	0
57	MG	A	3572	1/1	0.64	0.16	70,70,70,70	0
57	MG	A	3549	1/1	0.64	0.32	75,75,75,75	0
57	MG	A	3216	1/1	0.64	0.18	62,62,62,62	0
57	MG	A	3011	1/1	0.64	0.22	79,79,79,79	0
57	MG	A	3361	1/1	0.66	0.20	84,84,84,84	0
57	MG	A	3560	1/1	0.67	0.14	79,79,79,79	0
57	MG	A	3002	1/1	0.67	0.11	50,50,50,50	0
57	MG	A	3158	1/1	0.67	0.35	97,97,97,97	0
57	MG	A	3532	1/1	0.68	0.20	66,66,66,66	0
57	MG	A	3240	1/1	0.68	0.25	79,79,79,79	0
57	MG	A	3319	1/1	0.68	0.16	31,31,31,31	0
57	MG	A	3357	1/1	0.69	0.14	69,69,69,69	0
57	MG	a	3459	1/1	0.69	0.13	91,91,91,91	0
57	MG	B	214	1/1	0.70	0.22	83,83,83,83	0
57	MG	a	3371	1/1	0.70	0.21	65,65,65,65	0
57	MG	a	3392	1/1	0.70	0.22	65,65,65,65	0
57	MG	U	203	1/1	0.70	0.18	67,67,67,67	0
57	MG	A	3281	1/1	0.71	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	A	3603	1/1	0.71	0.14	82,82,82,82	0
57	MG	f	201	1/1	0.71	0.20	92,92,92,92	0
57	MG	A	3600	1/1	0.72	0.19	64,64,64,64	0
57	MG	A	3040	1/1	0.72	0.11	58,58,58,58	0
57	MG	A	3605	1/1	0.72	0.14	70,70,70,70	0
57	MG	A	3441	1/1	0.72	0.12	73,73,73,73	0
57	MG	a	3369	1/1	0.72	0.20	60,60,60,60	0
57	MG	A	3059	1/1	0.72	0.17	66,66,66,66	0
57	MG	A	3571	1/1	0.72	0.13	89,89,89,89	0
57	MG	a	3419	1/1	0.72	0.19	72,72,72,72	0
57	MG	A	3134	1/1	0.72	0.15	67,67,67,67	0
57	MG	a	3484	1/1	0.72	0.20	67,67,67,67	0
57	MG	A	3330	1/1	0.72	0.22	55,55,55,55	0
60	PHE	w	107	11/12	0.72	0.29	56,72,80,81	0
57	MG	A	3614	1/1	0.73	0.10	75,75,75,75	0
57	MG	A	3629	1/1	0.73	0.20	70,70,70,70	0
57	MG	A	3291	1/1	0.74	0.17	60,60,60,60	0
57	MG	A	3451	1/1	0.74	0.11	82,82,82,82	0
57	MG	A	3253	1/1	0.74	0.18	66,66,66,66	0
57	MG	A	3056	1/1	0.75	0.14	68,68,68,68	0
57	MG	a	3410	1/1	0.75	0.14	45,45,45,45	0
57	MG	A	3087	1/1	0.75	0.15	58,58,58,58	0
57	MG	a	3330	1/1	0.75	0.20	63,63,63,63	0
57	MG	a	3340	1/1	0.75	0.12	81,81,81,81	0
57	MG	A	3273	1/1	0.75	0.26	77,77,77,77	0
57	MG	A	3578	1/1	0.75	0.17	64,64,64,64	0
57	MG	X	101	1/1	0.76	0.14	72,72,72,72	0
57	MG	a	3390	1/1	0.76	0.18	45,45,45,45	0
57	MG	A	3586	1/1	0.76	0.20	55,55,55,55	0
57	MG	a	3400	1/1	0.76	0.30	61,61,61,61	0
57	MG	A	3135	1/1	0.76	0.23	54,54,54,54	0
57	MG	A	3461	1/1	0.76	0.17	59,59,59,59	0
57	MG	a	3436	1/1	0.76	0.12	66,66,66,66	0
57	MG	A	3328	1/1	0.76	0.17	62,62,62,62	0
57	MG	A	3577	1/1	0.76	0.22	72,72,72,72	0
57	MG	A	3213	1/1	0.76	0.18	67,67,67,67	0
57	MG	a	3370	1/1	0.76	0.17	66,66,66,66	0
57	MG	a	3328	1/1	0.77	0.21	60,60,60,60	0
57	MG	A	3602	1/1	0.77	0.14	73,73,73,73	0
57	MG	A	3029	1/1	0.77	0.18	52,52,52,52	0
57	MG	a	3350	1/1	0.77	0.23	73,73,73,73	0
57	MG	a	3358	1/1	0.77	0.26	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	A	3153	1/1	0.77	0.22	82,82,82,82	0
57	MG	0	102	1/1	0.77	0.07	61,61,61,61	0
57	MG	A	3491	1/1	0.77	0.17	72,72,72,72	0
57	MG	y	702	1/1	0.77	0.19	75,75,75,75	0
57	MG	A	3293	1/1	0.77	0.22	51,51,51,51	0
57	MG	A	3101	1/1	0.78	0.20	74,74,74,74	0
57	MG	A	3108	1/1	0.78	0.12	54,54,54,54	0
57	MG	A	3267	1/1	0.78	0.16	59,59,59,59	0
57	MG	a	3391	1/1	0.78	0.19	72,72,72,72	0
57	MG	A	3124	1/1	0.78	0.12	54,54,54,54	0
57	MG	A	3555	1/1	0.78	0.17	69,69,69,69	0
57	MG	A	3360	1/1	0.78	0.10	60,60,60,60	0
57	MG	A	3209	1/1	0.78	0.14	71,71,71,71	0
57	MG	A	3062	1/1	0.78	0.16	42,42,42,42	0
57	MG	A	3068	1/1	0.78	0.24	56,56,56,56	0
57	MG	a	3472	1/1	0.78	0.10	61,61,61,61	0
57	MG	A	3231	1/1	0.78	0.14	48,48,48,48	0
57	MG	A	3004	1/1	0.78	0.21	55,55,55,55	0
57	MG	A	3326	1/1	0.78	0.24	69,69,69,69	0
57	MG	B	208	1/1	0.78	0.12	74,74,74,74	0
57	MG	A	3272	1/1	0.79	0.10	62,62,62,62	0
57	MG	D	302	1/1	0.79	0.18	74,74,74,74	0
57	MG	F	301	1/1	0.79	0.12	71,71,71,71	0
57	MG	A	3355	1/1	0.79	0.11	84,84,84,84	0
57	MG	A	3287	1/1	0.79	0.12	54,54,54,54	0
57	MG	A	3060	1/1	0.79	0.25	81,81,81,81	0
57	MG	A	3075	1/1	0.79	0.14	67,67,67,67	0
57	MG	a	3361	1/1	0.79	0.21	73,73,73,73	0
57	MG	a	3332	1/1	0.80	0.09	45,45,45,45	0
57	MG	A	3084	1/1	0.80	0.09	57,57,57,57	0
57	MG	A	3045	1/1	0.80	0.22	68,68,68,68	0
57	MG	A	3617	1/1	0.80	0.11	65,65,65,65	0
57	MG	A	3137	1/1	0.80	0.13	59,59,59,59	0
57	MG	A	3627	1/1	0.80	0.18	91,91,91,91	0
57	MG	A	3284	1/1	0.80	0.20	67,67,67,67	0
57	MG	A	3054	1/1	0.80	0.19	71,71,71,71	0
57	MG	A	3366	1/1	0.80	0.13	58,58,58,58	0
57	MG	A	3104	1/1	0.80	0.16	64,64,64,64	0
57	MG	A	3433	1/1	0.80	0.19	64,64,64,64	0
57	MG	A	3008	1/1	0.80	0.18	80,80,80,80	0
57	MG	A	3315	1/1	0.80	0.15	56,56,56,56	0
57	MG	A	3259	1/1	0.80	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	A	3160	1/1	0.80	0.27	61,61,61,61	0
57	MG	A	3482	1/1	0.80	0.11	67,67,67,67	0
57	MG	A	3489	1/1	0.80	0.18	55,55,55,55	0
57	MG	a	3480	1/1	0.80	0.17	77,77,77,77	0
57	MG	A	3165	1/1	0.80	0.34	60,60,60,60	0
57	MG	a	3323	1/1	0.80	0.15	69,69,69,69	0
57	MG	A	3502	1/1	0.80	0.18	56,56,56,56	0
57	MG	A	3081	1/1	0.80	0.17	61,61,61,61	0
57	MG	A	3404	1/1	0.81	0.14	57,57,57,57	0
57	MG	A	3405	1/1	0.81	0.17	61,61,61,61	0
