wwPDB X-ray Structure Validation Summary Report (i)

Feb 25, 2024 – 01:21 PM EST

PDB ID	:	5J8B
Title	:	Crystal structure of Elongation Factor 4 (EF-4/LepA) in complex with GDPCP bound to the Thermus thermophilus 70S ribosome
Authors	:	Gagnon, M.G.; Lin, J.; Steitz, T.A.
Deposited on	:	2016-04-07
Resolution	:	2.60 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

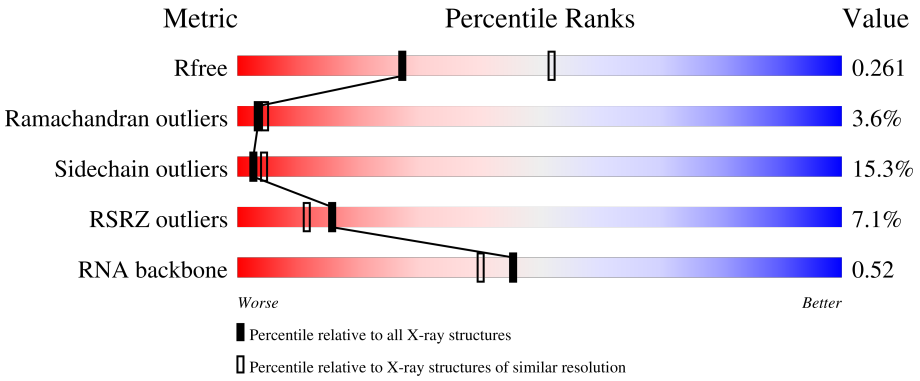
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 >=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 <=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	5% 78% 18%
2	B	121	87% 12%
3	C	228	26% 45% 14% 40%
4	D	276	88% 11%
5	E	206	2% 85% 13%

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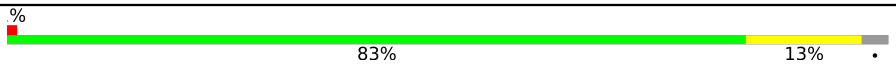
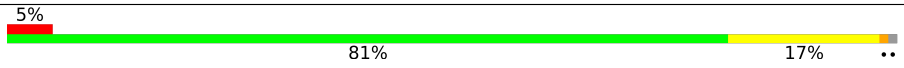
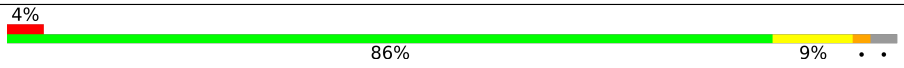
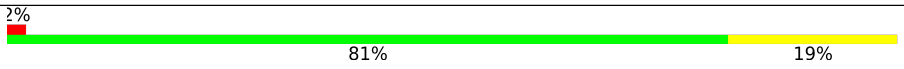
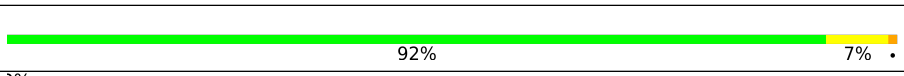
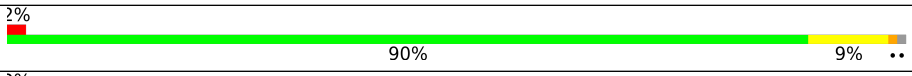
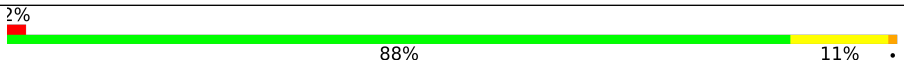
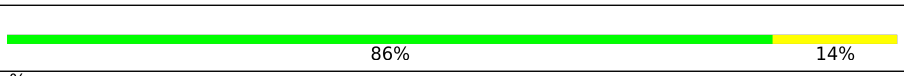
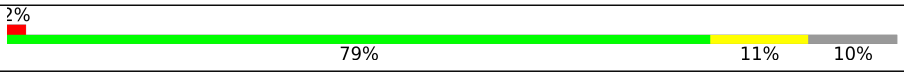
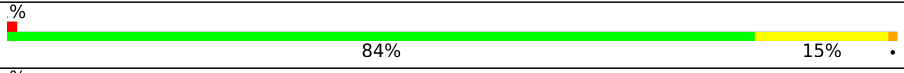
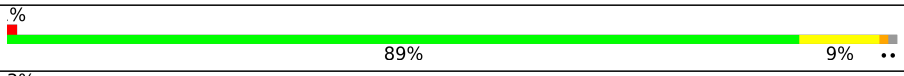
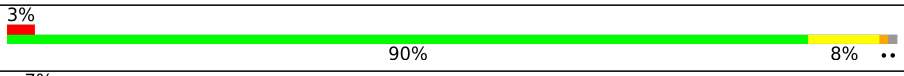
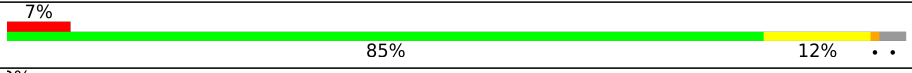
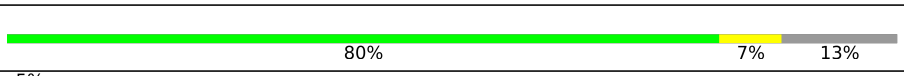
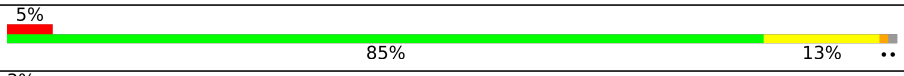
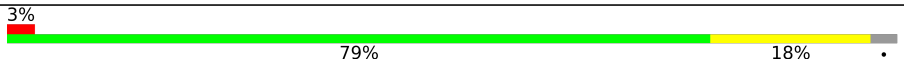
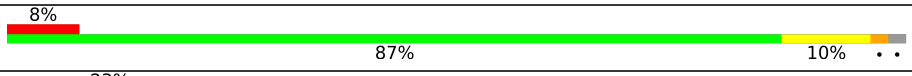
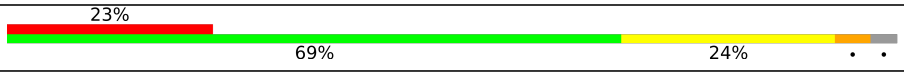
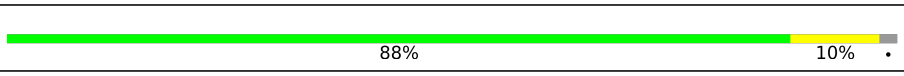
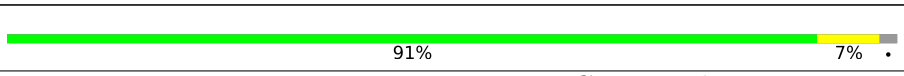
Mol	Chain	Length	Quality of chain
6	F	210	
7	G	182	
8	H	180	
9	J	173	
10	K	147	
11	N	140	
12	O	122	
13	P	150	
14	Q	141	
15	R	118	
16	S	112	
17	T	146	
18	U	118	
19	V	101	
20	W	113	
21	X	96	
22	Y	110	
23	Z	206	
24	0	85	
25	1	98	
26	2	72	
27	3	60	
28	4	71	
29	5	60	
30	6	54	

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Mol	Chain	Length	Quality of chain
31	7	49	4% 82% 16%
32	8	65	91% 8%
33	9	37	5% 86% 14%
34	a	1521	5% 79% 17%
35	b	256	12% 71% 17% 10%
36	c	239	3% 78% 8% 14%
37	d	209	3% 86% 13%
38	e	162	2% 79% 12% 9%
39	f	101	7% 82% 16%
40	g	156	8% 84% 15%
41	h	138	88% 10%
42	i	128	2% 81% 18%
43	j	105	17% 72% 18% 9%
44	k	129	2% 81% 7% 12%
45	l	132	83% 8% 8%
46	m	126	10% 81% 12% 6%
47	n	61	85% 11%
48	o	89	2% 89% 9%
49	p	88	6% 81% 13% 7%
50	q	105	80% 12% 6%
51	r	88	3% 67% 10% 23%
52	s	93	8% 73% 14% 11%
53	t	106	78% 10% 9%
54	u	27	78% 7% 15%
55	v	24	4% 46% 8% 46%

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Mol	Chain	Length	Quality of chain
56	w	76	42% 53% 34% 11%
57	x	77	5% 74% 21% 5%
58	y	76	21% 51% 33% 13%
59	z	679	8% 78% 18%

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
56	5MU	w	54	-	-	-	X
60	MG	A	3004	-	-	-	X
60	MG	A	3050	-	-	-	X
60	MG	A	3094	-	-	-	X
60	MG	A	3100	-	-	-	X
60	MG	A	3144	-	-	-	X
60	MG	A	3157	-	-	-	X
60	MG	A	3169	-	-	-	X
60	MG	A	3217	-	-	-	X
60	MG	A	3223	-	-	-	X
60	MG	A	3234	-	-	-	X
60	MG	A	3236	-	-	-	X
60	MG	A	3237	-	-	-	X
60	MG	A	3242	-	-	-	X
60	MG	A	3267	-	-	-	X
60	MG	A	3277	-	-	-	X
60	MG	A	3283	-	-	-	X
60	MG	A	3391	-	-	-	X
60	MG	A	3573	-	-	-	X
60	MG	A	3577	-	-	-	X
60	MG	A	3586	-	-	-	X
60	MG	A	3624	-	-	-	X
60	MG	B	201	-	-	-	X
60	MG	V	202	-	-	-	X
60	MG	a	1614	-	-	-	X
60	MG	a	1615	-	-	-	X
60	MG	a	1620	-	-	-	X
60	MG	a	1636	-	-	-	X
60	MG	a	1638	-	-	-	X
60	MG	a	1643	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	a	1665	-	-	-	X
60	MG	a	1666	-	-	-	X
60	MG	a	1718	-	-	-	X
60	MG	a	1785	-	-	-	X
60	MG	x	106	-	-	-	X

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 155465 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	2874	61902	27550	11582	19897	2873	11	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 L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	136	1024	644	190	189	1	1	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L10.