57	MG	A	3276	1/1	0.81	0.12	73,73,73,73	0
57	MG	a	3407	1/1	0.81	0.11	82,82,82,82	0
57	MG	E	304	1/1	0.81	0.18	55,55,55,55	0
57	MG	a	3334	1/1	0.81	0.20	43,43,43,43	0
57	MG	A	3498	1/1	0.81	0.18	76,76,76,76	0
57	MG	A	3260	1/1	0.81	0.12	68,68,68,68	0
57	MG	A	3032	1/1	0.81	0.19	50,50,50,50	0
57	MG	A	3436	1/1	0.81	0.17	87,87,87,87	0
57	MG	A	3245	1/1	0.81	0.22	56,56,56,56	0
57	MG	5	101	1/1	0.81	0.35	69,69,69,69	0
57	MG	A	3129	1/1	0.81	0.13	48,48,48,48	0
57	MG	A	3113	1/1	0.81	0.20	63,63,63,63	0
57	MG	A	3309	1/1	0.82	0.13	52,52,52,52	0
57	MG	A	3246	1/1	0.82	0.20	49,49,49,49	0
57	MG	A	3093	1/1	0.82	0.22	81,81,81,81	0
57	MG	A	3156	1/1	0.82	0.17	86,86,86,86	0
57	MG	a	3393	1/1	0.82	0.31	69,69,69,69	0
57	MG	B	209	1/1	0.82	0.10	70,70,70,70	0
57	MG	a	3327	1/1	0.82	0.14	62,62,62,62	0
57	MG	B	210	1/1	0.82	0.11	68,68,68,68	0
57	MG	A	3563	1/1	0.82	0.15	73,73,73,73	0
57	MG	A	3177	1/1	0.82	0.14	65,65,65,65	0
57	MG	A	3262	1/1	0.82	0.11	63,63,63,63	0
57	MG	A	3126	1/1	0.82	0.17	60,60,60,60	0
57	MG	P	202	1/1	0.82	0.21	86,86,86,86	0
57	MG	A	3244	1/1	0.82	0.18	59,59,59,59	0
57	MG	W	201	1/1	0.82	0.14	77,77,77,77	0
57	MG	v	101	1/1	0.82	0.25	89,89,89,89	0
57	MG	A	3531	1/1	0.82	0.16	91,91,91,91	0
57	MG	A	3150	1/1	0.82	0.16	74,74,74,74	0
57	MG	a	3362	1/1	0.83	0.11	73,73,73,73	0
57	MG	A	3226	1/1	0.83	0.30	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	A	3334	1/1	0.83	0.17	84,84,84,84	0
57	MG	A	3573	1/1	0.83	0.10	70,70,70,70	0
57	MG	a	3372	1/1	0.83	0.17	47,47,47,47	0
57	MG	A	3003	1/1	0.83	0.13	59,59,59,59	0
57	MG	B	206	1/1	0.83	0.16	75,75,75,75	0
57	MG	7	102	1/1	0.83	0.15	66,66,66,66	0
57	MG	A	3302	1/1	0.83	0.16	59,59,59,59	0
57	MG	A	3065	1/1	0.83	0.26	74,74,74,74	0
57	MG	a	3314	1/1	0.83	0.18	60,60,60,60	0
57	MG	A	3542	1/1	0.83	0.24	60,60,60,60	0
57	MG	A	3439	1/1	0.83	0.14	58,58,58,58	0
57	MG	A	3148	1/1	0.83	0.19	60,60,60,60	0
57	MG	B	215	1/1	0.83	0.11	114,114,114,114	0
57	MG	a	3463	1/1	0.83	0.12	45,45,45,45	0
57	MG	A	3444	1/1	0.83	0.24	48,48,48,48	0
57	MG	A	3263	1/1	0.83	0.17	55,55,55,55	0
57	MG	A	3031	1/1	0.83	0.21	70,70,70,70	0
57	MG	P	201	1/1	0.83	0.25	54,54,54,54	0
57	MG	w	101	1/1	0.83	0.19	60,60,60,60	0
57	MG	a	3354	1/1	0.83	0.19	51,51,51,51	0
57	MG	A	3376	1/1	0.83	0.13	67,67,67,67	0
57	MG	A	3121	1/1	0.83	0.20	62,62,62,62	0
57	MG	A	3243	1/1	0.84	0.18	58,58,58,58	0
57	MG	A	3173	1/1	0.84	0.15	57,57,57,57	0
57	MG	A	3133	1/1	0.84	0.18	44,44,44,44	0
57	MG	A	3092	1/1	0.84	0.24	67,67,67,67	0
57	MG	B	211	1/1	0.84	0.29	61,61,61,61	0
57	MG	B	213	1/1	0.84	0.11	81,81,81,81	0
57	MG	A	3570	1/1	0.84	0.12	57,57,57,57	0
57	MG	A	3061	1/1	0.84	0.20	54,54,54,54	0
57	MG	A	3258	1/1	0.84	0.12	43,43,43,43	0
57	MG	A	3005	1/1	0.84	0.24	40,40,40,40	0
57	MG	a	3380	1/1	0.84	0.20	57,57,57,57	0
57	MG	A	3574	1/1	0.84	0.18	57,57,57,57	0
57	MG	A	3465	1/1	0.84	0.13	68,68,68,68	0
57	MG	A	3466	1/1	0.84	0.16	67,67,67,67	0
57	MG	A	3474	1/1	0.84	0.15	51,51,51,51	0
57	MG	A	3478	1/1	0.84	0.09	65,65,65,65	0
57	MG	A	3215	1/1	0.84	0.26	66,66,66,66	0
57	MG	A	3365	1/1	0.84	0.13	51,51,51,51	0
57	MG	A	3299	1/1	0.84	0.16	64,64,64,64	0
57	MG	A	3604	1/1	0.84	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	A	3138	1/1	0.84	0.30	77,77,77,77	0
57	MG	A	3402	1/1	0.84	0.08	50,50,50,50	0
57	MG	A	3142	1/1	0.84	0.08	84,84,84,84	0
57	MG	A	3161	1/1	0.84	0.10	67,67,67,67	0
57	MG	A	3239	1/1	0.84	0.24	56,56,56,56	0
57	MG	A	3543	1/1	0.84	0.10	71,71,71,71	0
57	MG	A	3423	1/1	0.84	0.17	59,59,59,59	0
57	MG	A	3431	1/1	0.84	0.14	69,69,69,69	0
57	MG	B	204	1/1	0.84	0.16	85,85,85,85	0
57	MG	A	3119	1/1	0.84	0.20	50,50,50,50	0
57	MG	A	3023	1/1	0.85	0.10	48,48,48,48	0
57	MG	A	3218	1/1	0.85	0.23	32,32,32,32	0
57	MG	A	3114	1/1	0.85	0.34	57,57,57,57	0
57	MG	B	218	1/1	0.85	0.15	74,74,74,74	0
57	MG	A	3261	1/1	0.85	0.15	61,61,61,61	0
57	MG	A	3393	1/1	0.85	0.24	57,57,57,57	0
57	MG	A	3152	1/1	0.85	0.26	68,68,68,68	0
57	MG	A	3102	1/1	0.85	0.12	59,59,59,59	0
57	MG	A	3182	1/1	0.85	0.10	53,53,53,53	0
57	MG	A	3505	1/1	0.85	0.21	68,68,68,68	0
57	MG	A	3266	1/1	0.85	0.20	61,61,61,61	0
57	MG	A	3242	1/1	0.85	0.12	63,63,63,63	0
57	MG	A	3269	1/1	0.85	0.14	54,54,54,54	0
57	MG	A	3120	1/1	0.85	0.25	52,52,52,52	0
57	MG	a	3403	1/1	0.85	0.10	61,61,61,61	0
57	MG	a	3405	1/1	0.85	0.18	70,70,70,70	0
57	MG	A	3203	1/1	0.85	0.16	53,53,53,53	0
57	MG	a	3409	1/1	0.85	0.13	74,74,74,74	0
57	MG	6	101	1/1	0.85	0.20	64,64,64,64	0
57	MG	A	3044	1/1	0.85	0.20	72,72,72,72	0
57	MG	a	3430	1/1	0.85	0.12	65,65,65,65	0
57	MG	a	3434	1/1	0.85	0.16	54,54,54,54	0
57	MG	A	3343	1/1	0.85	0.10	69,69,69,69	0
57	MG	a	3455	1/1	0.85	0.11	67,67,67,67	0
57	MG	A	3557	1/1	0.85	0.17	60,60,60,60	0
57	MG	A	3628	1/1	0.85	0.13	87,87,87,87	0
57	MG	a	3468	1/1	0.85	0.13	69,69,69,69	0
57	MG	A	3352	1/1	0.85	0.13	47,47,47,47	0
57	MG	A	3278	1/1	0.85	0.34	64,64,64,64	0
57	MG	A	3449	1/1	0.85	0.17	51,51,51,51	0
57	MG	e	201	1/1	0.85	0.16	69,69,69,69	0
57	MG	A	3565	1/1	0.85	0.08	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	l	201	1/1	0.85	0.12	61,61,61,61	0
57	MG	A	3450	1/1	0.85	0.09	57,57,57,57	0
57	MG	A	3279	1/1	0.85	0.11	55,55,55,55	0
57	MG	A	3095	1/1	0.85	0.27	63,63,63,63	0
57	MG	A	3112	1/1	0.85	0.25	66,66,66,66	0
57	MG	a	3388	1/1	0.86	0.11	59,59,59,59	0
57	MG	A	3250	1/1	0.86	0.24	58,58,58,58	0
57	MG	A	3171	1/1	0.86	0.08	37,37,37,37	0
57	MG	A	3096	1/1	0.86	0.20	58,58,58,58	0
57	MG	A	3219	1/1	0.86	0.21	61,61,61,61	0
57	MG	a	3310	1/1	0.86	0.09	52,52,52,52	0
57	MG	A	3117	1/1	0.86	0.34	50,50,50,50	0
57	MG	A	3477	1/1	0.86	0.14	65,65,65,65	0
57	MG	a	3325	1/1	0.86	0.35	55,55,55,55	0
57	MG	A	3180	1/1	0.86	0.26	44,44,44,44	0
57	MG	A	3481	1/1	0.86	0.12	65,65,65,65	0
57	MG	a	3329	1/1	0.86	0.17	46,46,46,46	0
57	MG	A	3066	1/1	0.86	0.13	56,56,56,56	0
57	MG	A	3086	1/1	0.86	0.20	50,50,50,50	0
57	MG	A	3197	1/1	0.86	0.20	40,40,40,40	0
57	MG	A	3624	1/1	0.86	0.10	52,52,52,52	0
57	MG	F	302	1/1	0.86	0.37	52,52,52,52	0
57	MG	A	3039	1/1	0.86	0.23	59,59,59,59	0
57	MG	a	3467	1/1	0.86	0.12	62,62,62,62	0
57	MG	A	3064	1/1	0.86	0.22	50,50,50,50	0
57	MG	a	3360	1/1	0.86	0.27	40,40,40,40	0
57	MG	a	3475	1/1	0.86	0.22	38,38,38,38	0
57	MG	A	3076	1/1	0.86	0.10	41,41,41,41	0
57	MG	V	202	1/1	0.86	0.23	51,51,51,51	0
57	MG	A	3034	1/1	0.86	0.16	71,71,71,71	0
57	MG	A	3632	1/1	0.86	0.12	63,63,63,63	0
57	MG	A	3635	1/1	0.86	0.14	69,69,69,69	0
57	MG	A	3248	1/1	0.86	0.31	57,57,57,57	0
57	MG	a	3378	1/1	0.86	0.20	39,39,39,39	0
57	MG	A	3383	1/1	0.86	0.15	55,55,55,55	0
57	MG	a	3383	1/1	0.86	0.16	56,56,56,56	0
57	MG	A	3425	1/1	0.87	0.14	62,62,62,62	0
57	MG	G	202	1/1	0.87	0.20	67,67,67,67	0
57	MG	A	3506	1/1	0.87	0.11	49,49,49,49	0
57	MG	A	3511	1/1	0.87	0.11	99,99,99,99	0
57	MG	R	201	1/1	0.87	0.12	67,67,67,67	0
57	MG	A	3236	1/1	0.87	0.36	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	V	201	1/1	0.87	0.08	53,53,53,53	0
57	MG	A	3346	1/1	0.87	0.17	68,68,68,68	0
57	MG	A	3125	1/1	0.87	0.20	31,31,31,31	0
57	MG	A	3353	1/1	0.87	0.24	79,79,79,79	0
57	MG	A	3036	1/1	0.87	0.17	74,74,74,74	0
57	MG	A	3615	1/1	0.87	0.12	50,50,50,50	0
57	MG	A	3551	1/1	0.87	0.12	63,63,63,63	0
57	MG	A	3147	1/1	0.87	0.16	64,64,64,64	0
57	MG	A	3288	1/1	0.87	0.18	60,60,60,60	0
57	MG	A	3162	1/1	0.87	0.13	71,71,71,71	0
57	MG	x	3002	1/1	0.87	0.19	101,101,101,101	0
57	MG	A	3212	1/1	0.87	0.10	55,55,55,55	0
57	MG	a	3418	1/1	0.87	0.13	67,67,67,67	0
57	MG	A	3103	1/1	0.87	0.21	56,56,56,56	0
57	MG	A	3166	1/1	0.87	0.21	57,57,57,57	0
57	MG	A	3271	1/1	0.87	0.22	57,57,57,57	0
57	MG	a	3324	1/1	0.87	0.29	40,40,40,40	0
57	MG	a	3440	1/1	0.87	0.12	69,69,69,69	0
57	MG	a	3445	1/1	0.87	0.20	66,66,66,66	0
57	MG	a	3446	1/1	0.87	0.12	68,68,68,68	0
57	MG	A	3132	1/1	0.87	0.30	48,48,48,48	0
57	MG	A	3384	1/1	0.87	0.23	51,51,51,51	0
57	MG	A	3046	1/1	0.87	0.14	55,55,55,55	0
57	MG	A	3398	1/1	0.87	0.14	43,43,43,43	0
57	MG	A	3275	1/1	0.87	0.19	63,63,63,63	0
57	MG	A	3052	1/1	0.87	0.19	59,59,59,59	0
57	MG	A	3020	1/1	0.87	0.16	50,50,50,50	0
57	MG	A	3088	1/1	0.87	0.16	63,63,63,63	0
57	MG	a	3481	1/1	0.87	0.21	46,46,46,46	0
57	MG	a	3348	1/1	0.87	0.14	53,53,53,53	0
57	MG	A	3419	1/1	0.87	0.15	74,74,74,74	0
57	MG	A	3342	1/1	0.87	0.09	61,61,61,61	0
57	MG	a	3356	1/1	0.87	0.20	49,49,49,49	0
57	MG	A	3589	1/1	0.87	0.13	46,46,46,46	0
57	MG	A	3593	1/1	0.87	0.18	41,41,41,41	0
57	MG	A	3595	1/1	0.87	0.16	63,63,63,63	0
57	MG	A	3596	1/1	0.87	0.11	45,45,45,45	0
57	MG	A	3515	1/1	0.88	0.14	48,48,48,48	0
57	MG	A	3434	1/1	0.88	0.11	56,56,56,56	0
57	MG	Q	204	1/1	0.88	0.18	56,56,56,56	0
57	MG	Q	205	1/1	0.88	0.15	55,55,55,55	0
57	MG	A	3107	1/1	0.88	0.32	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	U	201	1/1	0.88	0.23	72,72,72,72	0
57	MG	A	3053	1/1	0.88	0.30	61,61,61,61	0
57	MG	A	3294	1/1	0.88	0.11	44,44,44,44	0
57	MG	A	3546	1/1	0.88	0.16	53,53,53,53	0
57	MG	A	3297	1/1	0.88	0.23	67,67,67,67	0
57	MG	A	3610	1/1	0.88	0.14	61,61,61,61	0
57	MG	Z	301	1/1	0.88	0.12	66,66,66,66	0
57	MG	A	3550	1/1	0.88	0.14	58,58,58,58	0
57	MG	A	3270	1/1	0.88	0.26	61,61,61,61	0
57	MG	A	3552	1/1	0.88	0.12	64,64,64,64	0
57	MG	A	3620	1/1	0.88	0.18	49,49,49,49	0
57	MG	A	3097	1/1	0.88	0.22	60,60,60,60	0
57	MG	A	3305	1/1	0.88	0.17	70,70,70,70	0
57	MG	A	3370	1/1	0.88	0.14	64,64,64,64	0
57	MG	A	3371	1/1	0.88	0.13	53,53,53,53	0
57	MG	A	3010	1/1	0.88	0.14	41,41,41,41	0
57	MG	A	3631	1/1	0.88	0.11	87,87,87,87	0
57	MG	A	3254	1/1	0.88	0.31	67,67,67,67	0
57	MG	A	3469	1/1	0.88	0.10	54,54,54,54	0
57	MG	A	3471	1/1	0.88	0.19	56,56,56,56	0
57	MG	A	3472	1/1	0.88	0.08	53,53,53,53	0
57	MG	A	3255	1/1	0.88	0.33	57,57,57,57	0
57	MG	A	3185	1/1	0.88	0.34	63,63,63,63	0
57	MG	A	3277	1/1	0.88	0.25	71,71,71,71	0
57	MG	A	3042	1/1	0.88	0.17	92,92,92,92	0