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

- Molecule 10 is a protein called 50S ribosomal protein L11.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

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

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	107	Total	C	N	O	S	1	0	0
			806	517	152	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	94	Total	C	N	O	S	0	0	0
			784	499	150	134	1			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	0	74	Total	C	N	O	S	0	0	0
			591	366	126	98	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	69	Total	C	N	O	S	0	0	0
			557	350	101	101	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	a	1498	Total	C	N	O	P	4	0	0
			32207	14334	5973	10402	1498			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 56 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	w	74	Total	C	N	O	P	S	1	0	0
			1586	713	285	513	73	2			

- Molecule 57 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	x	77	Total	C	N	O	P	S	3	0	0
			1645	734	297	536	77	1			

- Molecule 58 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
58	y	74	Total	C	N	O	P	S	0	0	0
			1580	706	285	515	73	1			

- Molecule 59 is a protein called GDPCP fused to the N-terminus of the ribosomal protein L9,Elongation factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	z	671	Total	C	N	O	S	0	0	0
			5200	3333	897	961	9			

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	A	644	Total	Mg	0	0
			644	644		
60	B	18	Total	Mg	0	0
			18	18		
60	D	6	Total	Mg	0	0
			6	6		
60	E	5	Total	Mg	0	0
			5	5		
60	F	6	Total	Mg	0	0
			6	6		
60	G	2	Total	Mg	0	0
			2	2		
60	H	1	Total	Mg	0	0
			1	1		
60	N	1	Total	Mg	0	0
			1	1		
60	O	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	P	3	Total Mg 3 3	0	0
60	Q	2	Total Mg 2 2	0	0
60	R	2	Total Mg 2 2	0	0
60	U	1	Total Mg 1 1	0	0
60	V	2	Total Mg 2 2	0	0
60	W	1	Total Mg 1 1	0	0
60	X	1	Total Mg 1 1	0	0
60	Z	1	Total Mg 1 1	0	0
60	0	4	Total Mg 4 4	0	0
60	5	2	Total Mg 2 2	0	0
60	6	2	Total Mg 2 2	0	0
60	7	1	Total Mg 1 1	0	0
60	8	1	Total Mg 1 1	0	0
60	9	1	Total Mg 1 1	0	0
60	a	188	Total Mg 188 188	0	0
60	d	1	Total Mg 1 1	0	0
60	e	1	Total Mg 1 1	0	0
60	f	1	Total Mg 1 1	0	0
60	l	1	Total Mg 1 1	0	0
60	m	2	Total Mg 2 2	0	0
60	n	3	Total Mg 3 3	0	0

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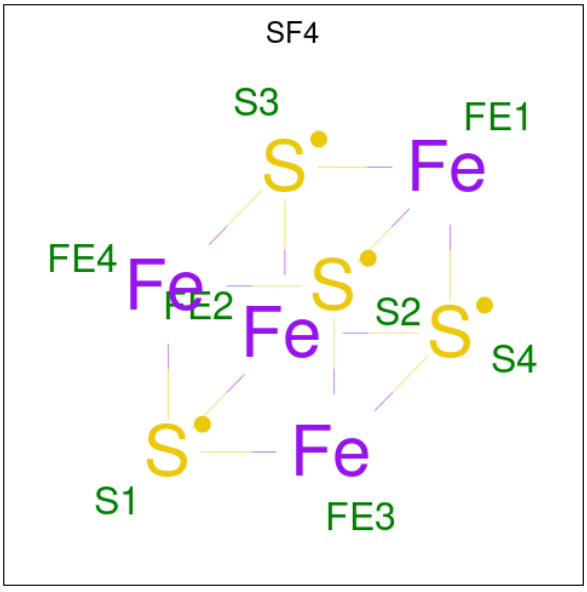
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	v	2	Total Mg 2 2	0	0
60	x	9	Total Mg 9 9	0	0
60	z	2	Total Mg 2 2	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

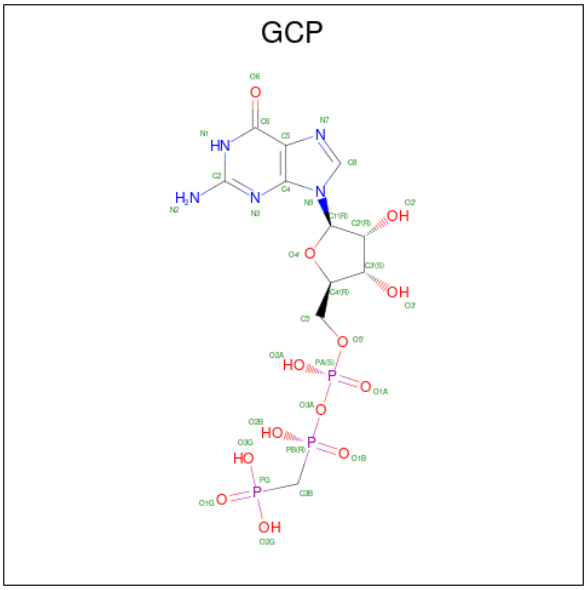
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	Y	1	Total Zn 1 1	0	0
61	4	1	Total Zn 1 1	0	0
61	5	1	Total Zn 1 1	0	0
61	6	1	Total Zn 1 1	0	0
61	9	1	Total Zn 1 1	0	0
61	n	1	Total Zn 1 1	0	0

- Molecule 62 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 63 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	z	1	Total C N O P 32 11 5 13 3	0	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	A	715	Total O 715 715	0	0
64	B	32	Total O 32 32	0	0
64	D	4	Total O 4 4	0	0
64	E	6	Total O 6 6	0	0
64	F	5	Total O 5 5	0	0
64	H	1	Total O 1 1	0	0
64	N	1	Total O 1 1	0	0

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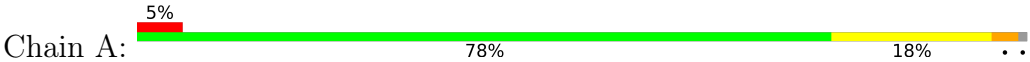
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	O	3	Total O 3 3	0	0
64	P	8	Total O 8 8	0	0
64	Q	3	Total O 3 3	0	0
64	T	2	Total O 2 2	0	0
64	U	3	Total O 3 3	0	0
64	V	1	Total O 1 1	0	0
64	0	3	Total O 3 3	0	0
64	1	1	Total O 1 1	0	0
64	3	1	Total O 1 1	0	0
64	7	1	Total O 1 1	0	0
64	8	4	Total O 4 4	0	0
64	a	165	Total O 165 165	0	0
64	l	1	Total O 1 1	0	0
64	p	1	Total O 1 1	0	0
64	v	3	Total O 3 3	0	0
64	w	1	Total O 1 1	0	0
64	z	1	Total O 1 1	0	0

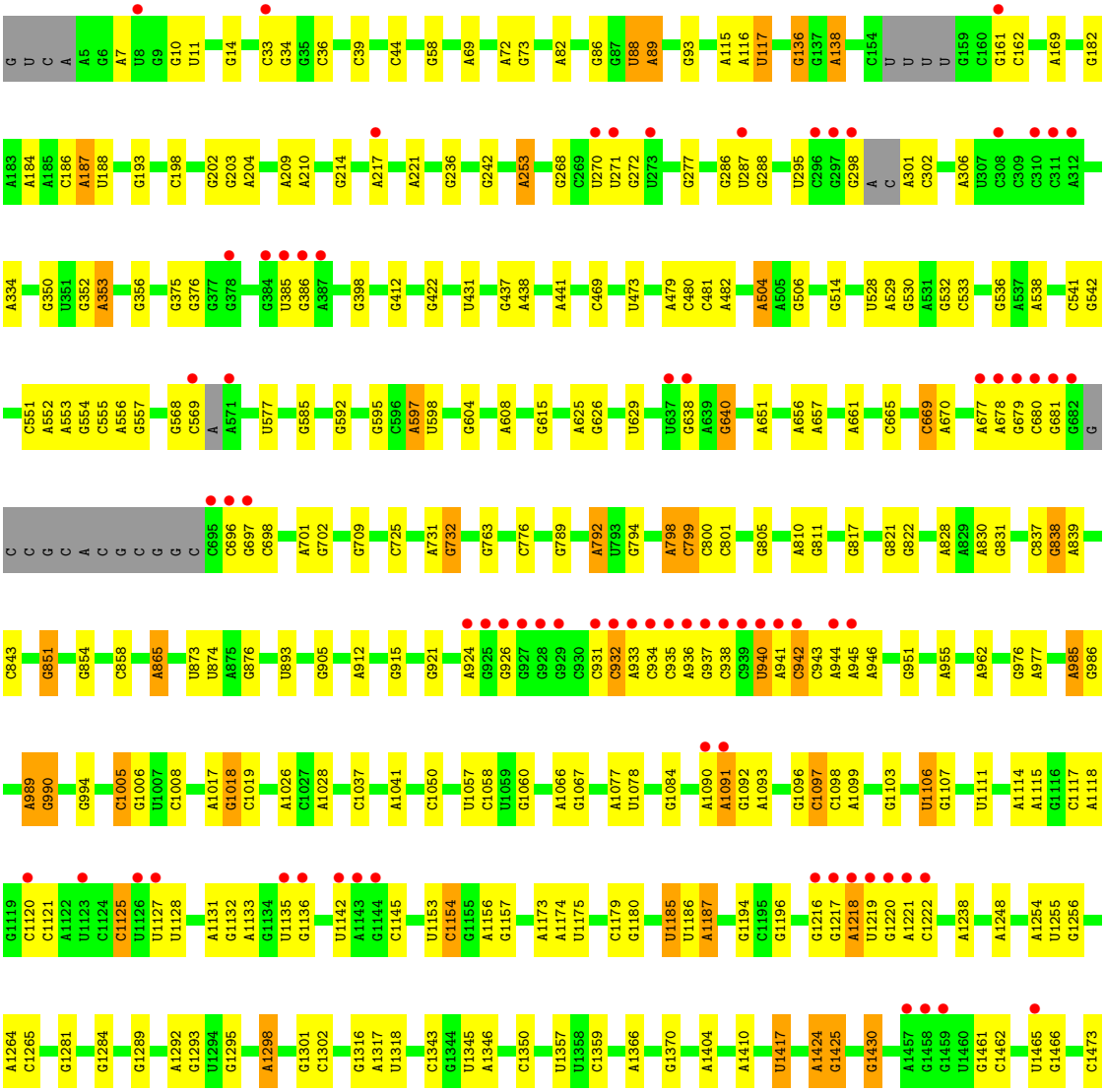
3 Residue-property plots (i)