57	MG	A	3116	1/1	0.88	0.23	50,50,50,50	0
57	MG	A	3341	1/1	0.88	0.12	57,57,57,57	0
57	MG	a	3346	1/1	0.88	0.14	50,50,50,50	0
57	MG	A	3130	1/1	0.88	0.21	43,43,43,43	0
57	MG	A	3164	1/1	0.88	0.20	51,51,51,51	0
57	MG	A	3025	1/1	0.88	0.16	60,60,60,60	0
57	MG	A	3592	1/1	0.88	0.15	67,67,67,67	0
57	MG	A	3348	1/1	0.88	0.13	71,71,71,71	0
57	MG	A	3151	1/1	0.88	0.17	43,43,43,43	0
57	MG	A	3073	1/1	0.88	0.21	56,56,56,56	0
57	MG	A	3597	1/1	0.88	0.20	65,65,65,65	0
57	MG	G	203	1/1	0.88	0.15	69,69,69,69	0
57	MG	A	3426	1/1	0.89	0.17	55,55,55,55	0
57	MG	A	3598	1/1	0.89	0.14	74,74,74,74	0
57	MG	A	3599	1/1	0.89	0.17	57,57,57,57	0
57	MG	A	3476	1/1	0.89	0.14	50,50,50,50	0
57	MG	A	3058	1/1	0.89	0.27	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	a	3301	1/1	0.89	0.16	49,49,49,49	0
57	MG	A	3222	1/1	0.89	0.20	33,33,33,33	0
57	MG	A	3224	1/1	0.89	0.17	51,51,51,51	0
57	MG	a	3319	1/1	0.89	0.21	39,39,39,39	0
57	MG	a	3320	1/1	0.89	0.11	39,39,39,39	0
57	MG	a	3322	1/1	0.89	0.11	50,50,50,50	0
57	MG	A	3331	1/1	0.89	0.19	54,54,54,54	0
57	MG	A	3006	1/1	0.89	0.16	57,57,57,57	0
57	MG	A	3490	1/1	0.89	0.12	47,47,47,47	0
57	MG	A	3194	1/1	0.89	0.17	34,34,34,34	0
57	MG	a	3422	1/1	0.89	0.09	50,50,50,50	0
57	MG	a	3425	1/1	0.89	0.19	47,47,47,47	0
57	MG	a	3428	1/1	0.89	0.18	46,46,46,46	0
57	MG	A	3085	1/1	0.89	0.24	52,52,52,52	0
57	MG	A	3167	1/1	0.89	0.14	65,65,65,65	0
57	MG	a	3435	1/1	0.89	0.12	57,57,57,57	0
57	MG	A	3030	1/1	0.89	0.16	64,64,64,64	0
57	MG	A	3347	1/1	0.89	0.12	75,75,75,75	0
57	MG	Q	203	1/1	0.89	0.10	45,45,45,45	0
57	MG	a	3337	1/1	0.89	0.21	50,50,50,50	0
57	MG	A	3621	1/1	0.89	0.17	59,59,59,59	0
57	MG	a	3342	1/1	0.89	0.19	50,50,50,50	0
57	MG	A	3510	1/1	0.89	0.15	60,60,60,60	0
57	MG	A	3301	1/1	0.89	0.22	57,57,57,57	0
57	MG	R	202	1/1	0.89	0.17	53,53,53,53	0
57	MG	a	3470	1/1	0.89	0.10	56,56,56,56	0
57	MG	A	3455	1/1	0.89	0.20	73,73,73,73	0
57	MG	A	3525	1/1	0.89	0.10	54,54,54,54	0
57	MG	a	3477	1/1	0.89	0.12	68,68,68,68	0
57	MG	A	3159	1/1	0.89	0.13	78,78,78,78	0
57	MG	A	3175	1/1	0.89	0.15	46,46,46,46	0
57	MG	A	3535	1/1	0.89	0.15	49,49,49,49	0
57	MG	A	3541	1/1	0.89	0.16	56,56,56,56	0
57	MG	A	3001	1/1	0.89	0.24	70,70,70,70	0
57	MG	A	3312	1/1	0.89	0.19	59,59,59,59	0
57	MG	A	3019	1/1	0.89	0.10	49,49,49,49	0
57	MG	0	103	1/1	0.89	0.11	61,61,61,61	0
57	MG	a	3377	1/1	0.89	0.08	85,85,85,85	0
57	MG	A	3050	1/1	0.89	0.16	39,39,39,39	0
57	MG	A	3591	1/1	0.90	0.10	66,66,66,66	0
57	MG	A	3452	1/1	0.90	0.16	53,53,53,53	0
57	MG	A	3410	1/1	0.90	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	A	3192	1/1	0.90	0.23	39,39,39,39	0
57	MG	A	3024	1/1	0.90	0.11	63,63,63,63	0
57	MG	A	3558	1/1	0.90	0.12	73,73,73,73	0
57	MG	A	3367	1/1	0.90	0.20	51,51,51,51	0
57	MG	A	3562	1/1	0.90	0.09	59,59,59,59	0
57	MG	a	3423	1/1	0.90	0.20	66,66,66,66	0
57	MG	a	3341	1/1	0.90	0.14	60,60,60,60	0
57	MG	A	3223	1/1	0.90	0.24	61,61,61,61	0
57	MG	A	3106	1/1	0.90	0.15	57,57,57,57	0
57	MG	A	3174	1/1	0.90	0.16	59,59,59,59	0
57	MG	A	3568	1/1	0.90	0.10	83,83,83,83	0
57	MG	A	3528	1/1	0.90	0.07	51,51,51,51	0
57	MG	A	3027	1/1	0.90	0.09	44,44,44,44	0
57	MG	A	3286	1/1	0.90	0.12	62,62,62,62	0
57	MG	a	3359	1/1	0.90	0.12	65,65,65,65	0
57	MG	A	3028	1/1	0.90	0.24	66,66,66,66	0
57	MG	a	3458	1/1	0.90	0.14	62,62,62,62	0
57	MG	9	101	1/1	0.90	0.12	57,57,57,57	0
57	MG	A	3237	1/1	0.90	0.23	51,51,51,51	0
57	MG	a	3368	1/1	0.90	0.21	44,44,44,44	0
57	MG	E	301	1/1	0.90	0.33	56,56,56,56	0
57	MG	a	3469	1/1	0.90	0.18	42,42,42,42	0
57	MG	A	3118	1/1	0.90	0.41	52,52,52,52	0
57	MG	a	3471	1/1	0.90	0.15	49,49,49,49	0
57	MG	A	3616	1/1	0.90	0.18	59,59,59,59	0
57	MG	a	3302	1/1	0.90	0.09	58,58,58,58	0
57	MG	a	3375	1/1	0.90	0.21	41,41,41,41	0
57	MG	a	3309	1/1	0.90	0.33	37,37,37,37	0
57	MG	A	3111	1/1	0.90	0.13	61,61,61,61	0
57	MG	A	3619	1/1	0.90	0.20	78,78,78,78	0
57	MG	a	3316	1/1	0.90	0.15	54,54,54,54	0
57	MG	A	3143	1/1	0.90	0.18	60,60,60,60	0
57	MG	A	3406	1/1	0.90	0.10	56,56,56,56	0
57	MG	A	3583	1/1	0.90	0.15	55,55,55,55	0
57	MG	w	102	1/1	0.90	0.17	49,49,49,49	0
57	MG	Q	202	1/1	0.90	0.20	51,51,51,51	0
57	MG	A	3091	1/1	0.90	0.18	63,63,63,63	0
57	MG	A	3497	1/1	0.90	0.13	50,50,50,50	0
57	MG	A	3140	1/1	0.91	0.15	57,57,57,57	0
57	MG	a	3373	1/1	0.91	0.16	63,63,63,63	0
57	MG	A	3241	1/1	0.91	0.08	42,42,42,42	0
57	MG	A	3333	1/1	0.91	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	A	3264	1/1	0.91	0.30	65,65,65,65	0
57	MG	A	3339	1/1	0.91	0.11	68,68,68,68	0
57	MG	a	3382	1/1	0.91	0.14	31,31,31,31	0
57	MG	A	3141	1/1	0.91	0.17	55,55,55,55	0
57	MG	A	3290	1/1	0.91	0.18	49,49,49,49	0
57	MG	A	3072	1/1	0.91	0.18	43,43,43,43	0
57	MG	A	3041	1/1	0.91	0.17	42,42,42,42	0
57	MG	A	3488	1/1	0.91	0.16	50,50,50,50	0
57	MG	A	3418	1/1	0.91	0.22	32,32,32,32	0
57	MG	a	3396	1/1	0.91	0.15	42,42,42,42	0
57	MG	A	3633	1/1	0.91	0.18	64,64,64,64	0