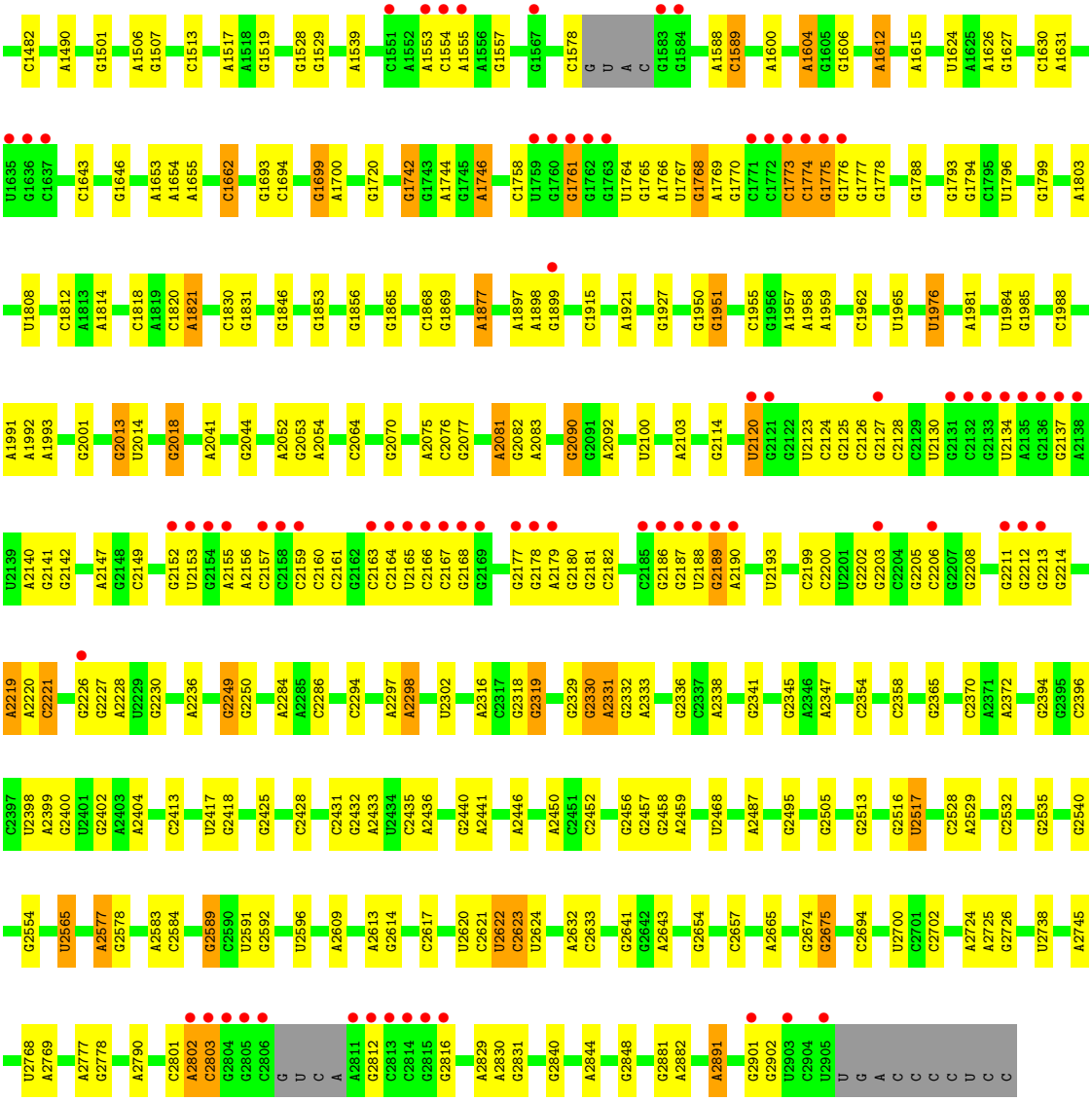
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

Chain A:

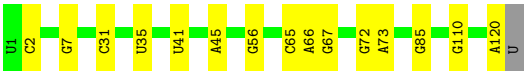






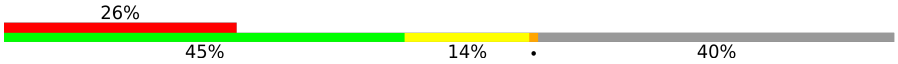
• Molecule 2: 5S Ribosomal RNA

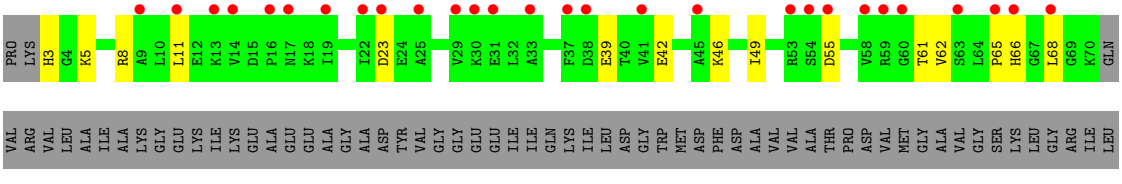
Chain B:

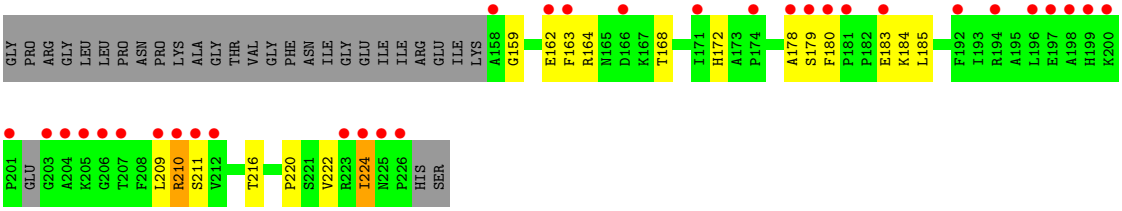


• Molecule 3: 50S ribosomal protein L1

Chain C:

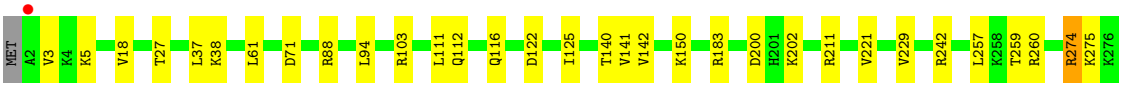






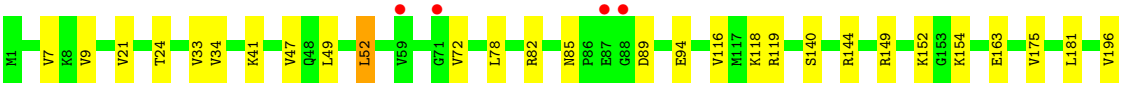
• Molecule 4: 50S ribosomal protein L2

Chain D:



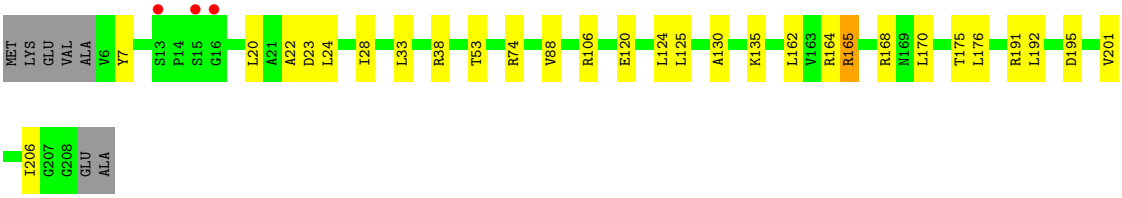
• Molecule 5: 50S ribosomal protein L3

Chain E:



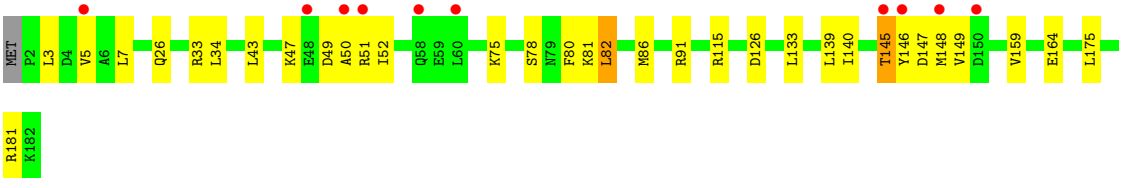
• Molecule 6: 50S ribosomal protein L4

Chain F:



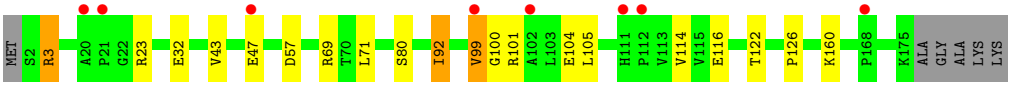
• Molecule 7: 50S ribosomal protein L5

Chain G:

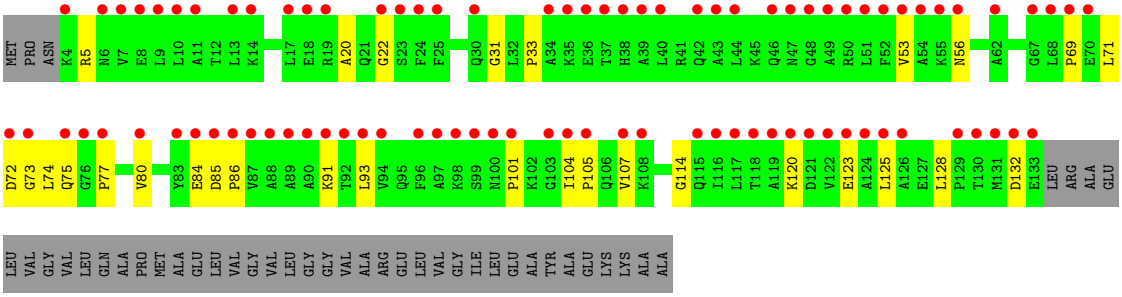


• Molecule 8: 50S ribosomal protein L6

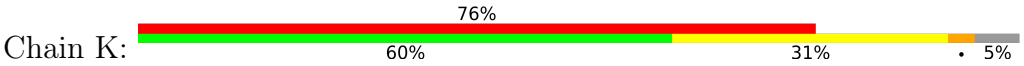
Chain H:

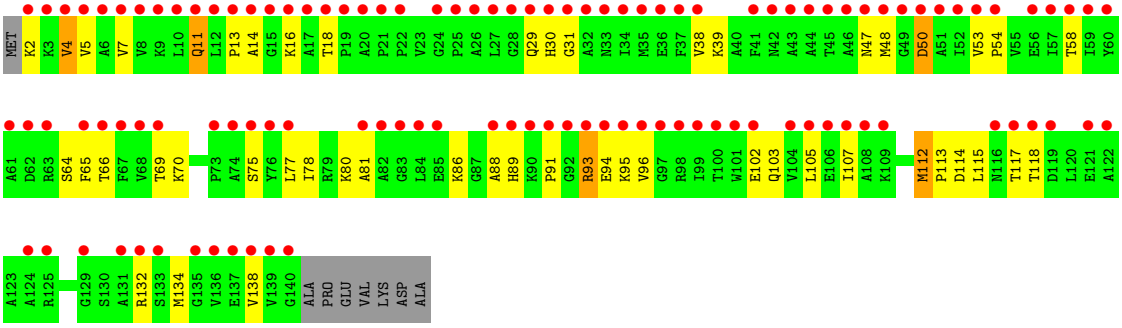


• Molecule 9: 50S ribosomal protein L10

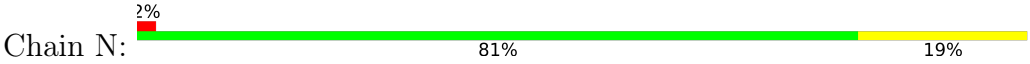


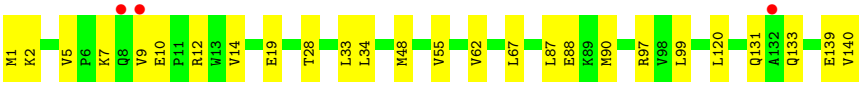
• Molecule 10: 50S ribosomal protein L11



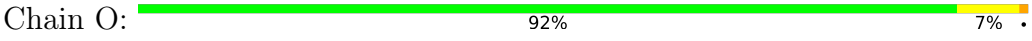


• Molecule 11: 50S ribosomal protein L13

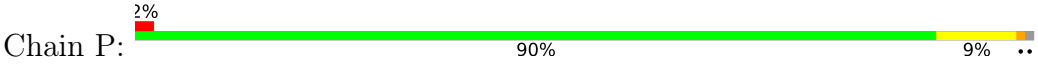


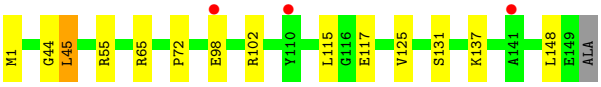


• Molecule 12: 50S ribosomal protein L14

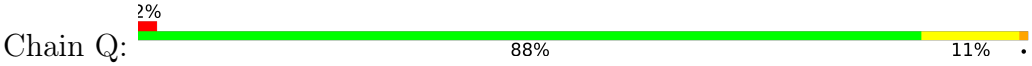


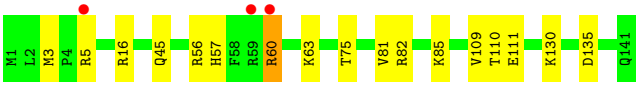
• Molecule 13: 50S ribosomal protein L15



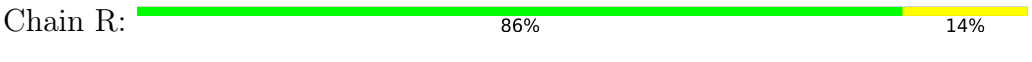


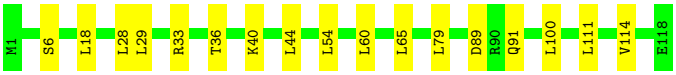
• Molecule 14: 50S ribosomal protein L16



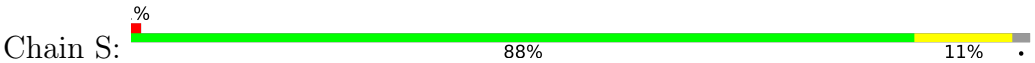


• Molecule 15: 50S ribosomal protein L17

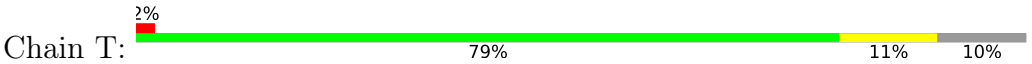


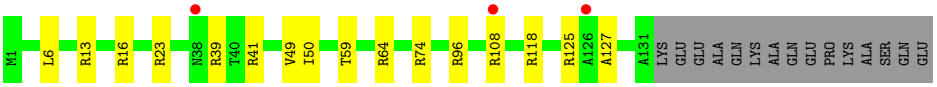


• Molecule 16: 50S ribosomal protein L18

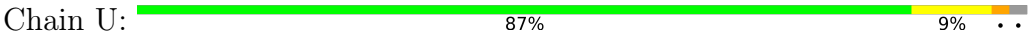


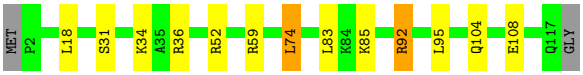
• Molecule 17: 50S ribosomal protein L19



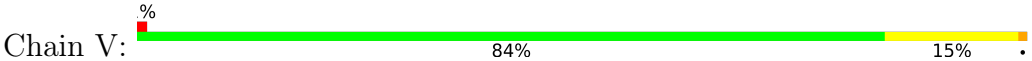


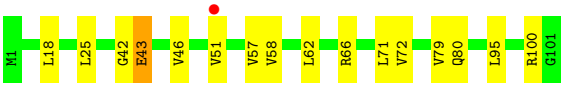
• Molecule 18: 50S ribosomal protein L20





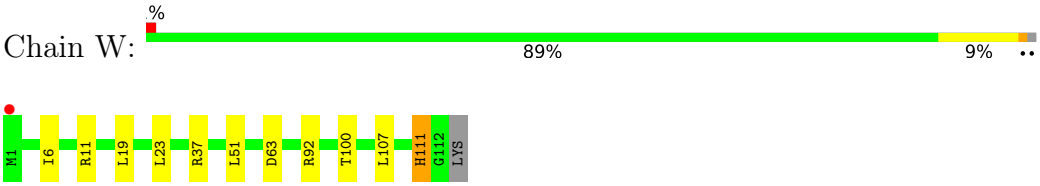
• Molecule 19: 50S ribosomal protein L21





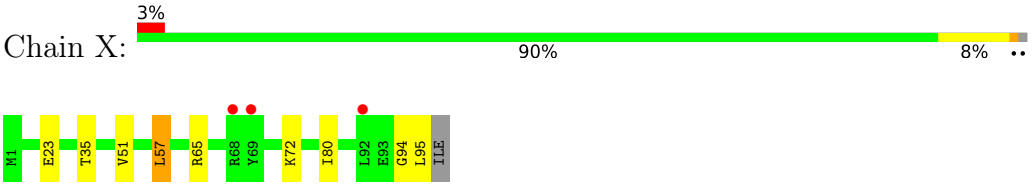
• Molecule 20: 50S ribosomal protein L22

Chain W:



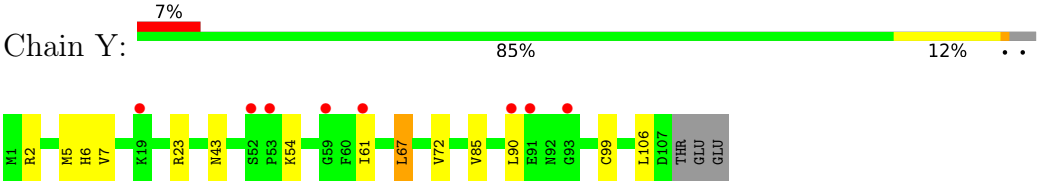
• Molecule 21: 50S ribosomal protein L23

Chain X:



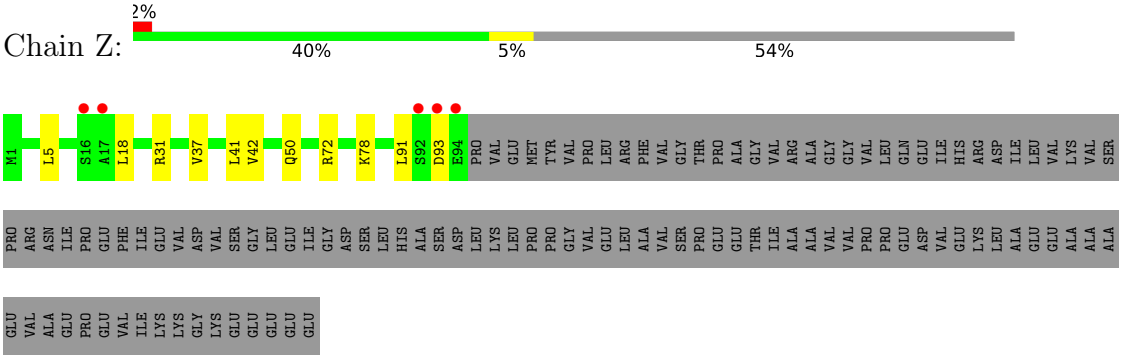
• Molecule 22: 50S ribosomal protein L24

Chain Y:



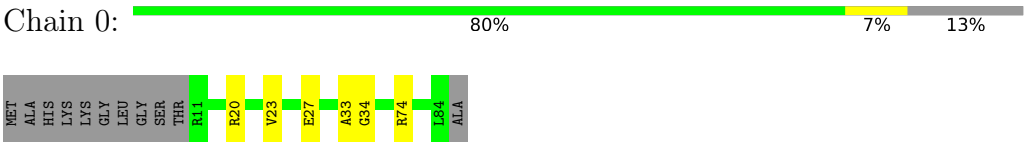
• Molecule 23: 50S ribosomal protein L25

Chain Z:



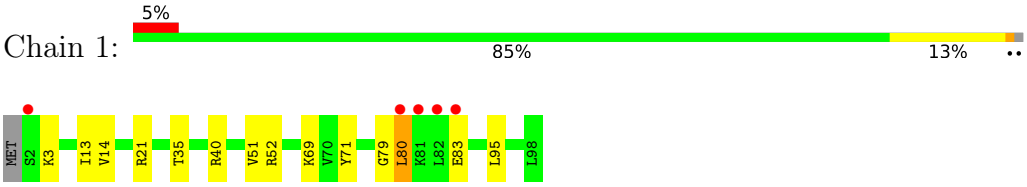
• Molecule 24: 50S ribosomal protein L27

Chain 0:



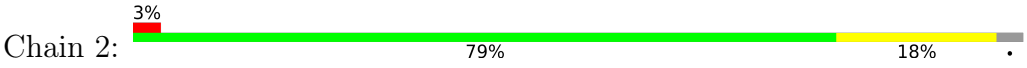
• Molecule 25: 50S ribosomal protein L28

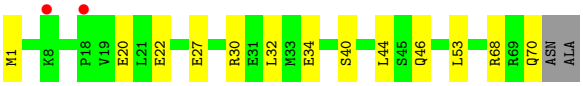
Chain 1:



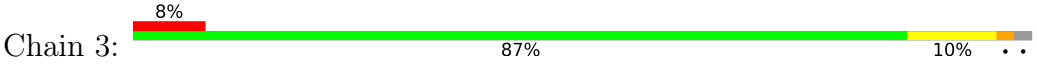
• Molecule 26: 50S ribosomal protein L29

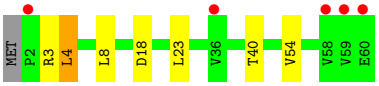
Chain 2:



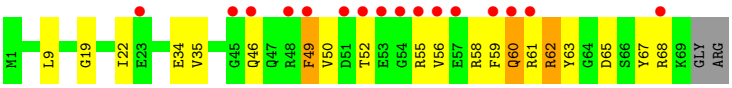


• Molecule 27: 50S ribosomal protein L30

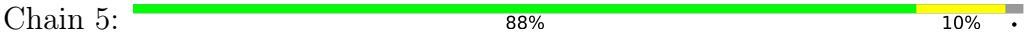


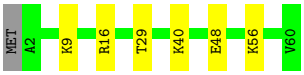


• Molecule 28: 50S ribosomal protein L31

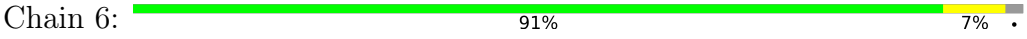


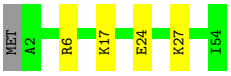
• Molecule 29: 50S ribosomal protein L32



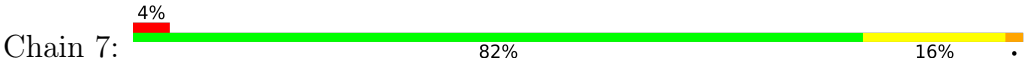


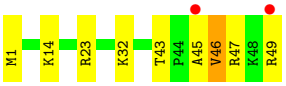
• Molecule 30: 50S ribosomal protein L33



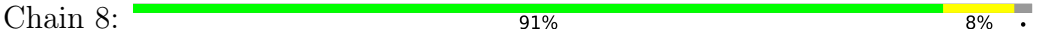


• Molecule 31: 50S ribosomal protein L34

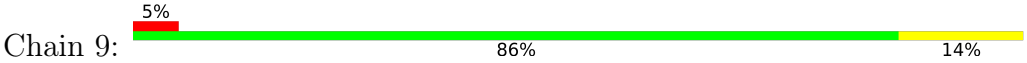


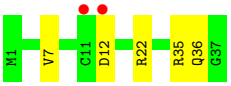


• Molecule 32: 50S ribosomal protein L35



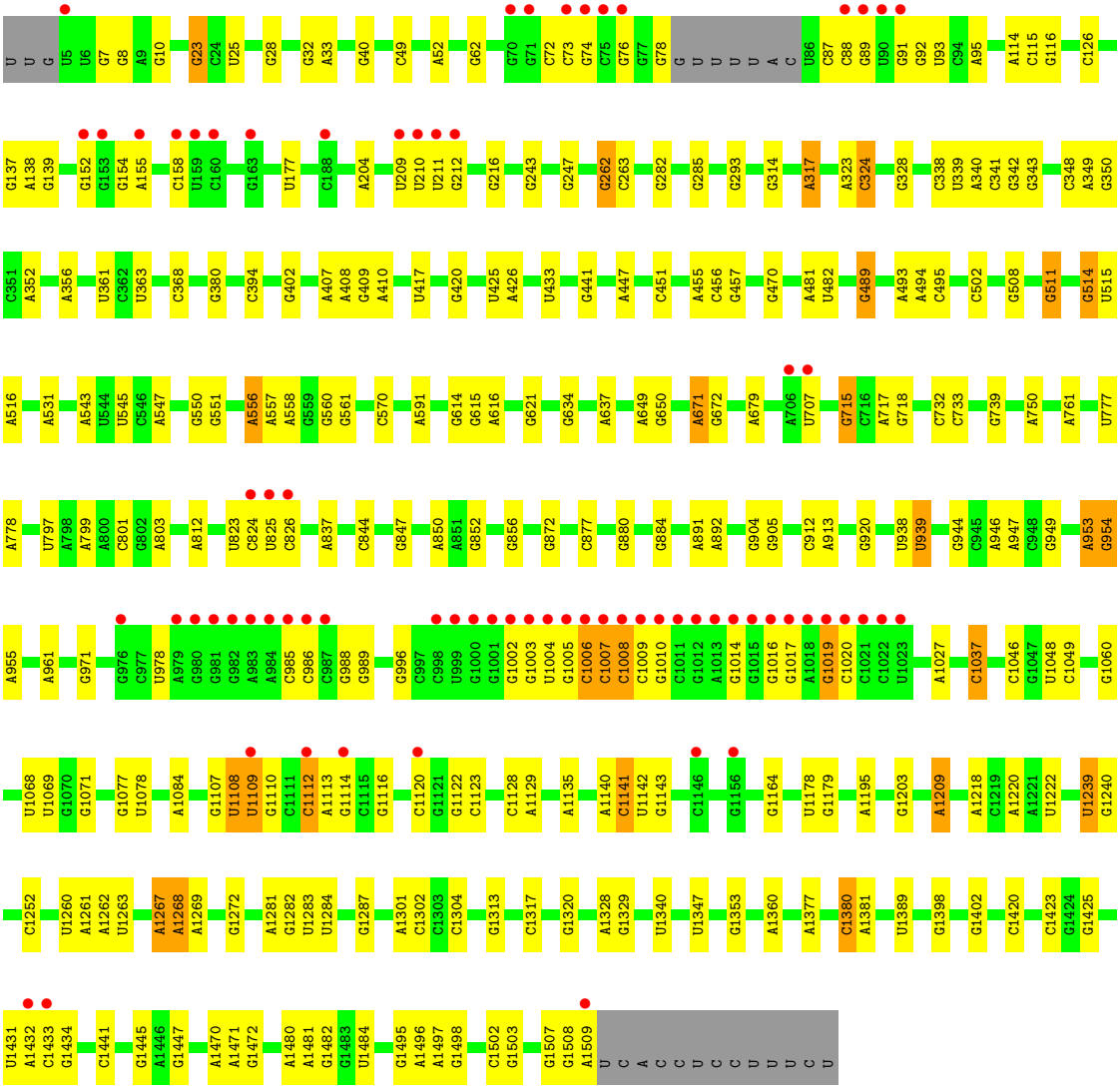
• Molecule 33: 50S ribosomal protein L36