57	MG	A	3217	1/1	0.91	0.30	50,50,50,50	0
57	MG	A	3144	1/1	0.91	0.15	38,38,38,38	0
57	MG	B	205	1/1	0.91	0.15	81,81,81,81	0
57	MG	A	3493	1/1	0.91	0.20	33,33,33,33	0
57	MG	A	3007	1/1	0.91	0.12	46,46,46,46	0
57	MG	a	3416	1/1	0.91	0.16	61,61,61,61	0
57	MG	a	3311	1/1	0.91	0.14	51,51,51,51	0
57	MG	A	3109	1/1	0.91	0.10	52,52,52,52	0
57	MG	A	3251	1/1	0.91	0.13	35,35,35,35	0
57	MG	A	3015	1/1	0.91	0.12	43,43,43,43	0
57	MG	A	3079	1/1	0.91	0.21	63,63,63,63	0
57	MG	a	3426	1/1	0.91	0.09	69,69,69,69	0
57	MG	a	3427	1/1	0.91	0.24	50,50,50,50	0
57	MG	A	3358	1/1	0.91	0.10	63,63,63,63	0
57	MG	A	3311	1/1	0.91	0.26	52,52,52,52	0
57	MG	A	3512	1/1	0.91	0.10	51,51,51,51	0
57	MG	B	217	1/1	0.91	0.17	67,67,67,67	0
57	MG	A	3123	1/1	0.91	0.10	51,51,51,51	0
57	MG	A	3314	1/1	0.91	0.14	54,54,54,54	0
57	MG	a	3444	1/1	0.91	0.10	53,53,53,53	0
57	MG	D	303	1/1	0.91	0.58	49,49,49,49	0
57	MG	D	305	1/1	0.91	0.06	37,37,37,37	0
57	MG	A	3442	1/1	0.91	0.10	56,56,56,56	0
57	MG	A	3199	1/1	0.91	0.19	42,42,42,42	0
57	MG	a	3335	1/1	0.91	0.21	37,37,37,37	0
57	MG	a	3460	1/1	0.91	0.12	52,52,52,52	0
57	MG	a	3462	1/1	0.91	0.08	74,74,74,74	0
57	MG	A	3018	1/1	0.91	0.11	49,49,49,49	0
57	MG	a	3338	1/1	0.91	0.13	66,66,66,66	0
57	MG	A	3533	1/1	0.91	0.13	47,47,47,47	0
57	MG	F	305	1/1	0.91	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	G	201	1/1	0.91	0.09	71,71,71,71	0
57	MG	A	3368	1/1	0.91	0.09	47,47,47,47	0
57	MG	A	3538	1/1	0.91	0.09	40,40,40,40	0
57	MG	a	3474	1/1	0.91	0.10	64,64,64,64	0
57	MG	A	3322	1/1	0.91	0.12	61,61,61,61	0
57	MG	a	3476	1/1	0.91	0.07	50,50,50,50	0
57	MG	A	3325	1/1	0.91	0.16	52,52,52,52	0
57	MG	A	3373	1/1	0.91	0.06	64,64,64,64	0
57	MG	A	3457	1/1	0.91	0.10	41,41,41,41	0
57	MG	A	3375	1/1	0.91	0.07	55,55,55,55	0
57	MG	a	3485	1/1	0.91	0.13	51,51,51,51	0
57	MG	A	3464	1/1	0.91	0.10	49,49,49,49	0
57	MG	A	3204	1/1	0.91	0.06	43,43,43,43	0
57	MG	A	3612	1/1	0.91	0.11	53,53,53,53	0
57	MG	l	202	1/1	0.91	0.20	61,61,61,61	0
57	MG	a	3364	1/1	0.91	0.26	56,56,56,56	0
57	MG	A	3613	1/1	0.91	0.16	52,52,52,52	0
57	MG	A	3069	1/1	0.91	0.21	46,46,46,46	0
57	MG	A	3553	1/1	0.91	0.06	40,40,40,40	0
57	MG	A	3467	1/1	0.91	0.20	52,52,52,52	0
57	MG	A	3409	1/1	0.92	0.21	60,60,60,60	0
57	MG	A	3043	1/1	0.92	0.08	59,59,59,59	0
57	MG	A	3412	1/1	0.92	0.12	45,45,45,45	0
57	MG	a	3397	1/1	0.92	0.25	27,27,27,27	0
57	MG	A	3414	1/1	0.92	0.16	31,31,31,31	0
57	MG	A	3257	1/1	0.92	0.12	50,50,50,50	0
57	MG	a	3404	1/1	0.92	0.23	38,38,38,38	0
57	MG	B	212	1/1	0.92	0.10	75,75,75,75	0
57	MG	A	3344	1/1	0.92	0.06	53,53,53,53	0
57	MG	A	3183	1/1	0.92	0.17	54,54,54,54	0
57	MG	A	3090	1/1	0.92	0.19	38,38,38,38	0
57	MG	a	3321	1/1	0.92	0.10	48,48,48,48	0
57	MG	B	216	1/1	0.92	0.12	86,86,86,86	0
57	MG	A	3071	1/1	0.92	0.13	41,41,41,41	0
57	MG	a	3421	1/1	0.92	0.09	61,61,61,61	0
57	MG	A	3350	1/1	0.92	0.12	63,63,63,63	0
57	MG	A	3432	1/1	0.92	0.13	58,58,58,58	0
57	MG	A	3188	1/1	0.92	0.17	44,44,44,44	0
57	MG	A	3295	1/1	0.92	0.15	30,30,30,30	0
57	MG	A	3518	1/1	0.92	0.07	65,65,65,65	0
57	MG	E	302	1/1	0.92	0.07	35,35,35,35	0
57	MG	a	3331	1/1	0.92	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	A	3296	1/1	0.92	0.25	52,52,52,52	0
57	MG	A	3051	1/1	0.92	0.17	43,43,43,43	0
57	MG	A	3356	1/1	0.92	0.19	57,57,57,57	0
57	MG	A	3440	1/1	0.92	0.19	74,74,74,74	0
57	MG	A	3228	1/1	0.92	0.18	62,62,62,62	0
57	MG	A	3149	1/1	0.92	0.21	53,53,53,53	0
57	MG	A	3235	1/1	0.92	0.09	48,48,48,48	0
57	MG	A	3196	1/1	0.92	0.22	44,44,44,44	0
57	MG	a	3345	1/1	0.92	0.12	47,47,47,47	0
57	MG	A	3122	1/1	0.92	0.09	35,35,35,35	0
57	MG	A	3310	1/1	0.92	0.08	45,45,45,45	0
57	MG	A	3611	1/1	0.92	0.18	52,52,52,52	0
57	MG	A	3544	1/1	0.92	0.08	55,55,55,55	0
57	MG	A	3268	1/1	0.92	0.10	58,58,58,58	0
57	MG	A	3198	1/1	0.92	0.18	55,55,55,55	0
57	MG	A	3009	1/1	0.92	0.21	50,50,50,50	0
57	MG	R	203	1/1	0.92	0.12	44,44,44,44	0
57	MG	A	3105	1/1	0.92	0.06	35,35,35,35	0
57	MG	U	202	1/1	0.92	0.11	62,62,62,62	0
57	MG	a	3473	1/1	0.92	0.22	43,43,43,43	0
57	MG	A	3462	1/1	0.92	0.10	53,53,53,53	0
57	MG	A	3372	1/1	0.92	0.10	59,59,59,59	0
57	MG	A	3318	1/1	0.92	0.19	60,60,60,60	0
57	MG	A	3139	1/1	0.92	0.16	62,62,62,62	0
57	MG	A	3207	1/1	0.92	0.09	40,40,40,40	0
57	MG	A	3154	1/1	0.92	0.14	60,60,60,60	0
57	MG	A	3210	1/1	0.92	0.20	56,56,56,56	0
57	MG	A	3211	1/1	0.92	0.23	55,55,55,55	0
57	MG	A	3247	1/1	0.92	0.25	66,66,66,66	0
57	MG	A	3155	1/1	0.92	0.20	44,44,44,44	0
57	MG	A	3115	1/1	0.92	0.08	48,48,48,48	0
57	MG	A	3067	1/1	0.92	0.20	70,70,70,70	0
57	MG	A	3063	1/1	0.92	0.12	62,62,62,62	0
57	MG	a	3387	1/1	0.92	0.05	55,55,55,55	0
57	MG	w	106	1/1	0.92	0.20	45,45,45,45	0
57	MG	A	3407	1/1	0.92	0.07	38,38,38,38	0
57	MG	y	701	1/1	0.92	0.20	68,68,68,68	0
57	MG	A	3487	1/1	0.92	0.16	60,60,60,60	0
57	MG	A	3181	1/1	0.92	0.12	35,35,35,35	0
61	GDP	y	703	28/28	0.92	0.11	91,120,142,146	0
57	MG	A	3509	1/1	0.93	0.19	51,51,51,51	0