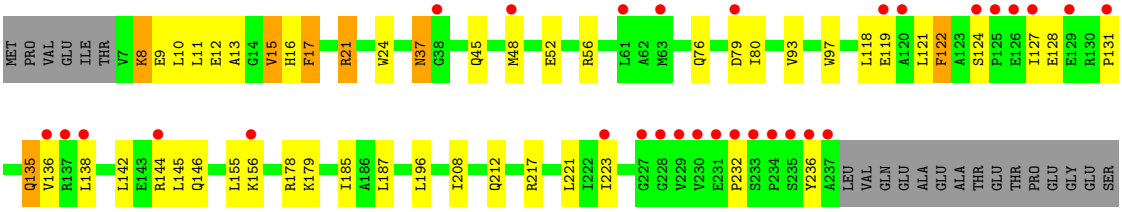
• Molecule 34: 16S Ribosomal RNA

Chain a:



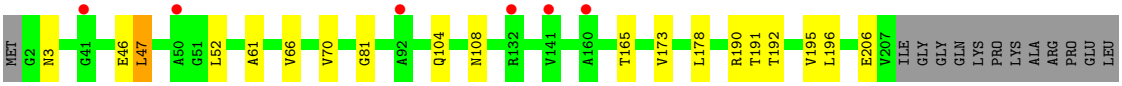
• Molecule 35: 30S ribosomal protein S2

Chain b:



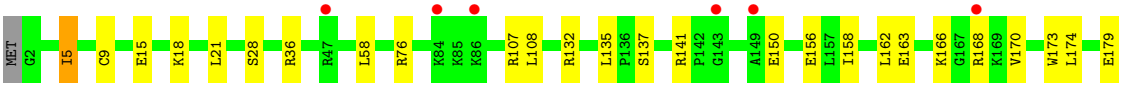
• Molecule 36: 30S ribosomal protein S3

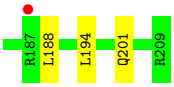
Chain c:



• Molecule 37: 30S ribosomal protein S4

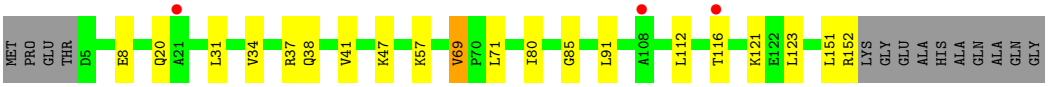
Chain d:





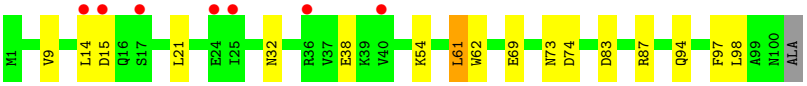
• Molecule 38: 30S ribosomal protein S5

Chain e:



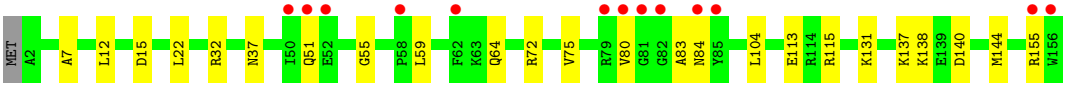
• Molecule 39: 30S ribosomal protein S6

Chain f:



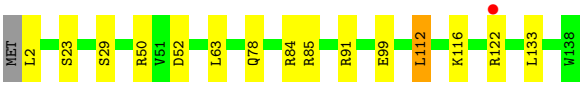
• Molecule 40: 30S ribosomal protein S7

Chain g:

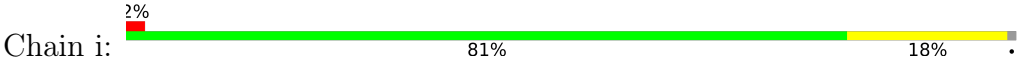


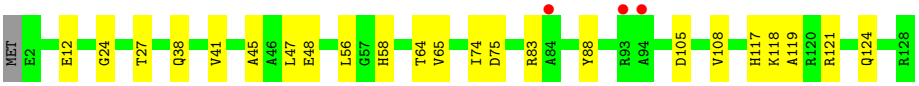
• Molecule 41: 30S ribosomal protein S8

Chain h:



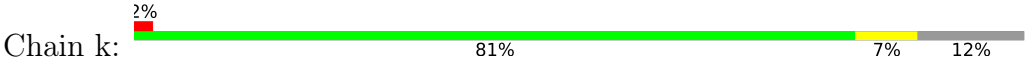
• Molecule 42: 30S ribosomal protein S9

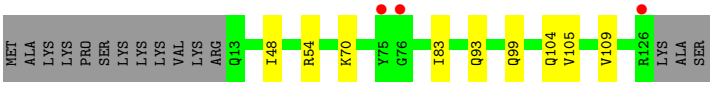




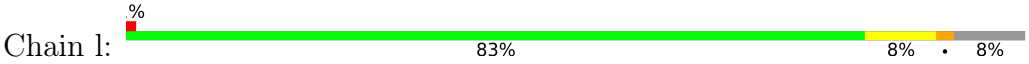
• Molecule 43: 30S ribosomal protein S10

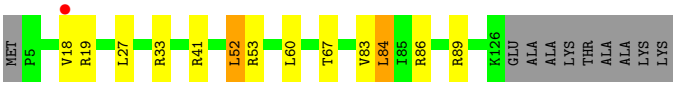
• Molecule 44: 30S ribosomal protein S11



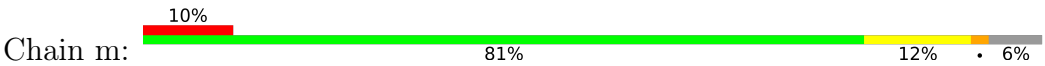


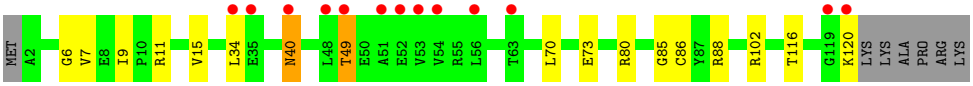
• Molecule 45: 30S ribosomal protein S12



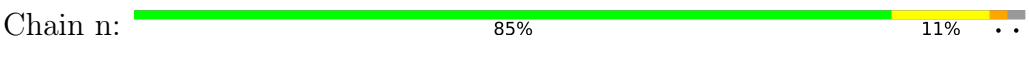


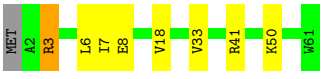
• Molecule 46: 30S ribosomal protein S13





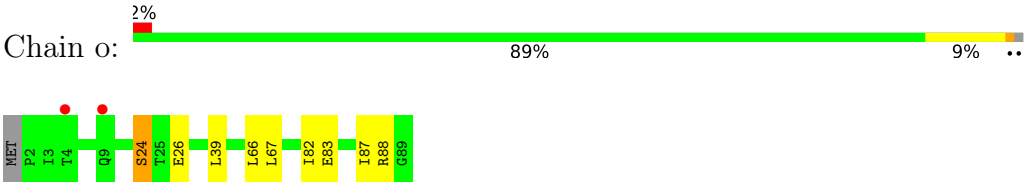
• Molecule 47: 30S ribosomal protein S14 type Z





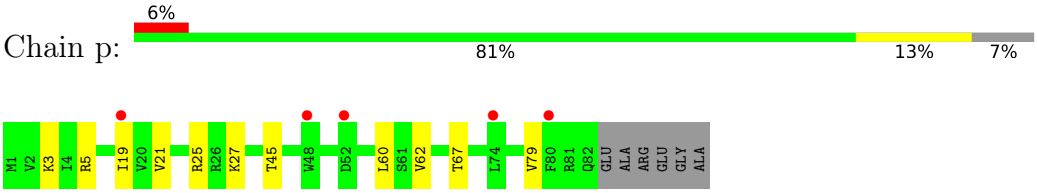
• Molecule 48: 30S ribosomal protein S15

Chain o:



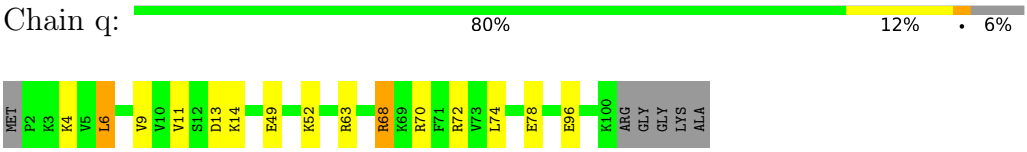
• Molecule 49: 30S ribosomal protein S16

Chain p:



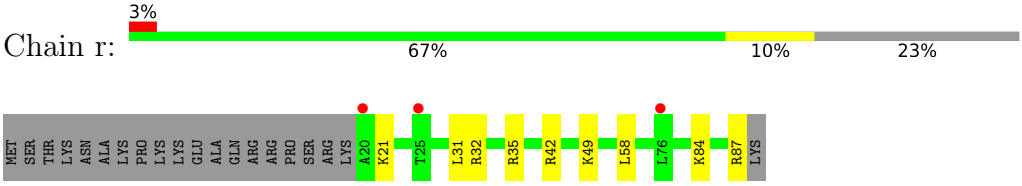
• Molecule 50: 30S ribosomal protein S17

Chain q:



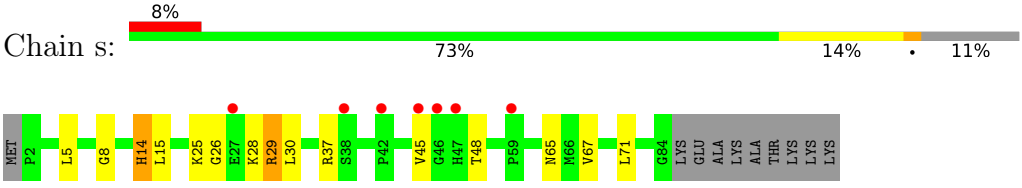
• Molecule 51: 30S ribosomal protein S18