57	MG	A	3392	1/1	0.93	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	A	3575	1/1	0.93	0.14	70,70,70,70	0
57	MG	a	3304	1/1	0.93	0.13	55,55,55,55	0
57	MG	a	3306	1/1	0.93	0.20	55,55,55,55	0
57	MG	a	3395	1/1	0.93	0.19	32,32,32,32	0
57	MG	A	3214	1/1	0.93	0.21	52,52,52,52	0
57	MG	A	3349	1/1	0.93	0.09	39,39,39,39	0
57	MG	A	3136	1/1	0.93	0.10	49,49,49,49	0
57	MG	a	3313	1/1	0.93	0.11	61,61,61,61	0
57	MG	A	3580	1/1	0.93	0.17	67,67,67,67	0
57	MG	A	3516	1/1	0.93	0.15	55,55,55,55	0
57	MG	A	3517	1/1	0.93	0.14	51,51,51,51	0
57	MG	A	3169	1/1	0.93	0.22	57,57,57,57	0
57	MG	A	3590	1/1	0.93	0.13	59,59,59,59	0
57	MG	a	3413	1/1	0.93	0.06	54,54,54,54	0
57	MG	A	3047	1/1	0.93	0.14	39,39,39,39	0
57	MG	A	3200	1/1	0.93	0.12	44,44,44,44	0
57	MG	A	3463	1/1	0.93	0.14	46,46,46,46	0
57	MG	a	3420	1/1	0.93	0.10	62,62,62,62	0
57	MG	A	3201	1/1	0.93	0.14	63,63,63,63	0
57	MG	a	3326	1/1	0.93	0.16	48,48,48,48	0
57	MG	A	3172	1/1	0.93	0.24	31,31,31,31	0
57	MG	A	3131	1/1	0.93	0.10	53,53,53,53	0
57	MG	E	303	1/1	0.93	0.12	41,41,41,41	0
57	MG	A	3536	1/1	0.93	0.12	39,39,39,39	0
57	MG	A	3206	1/1	0.93	0.07	65,65,65,65	0
57	MG	A	3082	1/1	0.93	0.42	53,53,53,53	0
57	MG	F	304	1/1	0.93	0.17	60,60,60,60	0
57	MG	A	3190	1/1	0.93	0.19	38,38,38,38	0
57	MG	a	3336	1/1	0.93	0.24	62,62,62,62	0
57	MG	A	3230	1/1	0.93	0.18	46,46,46,46	0
57	MG	A	3252	1/1	0.93	0.21	58,58,58,58	0
57	MG	A	3545	1/1	0.93	0.19	64,64,64,64	0
57	MG	N	201	1/1	0.93	0.12	57,57,57,57	0
57	MG	a	3447	1/1	0.93	0.20	36,36,36,36	0
57	MG	a	3454	1/1	0.93	0.18	39,39,39,39	0
57	MG	A	3422	1/1	0.93	0.10	52,52,52,52	0
57	MG	A	3547	1/1	0.93	0.06	60,60,60,60	0
57	MG	A	3298	1/1	0.93	0.09	58,58,58,58	0
57	MG	A	3335	1/1	0.93	0.07	56,56,56,56	0
57	MG	a	3461	1/1	0.93	0.08	44,44,44,44	0
57	MG	a	3349	1/1	0.93	0.23	47,47,47,47	0
57	MG	A	3479	1/1	0.93	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	a	3352	1/1	0.93	0.18	59,59,59,59	0
57	MG	A	3098	1/1	0.93	0.10	48,48,48,48	0
57	MG	A	3232	1/1	0.93	0.17	36,36,36,36	0
57	MG	A	3483	1/1	0.93	0.12	55,55,55,55	0
57	MG	A	3099	1/1	0.93	0.13	34,34,34,34	0
57	MG	A	3556	1/1	0.93	0.09	55,55,55,55	0
57	MG	A	3195	1/1	0.93	0.15	41,41,41,41	0
57	MG	A	3374	1/1	0.93	0.10	58,58,58,58	0
57	MG	A	3559	1/1	0.93	0.08	46,46,46,46	0
57	MG	A	3308	1/1	0.93	0.09	56,56,56,56	0
57	MG	A	3561	1/1	0.93	0.08	54,54,54,54	0
57	MG	A	3345	1/1	0.93	0.11	44,44,44,44	0
57	MG	A	3379	1/1	0.93	0.16	50,50,50,50	0
57	MG	A	3037	1/1	0.93	0.12	61,61,61,61	0
57	MG	A	3238	1/1	0.93	0.17	45,45,45,45	0
57	MG	a	3487	1/1	0.93	0.15	35,35,35,35	0
57	MG	A	3567	1/1	0.93	0.11	47,47,47,47	0
57	MG	a	3376	1/1	0.93	0.13	46,46,46,46	0
57	MG	A	3499	1/1	0.93	0.07	60,60,60,60	0
57	MG	A	3385	1/1	0.93	0.12	57,57,57,57	0
57	MG	a	3379	1/1	0.93	0.14	30,30,30,30	0
57	MG	B	203	1/1	0.93	0.09	56,56,56,56	0
57	MG	w	105	1/1	0.93	0.22	29,29,29,29	0
57	MG	A	3387	1/1	0.93	0.08	53,53,53,53	0
57	MG	A	3390	1/1	0.93	0.15	46,46,46,46	0
57	MG	a	3384	1/1	0.93	0.12	49,49,49,49	0
57	MG	a	3385	1/1	0.93	0.10	33,33,33,33	0
57	MG	a	3386	1/1	0.93	0.27	41,41,41,41	0
57	MG	A	3507	1/1	0.93	0.10	46,46,46,46	0
57	MG	D	304	1/1	0.94	0.09	74,74,74,74	0
57	MG	A	3189	1/1	0.94	0.24	37,37,37,37	0
57	MG	A	3016	1/1	0.94	0.08	49,49,49,49	0
57	MG	A	3520	1/1	0.94	0.14	80,80,80,80	0
57	MG	A	3523	1/1	0.94	0.16	36,36,36,36	0
57	MG	A	3427	1/1	0.94	0.12	62,62,62,62	0
57	MG	A	3176	1/1	0.94	0.08	35,35,35,35	0
57	MG	A	3193	1/1	0.94	0.15	38,38,38,38	0
57	MG	F	303	1/1	0.94	0.10	36,36,36,36	0
57	MG	a	3441	1/1	0.94	0.10	62,62,62,62	0
57	MG	A	3021	1/1	0.94	0.14	34,34,34,34	0
57	MG	a	3315	1/1	0.94	0.20	60,60,60,60	0
57	MG	A	3168	1/1	0.94	0.30	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	A	3534	1/1	0.94	0.19	45,45,45,45	0
57	MG	a	3448	1/1	0.94	0.07	42,42,42,42	0
57	MG	a	3452	1/1	0.94	0.07	52,52,52,52	0
57	MG	A	3306	1/1	0.94	0.08	50,50,50,50	0
57	MG	A	3077	1/1	0.94	0.13	48,48,48,48	0
57	MG	a	3457	1/1	0.94	0.21	41,41,41,41	0
57	MG	A	3437	1/1	0.94	0.12	28,28,28,28	0
57	MG	A	3336	1/1	0.94	0.10	36,36,36,36	0
57	MG	A	3400	1/1	0.94	0.08	35,35,35,35	0
57	MG	Q	201	1/1	0.94	0.18	51,51,51,51	0
57	MG	A	3362	1/1	0.94	0.11	50,50,50,50	0
57	MG	A	3584	1/1	0.94	0.11	62,62,62,62	0
57	MG	a	3465	1/1	0.94	0.06	57,57,57,57	0
57	MG	A	3363	1/1	0.94	0.09	30,30,30,30	0
57	MG	A	3587	1/1	0.94	0.17	48,48,48,48	0
57	MG	B	201	1/1	0.94	0.07	51,51,51,51	0
57	MG	B	202	1/1	0.94	0.13	66,66,66,66	0
57	MG	A	3170	1/1	0.94	0.11	43,43,43,43	0
57	MG	A	3447	1/1	0.94	0.11	67,67,67,67	0
57	MG	A	3448	1/1	0.94	0.30	48,48,48,48	0
57	MG	A	3100	1/1	0.94	0.12	45,45,45,45	0
57	MG	A	3494	1/1	0.94	0.10	42,42,42,42	0
57	MG	A	3184	1/1	0.94	0.23	40,40,40,40	0
57	MG	A	3022	1/1	0.94	0.15	33,33,33,33	0
57	MG	A	3369	1/1	0.94	0.10	54,54,54,54	0
57	MG	A	3454	1/1	0.94	0.13	51,51,51,51	0
57	MG	a	3344	1/1	0.94	0.09	51,51,51,51	0
57	MG	A	3313	1/1	0.94	0.13	44,44,44,44	0
57	MG	a	3486	1/1	0.94	0.14	38,38,38,38	0
57	MG	a	3408	1/1	0.94	0.07	55,55,55,55	0
57	MG	A	3456	1/1	0.94	0.14	47,47,47,47	0
57	MG	A	3080	1/1	0.94	0.18	54,54,54,54	0
57	MG	a	3411	1/1	0.94	0.10	53,53,53,53	0
57	MG	a	3412	1/1	0.94	0.16	48,48,48,48	0
57	MG	m	201	1/1	0.94	0.07	35,35,35,35	0
57	MG	A	3187	1/1	0.94	0.24	47,47,47,47	0
57	MG	a	3414	1/1	0.94	0.14	50,50,50,50	0
57	MG	A	3415	1/1	0.94	0.17	42,42,42,42	0
57	MG	A	3221	1/1	0.94	0.19	58,58,58,58	0
57	MG	a	3353	1/1	0.94	0.20	48,48,48,48	0
57	MG	A	3274	1/1	0.94	0.11	45,45,45,45	0
57	MG	A	3026	1/1	0.94	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	a	3357	1/1	0.94	0.13	48,48,48,48	0
57	MG	A	3324	1/1	0.94	0.15	43,43,43,43	0
57	MG	A	3220	1/1	0.95	0.09	49,49,49,49	0
57	MG	A	3280	1/1	0.95	0.17	32,32,32,32	0
57	MG	A	3443	1/1	0.95	0.14	39,39,39,39	0
57	MG	A	3208	1/1	0.95	0.18	40,40,40,40	0
57	MG	A	3485	1/1	0.95	0.14	38,38,38,38	0
57	MG	A	3626	1/1	0.95	0.13	51,51,51,51	0
57	MG	A	3446	1/1	0.95	0.15	39,39,39,39	0
57	MG	A	3300	1/1	0.95	0.14	60,60,60,60	0
57	MG	A	3539	1/1	0.95	0.07	52,52,52,52	0
57	MG	A	3581	1/1	0.95	0.09	55,55,55,55	0
57	MG	A	3033	1/1	0.95	0.11	39,39,39,39	0
57	MG	a	3451	1/1	0.95	0.10	49,49,49,49	0
57	MG	a	3381	1/1	0.95	0.14	55,55,55,55	0
57	MG	A	3283	1/1	0.95	0.07	55,55,55,55	0
57	MG	A	3413	1/1	0.95	0.10	51,51,51,51	0
57	MG	A	3127	1/1	0.95	0.11	73,73,73,73	0
57	MG	A	3588	1/1	0.95	0.08	40,40,40,40	0
57	MG	A	3146	1/1	0.95	0.13	56,56,56,56	0
57	MG	A	3453	1/1	0.95	0.12	44,44,44,44	0
57	MG	A	3382	1/1	0.95	0.12	36,36,36,36	0
57	MG	A	3307	1/1	0.95	0.09	45,45,45,45	0
57	MG	A	3500	1/1	0.95	0.12	40,40,40,40	0
57	MG	A	3074	1/1	0.95	0.16	42,42,42,42	0
57	MG	A	3503	1/1	0.95	0.15	41,41,41,41	0
57	MG	A	3504	1/1	0.95	0.19	38,38,38,38	0
57	MG	a	3339	1/1	0.95	0.15	50,50,50,50	0
57	MG	A	3012	1/1	0.95	0.07	37,37,37,37	0
57	MG	a	3399	1/1	0.95	0.16	36,36,36,36	0
57	MG	A	3424	1/1	0.95	0.13	57,57,57,57	0
57	MG	a	3401	1/1	0.95	0.30	44,44,44,44	0
57	MG	A	3386	1/1	0.95	0.16	59,59,59,59	0
57	MG	A	3601	1/1	0.95	0.12	45,45,45,45	0
57	MG	A	3289	1/1	0.95	0.07	43,43,43,43	0
57	MG	A	3388	1/1	0.95	0.06	47,47,47,47	0
57	MG	a	3479	1/1	0.95	0.15	47,47,47,47	0
57	MG	a	3347	1/1	0.95	0.15	41,41,41,41	0
57	MG	A	3429	1/1	0.95	0.12	30,30,30,30	0
57	MG	A	3389	1/1	0.95	0.13	30,30,30,30	0
57	MG	7	103	1/1	0.95	0.08	57,57,57,57	0
57	MG	D	301	1/1	0.95	0.19	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	A	3070	1/1	0.95	0.08	57,57,57,57	0
57	MG	A	3178	1/1	0.95	0.17	31,31,31,31	0
57	MG	a	3415	1/1	0.95	0.14	62,62,62,62	0
57	MG	A	3364	1/1	0.95	0.07	61,61,61,61	0
57	MG	A	3292	1/1	0.95	0.23	54,54,54,54	0
57	MG	A	3179	1/1	0.95	0.16	43,43,43,43	0
57	MG	a	3303	1/1	0.95	0.13	58,58,58,58	0
57	MG	A	3521	1/1	0.95	0.07	60,60,60,60	0
57	MG	w	104	1/1	0.95	0.11	38,38,38,38	0
57	MG	A	3048	1/1	0.95	0.14	43,43,43,43	0
57	MG	A	3078	1/1	0.95	0.13	47,47,47,47	0
57	MG	a	3363	1/1	0.95	0.23	43,43,43,43	0
57	MG	A	3527	1/1	0.95	0.20	63,63,63,63	0
57	MG	a	3365	1/1	0.95	0.21	45,45,45,45	0
57	MG	A	3035	1/1	0.95	0.07	47,47,47,47	0
57	MG	a	3429	1/1	0.95	0.16	49,49,49,49	0
57	MG	a	3367	1/1	0.96	0.21	30,30,30,30	0
57	MG	A	3438	1/1	0.96	0.08	53,53,53,53	0
57	MG	a	3432	1/1	0.96	0.07	46,46,46,46	0
57	MG	A	3303	1/1	0.96	0.06	55,55,55,55	0
57	MG	A	3519	1/1	0.96	0.14	30,30,30,30	0
57	MG	A	3304	1/1	0.96	0.10	39,39,39,39	0
57	MG	a	3439	1/1	0.96	0.10	48,48,48,48	0
57	MG	A	3089	1/1	0.96	0.10	47,47,47,47	0
57	MG	A	3351	1/1	0.96	0.10	38,38,38,38	0
57	MG	a	3317	1/1	0.96	0.15	26,26,26,26	0
57	MG	a	3318	1/1	0.96	0.12	41,41,41,41	0
57	MG	A	3524	1/1	0.96	0.10	53,53,53,53	0
57	MG	A	3327	1/1	0.96	0.06	49,49,49,49	0
57	MG	A	3526	1/1	0.96	0.05	41,41,41,41	0
57	MG	a	3450	1/1	0.96	0.06	55,55,55,55	0
57	MG	A	3145	1/1	0.96	0.11	48,48,48,48	0
57	MG	A	3445	1/1	0.96	0.07	51,51,51,51	0
57	MG	A	3622	1/1	0.96	0.15	49,49,49,49	0
57	MG	A	3529	1/1	0.96	0.15	56,56,56,56	0
57	MG	A	3484	1/1	0.96	0.08	50,50,50,50	0
57	MG	A	3411	1/1	0.96	0.14	47,47,47,47	0
57	MG	A	3486	1/1	0.96	0.11	40,40,40,40	0
57	MG	A	3083	1/1	0.96	0.08	37,37,37,37	0
57	MG	A	3579	1/1	0.96	0.10	53,53,53,53	0
57	MG	A	3630	1/1	0.96	0.13	43,43,43,43	0
57	MG	A	3380	1/1	0.96	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	A	3202	1/1	0.96	0.30	50,50,50,50	0
57	MG	a	3466	1/1	0.96	0.15	60,60,60,60	0
57	MG	A	3128	1/1	0.96	0.08	45,45,45,45	0
57	MG	a	3394	1/1	0.96	0.12	32,32,32,32	0
57	MG	A	3055	1/1	0.96	0.10	45,45,45,45	0
57	MG	A	3585	1/1	0.96	0.06	47,47,47,47	0
57	MG	A	3225	1/1	0.96	0.16	36,36,36,36	0
57	MG	U	204	1/1	0.96	0.05	37,37,37,37	0
57	MG	A	3205	1/1	0.96	0.06	43,43,43,43	0
57	MG	A	3337	1/1	0.96	0.12	44,44,44,44	0
57	MG	A	3338	1/1	0.96	0.13	30,30,30,30	0
57	MG	A	3227	1/1	0.96	0.17	43,43,43,43	0
57	MG	A	3163	1/1	0.96	0.09	34,34,34,34	0