Chain r:



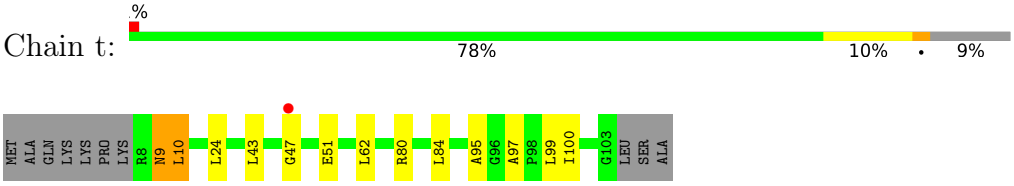
• Molecule 52: 30S ribosomal protein S19

Chain s:



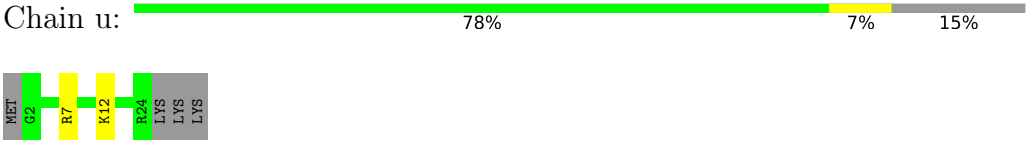
• Molecule 53: 30S ribosomal protein S20

Chain t:



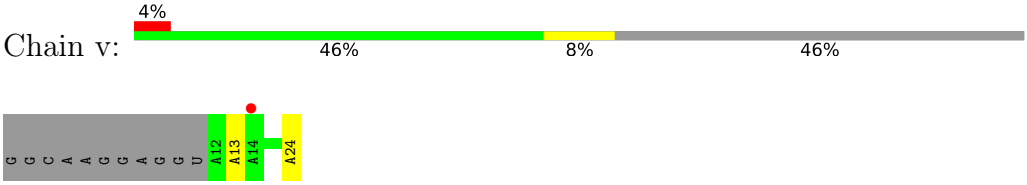
• Molecule 54: 30S ribosomal protein Thx

Chain u:



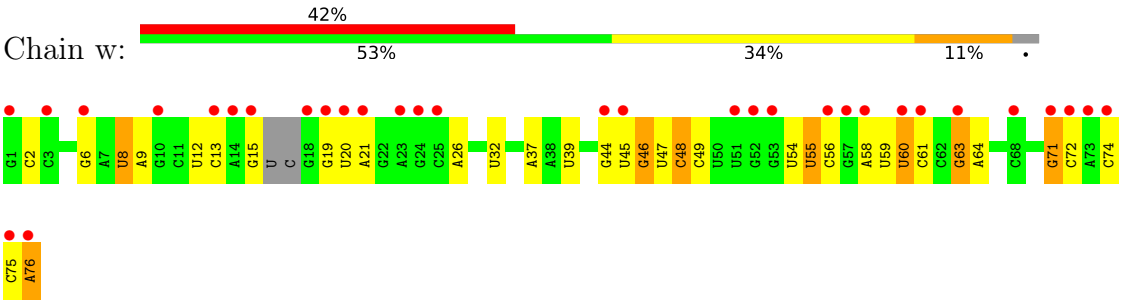
• Molecule 55: mRNA

Chain v:



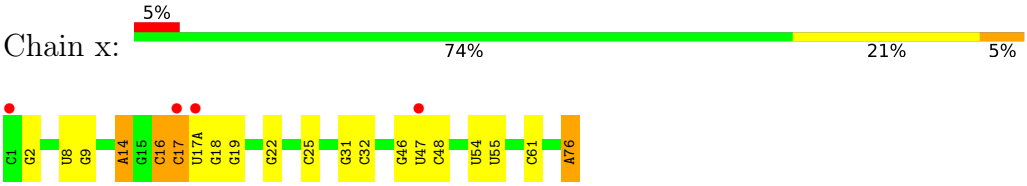
• Molecule 56: A-site tRNA

Chain w:



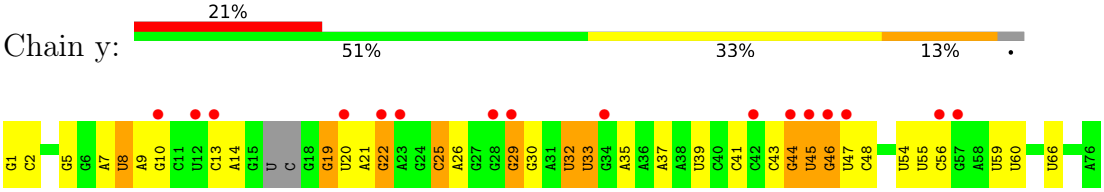
• Molecule 57: P-site tRNA

Chain x:



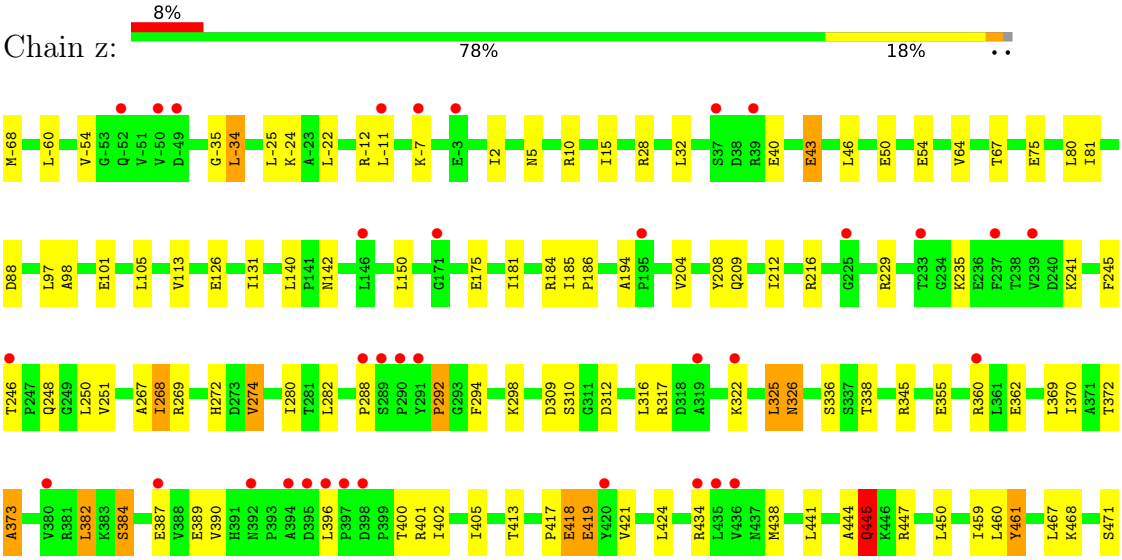
• Molecule 58: E-site tRNA

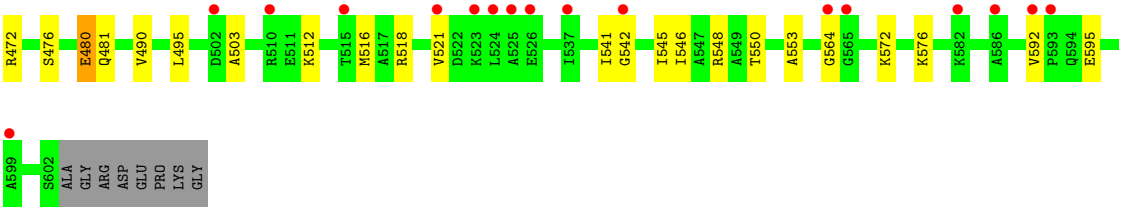
Chain y:



• Molecule 59: GDPCP fused to the N-terminus of the ribosomal protein L9,Elongation factor 4

Chain z:




R472
S476
E480
Q481
V490
L495
D502
A503
R510
E511
K512
T515
M516
A517
R518
V521
D522
K523
L524
A525
E526
I537
I541
G542
I545
I546
A547
R548
A549
T550
A553
G564
G565
K572
K576
K582
A586
V592
P593
Q594
E595
A599
S602
ALA
GLY
ARG
ASP
GLU
PRO
LYS
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	213.12Å 271.72Å 436.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.60 49.52 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.52-2.60) 98.7 (49.52-2.59)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, R_{free}	0.192 , 0.261 0.192 , 0.261	Depositor DCC
R_{free} test set	38580 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	155465	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GCP, 5MC, SF4, 5MU, MG, MIA, PSU, 4SU, 7MG, ZN

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	0.69	11/69327 (0.0%)	1.23	339/108217 (0.3%)
2	B	0.51	0/2878	1.00	1/4490 (0.0%)
3	C	0.36	0/1044	0.66	1/1413 (0.1%)
4	D	0.50	0/2186	0.73	1/2944 (0.0%)
5	E	0.45	0/1592	0.69	0/2149
6	F	0.46	0/1619	0.62	0/2193
7	G	0.38	0/1450	0.64	1/1959 (0.1%)
8	H	0.42	0/1356	0.63	0/1834
9	J	0.32	0/640	0.55	0/889
10	K	0.43	0/1044	0.65	1/1416 (0.1%)
11	N	0.41	0/1144	0.63	0/1543
12	O	0.49	0/943	0.68	1/1269 (0.1%)
13	P	0.47	0/1152	0.74	1/1533 (0.1%)
14	Q	0.46	0/1143	0.58	0/1527
15	R	0.38	0/982	0.66	0/1312
16	S	0.40	0/887	0.63	0/1180
17	T	0.43	0/1105	0.65	0/1477
18	U	0.46	0/977	0.69	2/1301 (0.2%)
19	V	0.48	0/782	0.68	1/1049 (0.1%)
20	W	0.46	0/897	0.63	0/1205
21	X	0.43	0/764	0.65	1/1025 (0.1%)
22	Y	0.43	0/819	0.66	1/1095 (0.1%)
23	Z	0.38	0/801	0.59	0/1079
24	0	0.43	0/599	0.64	0/798
25	1	0.52	0/762	0.74	1/1014 (0.1%)
26	2	0.38	0/590	0.58	0/781
27	3	0.38	0/474	0.69	1/635 (0.2%)
28	4	0.40	0/570	0.64	0/768
29	5	0.44	0/473	0.71	0/639
30	6	0.46	0/460	0.64	0/613
31	7	0.46	0/438	0.71	0/575
32	8	0.47	0/519	0.67	0/684