57	MG	a	3478	1/1	0.96	0.10	48,48,48,48	0
57	MG	A	3460	1/1	0.96	0.12	44,44,44,44	0
57	MG	A	3548	1/1	0.96	0.14	40,40,40,40	0
57	MG	A	3594	1/1	0.96	0.07	37,37,37,37	0
57	MG	a	3482	1/1	0.96	0.11	37,37,37,37	0
57	MG	A	3391	1/1	0.96	0.11	30,30,30,30	0
57	MG	A	3285	1/1	0.96	0.08	50,50,50,50	0
57	MG	a	3351	1/1	0.96	0.14	36,36,36,36	0
57	MG	A	3430	1/1	0.96	0.07	44,44,44,44	0
57	MG	A	3316	1/1	0.96	0.06	47,47,47,47	0
57	MG	8	101	1/1	0.96	0.13	66,66,66,66	0
57	MG	A	3396	1/1	0.96	0.13	38,38,38,38	0
57	MG	a	3417	1/1	0.96	0.12	37,37,37,37	0
57	MG	A	3508	1/1	0.96	0.05	46,46,46,46	0
57	MG	A	3229	1/1	0.96	0.12	46,46,46,46	0
57	MG	A	3399	1/1	0.96	0.17	29,29,29,29	0
57	MG	A	3014	1/1	0.96	0.07	39,39,39,39	0
57	MG	A	3321	1/1	0.96	0.08	41,41,41,41	0
57	MG	A	3513	1/1	0.96	0.13	41,41,41,41	0
57	MG	a	3424	1/1	0.96	0.06	43,43,43,43	0
57	MG	A	3606	1/1	0.96	0.07	55,55,55,55	0
57	MG	A	3110	1/1	0.96	0.06	42,42,42,42	0
57	MG	A	3473	1/1	0.96	0.09	46,46,46,46	0
57	MG	a	3366	1/1	0.96	0.15	38,38,38,38	0
57	MG	A	3049	1/1	0.97	0.08	41,41,41,41	0
57	MG	A	3420	1/1	0.97	0.12	31,31,31,31	0
57	MG	A	3403	1/1	0.97	0.06	40,40,40,40	0
57	MG	A	3332	1/1	0.97	0.09	39,39,39,39	0
57	MG	A	3094	1/1	0.97	0.13	31,31,31,31	0

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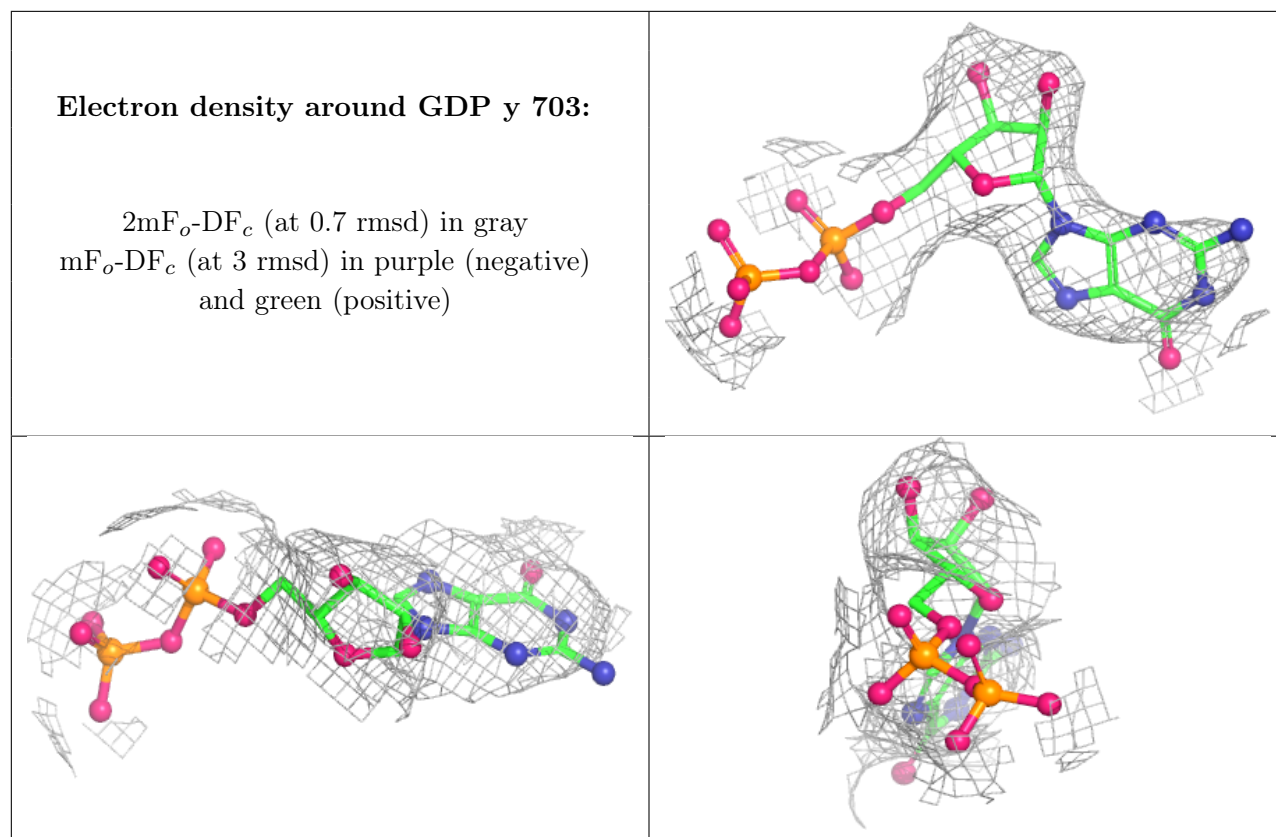
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	A	3256	1/1	0.97	0.10	55,55,55,55	0
57	MG	A	3582	1/1	0.97	0.07	63,63,63,63	0
57	MG	A	3359	1/1	0.97	0.05	45,45,45,45	0
57	MG	A	3249	1/1	0.97	0.04	31,31,31,31	0
57	MG	A	3191	1/1	0.97	0.24	33,33,33,33	0
57	MG	A	3013	1/1	0.97	0.09	52,52,52,52	0
57	MG	a	3355	1/1	0.97	0.13	39,39,39,39	0
57	MG	A	3233	1/1	0.97	0.10	53,53,53,53	0
57	MG	A	3468	1/1	0.97	0.10	48,48,48,48	0
57	MG	A	3377	1/1	0.97	0.15	44,44,44,44	0
57	MG	7	101	1/1	0.97	0.19	48,48,48,48	0
57	MG	A	3470	1/1	0.97	0.08	43,43,43,43	0
57	MG	a	3437	1/1	0.97	0.08	54,54,54,54	0
57	MG	A	3566	1/1	0.97	0.09	40,40,40,40	0
57	MG	O	201	1/1	0.97	0.05	38,38,38,38	0
57	MG	A	3317	1/1	0.97	0.10	31,31,31,31	0
57	MG	A	3340	1/1	0.97	0.07	65,65,65,65	0
57	MG	A	3495	1/1	0.97	0.12	40,40,40,40	0
57	MG	A	3329	1/1	0.97	0.10	40,40,40,40	0
57	MG	a	3333	1/1	0.97	0.23	51,51,51,51	0
57	MG	a	3406	1/1	0.97	0.13	52,52,52,52	0
57	MG	a	3449	1/1	0.97	0.11	50,50,50,50	0
57	MG	A	3623	1/1	0.97	0.07	52,52,52,52	0
57	MG	n	101	1/1	0.97	0.12	42,42,42,42	0
57	MG	A	3416	1/1	0.97	0.07	41,41,41,41	0
57	MG	A	3522	1/1	0.97	0.07	51,51,51,51	0
57	MG	w	103	1/1	0.97	0.15	38,38,38,38	0
57	MG	A	3475	1/1	0.97	0.09	55,55,55,55	0
57	MG	a	3305	1/1	0.97	0.12	46,46,46,46	0
57	MG	A	3234	1/1	0.97	0.24	48,48,48,48	0
57	MG	a	3374	1/1	0.97	0.21	30,30,30,30	0
57	MG	a	3307	1/1	0.97	0.05	35,35,35,35	0
57	MG	a	3308	1/1	0.97	0.06	41,41,41,41	0
57	MG	A	3501	1/1	0.97	0.14	46,46,46,46	0
57	MG	a	3343	1/1	0.97	0.14	29,29,29,29	0
57	MG	A	3395	1/1	0.98	0.07	31,31,31,31	0
57	MG	a	3453	1/1	0.98	0.03	41,41,41,41	0
57	MG	A	3537	1/1	0.98	0.07	32,32,32,32	0
57	MG	A	3428	1/1	0.98	0.06	36,36,36,36	0
57	MG	a	3456	1/1	0.98	0.06	59,59,59,59	0
57	MG	A	3496	1/1	0.98	0.08	47,47,47,47	0
57	MG	A	3540	1/1	0.98	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	A	3609	1/1	0.98	0.07	39,39,39,39	0
57	MG	A	3401	1/1	0.98	0.08	37,37,37,37	0
57	MG	a	3433	1/1	0.98	0.06	32,32,32,32	0
57	MG	A	3038	1/1	0.98	0.14	55,55,55,55	0
57	MG	A	3397	1/1	0.98	0.07	36,36,36,36	0
57	MG	a	3464	1/1	0.98	0.04	44,44,44,44	0
57	MG	a	3389	1/1	0.98	0.06	38,38,38,38	0
57	MG	A	3323	1/1	0.98	0.06	42,42,42,42	0
57	MG	A	3514	1/1	0.98	0.04	34,34,34,34	0
57	MG	A	3634	1/1	0.98	0.05	56,56,56,56	0
57	MG	A	3417	1/1	0.98	0.09	30,30,30,30	0
57	MG	A	3530	1/1	0.98	0.11	38,38,38,38	0
57	MG	A	3458	1/1	0.98	0.12	27,27,27,27	0
57	MG	A	3618	1/1	0.98	0.09	45,45,45,45	0
57	MG	A	3459	1/1	0.98	0.06	36,36,36,36	0
57	MG	a	3398	1/1	0.98	0.24	27,27,27,27	0
57	MG	A	3480	1/1	0.98	0.06	35,35,35,35	0
58	ZN	4	501	1/1	0.98	0.03	117,117,117,117	0
57	MG	A	3492	1/1	0.98	0.08	62,62,62,62	0
57	MG	A	3381	1/1	0.98	0.13	43,43,43,43	0
57	MG	a	3443	1/1	0.99	0.03	46,46,46,46	0
57	MG	A	3378	1/1	0.99	0.10	31,31,31,31	0
57	MG	A	3394	1/1	0.99	0.12	30,30,30,30	0
57	MG	A	3320	1/1	0.99	0.06	49,49,49,49	0
57	MG	A	3017	1/1	0.99	0.08	63,63,63,63	0
57	MG	a	3438	1/1	0.99	0.08	34,34,34,34	0
57	MG	a	3402	1/1	0.99	0.07	43,43,43,43	0
57	MG	a	3312	1/1	0.99	0.04	26,26,26,26	0
58	ZN	Y	501	1/1	0.99	0.03	92,92,92,92	0
57	MG	A	3421	1/1	0.99	0.07	40,40,40,40	0
58	ZN	5	102	1/1	0.99	0.02	70,70,70,70	0
58	ZN	9	102	1/1	0.99	0.03	72,72,72,72	0
59	SF4	d	501	8/8	0.99	0.05	48,60,64,65	0
57	MG	a	3442	1/1	0.99	0.03	45,45,45,45	0
57	MG	a	3483	1/1	0.99	0.11	39,39,39,39	0
58	ZN	6	102	1/1	1.00	0.02	70,70,70,70	0
57	MG	a	3431	1/1	1.00	0.03	41,41,41,41	0
58	ZN	n	102	1/1	1.00	0.01	61,61,61,61	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.