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	9	0.49	0/310	0.73	0/407
34	a	0.62	2/36053 (0.0%)	1.14	114/56270 (0.2%)
35	b	0.37	0/1885	0.61	0/2547
36	c	0.41	1/1574 (0.1%)	0.58	0/2127
37	d	0.38	0/1685	0.58	0/2262
38	e	0.42	0/1145	0.65	0/1543
39	f	0.39	0/819	0.57	0/1111
40	g	0.37	0/1246	0.54	0/1674
41	h	0.39	0/1108	0.64	1/1494 (0.1%)
42	i	0.39	0/1002	0.61	0/1346
43	j	0.38	0/711	0.55	0/968
44	k	0.38	0/844	0.60	0/1145
45	l	0.48	0/946	0.76	2/1274 (0.2%)
46	m	0.38	0/934	0.70	0/1256
47	n	0.46	0/501	0.65	0/664
48	o	0.39	0/739	0.61	0/985
49	p	0.37	0/697	0.65	0/939
50	q	0.44	0/836	0.68	1/1117 (0.1%)
51	r	0.38	0/560	0.62	0/746
52	s	0.35	0/665	0.68	0/897
53	t	0.39	0/726	0.64	0/961
54	u	0.44	0/203	0.64	0/266
55	v	0.71	0/310	1.31	3/480 (0.6%)
56	w	0.67	3/1602 (0.2%)	1.69	31/2493 (1.2%)
57	x	0.76	4/1747 (0.2%)	1.48	32/2723 (1.2%)
58	y	0.62	0/1628	1.49	31/2534 (1.2%)
59	z	0.40	0/5296	0.65	4/7179 (0.1%)
All	All	0.60	21/166189 (0.0%)	1.08	572/248014 (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
10	K	0	1
19	V	0	1
26	2	0	1
28	4	0	1
37	d	0	1
39	f	0	1
42	i	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
52	s	0	2
53	t	0	1
59	z	0	6
All	All	0	17

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	71	G	C6-N1	-10.59	1.32	1.39
56	w	71	G	N1-C2	-10.38	1.29	1.37
57	x	14	A	N7-C5	-8.86	1.33	1.39
1	A	353	A	N9-C4	-7.12	1.33	1.37
1	A	1091	A	C5-C6	-7.12	1.34	1.41

The worst 5 of 572 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	w	71	G	N3-C2-N2	23.02	136.02	119.90
56	w	71	G	C5-C6-O6	22.98	142.39	128.60
56	w	2	C	N1-C2-O2	21.56	131.84	118.90
56	w	71	G	N1-C2-N2	-21.15	97.16	116.20
1	A	1091	A	N9-C4-C5	-17.30	98.88	105.80

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	2	44	LEU	Peptide
28	4	65	ASP	Peptide
10	K	70	LYS	Peptide
19	V	43	GLU	Peptide
37	d	179	GLU	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	130/228 (57%)	94 (72%)	25 (19%)	11 (8%)	1 1
4	D	273/276 (99%)	255 (93%)	15 (6%)	3 (1%)	14 30
5	E	202/206 (98%)	188 (93%)	11 (5%)	3 (2%)	10 21
6	F	201/210 (96%)	184 (92%)	12 (6%)	5 (2%)	5 9
7	G	179/182 (98%)	162 (90%)	10 (6%)	7 (4%)	3 4
8	H	172/180 (96%)	148 (86%)	17 (10%)	7 (4%)	3 3
9	J	128/173 (74%)	76 (59%)	22 (17%)	30 (23%)	0 0
10	K	137/147 (93%)	85 (62%)	31 (23%)	21 (15%)	0 0
11	N	138/140 (99%)	129 (94%)	5 (4%)	4 (3%)	4 7
12	O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19 39
13	P	147/150 (98%)	129 (88%)	16 (11%)	2 (1%)	11 22
14	Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22 43
15	R	116/118 (98%)	111 (96%)	5 (4%)	0	100 100
16	S	108/112 (96%)	96 (89%)	10 (9%)	2 (2%)	8 15
17	T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	19 39
18	U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
19	V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	7 14
20	W	110/113 (97%)	105 (96%)	5 (4%)	0	100 100
21	X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14 30
22	Y	105/110 (96%)	89 (85%)	12 (11%)	4 (4%)	3 4
23	Z	92/206 (45%)	84 (91%)	8 (9%)	0	100 100
24	0	72/85 (85%)	67 (93%)	3 (4%)	2 (3%)	5 7
25	1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	4 6
26	2	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	10 21
27	3	57/60 (95%)	52 (91%)	5 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	4	67/71 (94%)	45 (67%)	15 (22%)	7 (10%)	0 0
29	5	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
30	6	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
31	7	47/49 (96%)	44 (94%)	1 (2%)	2 (4%)	2 3
32	8	62/65 (95%)	61 (98%)	1 (2%)	0	100 100
33	9	35/37 (95%)	35 (100%)	0	0	100 100
35	b	229/256 (90%)	192 (84%)	23 (10%)	14 (6%)	1 1
36	c	204/239 (85%)	177 (87%)	20 (10%)	7 (3%)	3 5
37	d	206/209 (99%)	187 (91%)	16 (8%)	3 (2%)	10 21
38	e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	7 13
39	f	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	4 6
40	g	153/156 (98%)	135 (88%)	13 (8%)	5 (3%)	4 6
41	h	135/138 (98%)	130 (96%)	5 (4%)	0	100 100
42	i	125/128 (98%)	113 (90%)	5 (4%)	7 (6%)	2 2
43	j	94/105 (90%)	79 (84%)	6 (6%)	9 (10%)	0 0
44	k	112/129 (87%)	107 (96%)	4 (4%)	1 (1%)	17 35
45	l	120/132 (91%)	112 (93%)	7 (6%)	1 (1%)	19 39
46	m	117/126 (93%)	102 (87%)	9 (8%)	6 (5%)	2 2
47	n	58/61 (95%)	57 (98%)	0	1 (2%)	9 18
48	o	86/89 (97%)	78 (91%)	5 (6%)	3 (4%)	3 5
49	p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	12 24
50	q	97/105 (92%)	86 (89%)	8 (8%)	3 (3%)	4 6
51	r	66/88 (75%)	60 (91%)	6 (9%)	0	100 100
52	s	81/93 (87%)	72 (89%)	4 (5%)	5 (6%)	1 1
53	t	94/106 (89%)	84 (89%)	4 (4%)	6 (6%)	1 1
54	u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
59	z	669/679 (98%)	568 (85%)	62 (9%)	39 (6%)	1 1
All	All	6534/7143 (92%)	5800 (89%)	497 (8%)	237 (4%)	3 4

5 of 237 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	65	PRO

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Mol	Chain	Res	Type
3	C	172	HIS
3	C	224	ILE
4	D	275	LYS
6	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	C	103/180 (57%)	79 (77%)	24 (23%)	1 1
4	D	215/218 (99%)	186 (86%)	29 (14%)	4 6
5	E	164/166 (99%)	138 (84%)	26 (16%)	2 4
6	F	160/166 (96%)	135 (84%)	25 (16%)	2 4
7	G	143/156 (92%)	116 (81%)	27 (19%)	1 2
8	H	144/148 (97%)	128 (89%)	16 (11%)	6 11
10	K	104/111 (94%)	71 (68%)	33 (32%)	0 0
11	N	118/119 (99%)	96 (81%)	22 (19%)	1 2
12	O	100/100 (100%)	91 (91%)	9 (9%)	9 18
13	P	115/116 (99%)	103 (90%)	12 (10%)	7 13
14	Q	111/111 (100%)	94 (85%)	17 (15%)	2 4
15	R	101/101 (100%)	84 (83%)	17 (17%)	2 3
16	S	87/88 (99%)	77 (88%)	10 (12%)	5 10
17	T	115/127 (91%)	100 (87%)	15 (13%)	4 7
18	U	93/94 (99%)	80 (86%)	13 (14%)	3 6
19	V	80/82 (98%)	67 (84%)	13 (16%)	2 3
20	W	90/92 (98%)	79 (88%)	11 (12%)	5 9
21	X	77/78 (99%)	69 (90%)	8 (10%)	7 13
22	Y	85/91 (93%)	75 (88%)	10 (12%)	5 9
23	Z	84/179 (47%)	73 (87%)	11 (13%)	4 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	0	59/67 (88%)	55 (93%)	4 (7%)	16 32
25	1	80/83 (96%)	69 (86%)	11 (14%)	3 6
26	2	65/67 (97%)	54 (83%)	11 (17%)	2 3
27	3	51/52 (98%)	44 (86%)	7 (14%)	3 6
28	4	60/63 (95%)	45 (75%)	15 (25%)	0 1
29	5	51/52 (98%)	45 (88%)	6 (12%)	5 9
30	6	51/52 (98%)	47 (92%)	4 (8%)	12 25
31	7	42/42 (100%)	34 (81%)	8 (19%)	1 2
32	8	53/55 (96%)	48 (91%)	5 (9%)	8 17
33	9	34/34 (100%)	29 (85%)	5 (15%)	3 5
35	b	193/220 (88%)	150 (78%)	43 (22%)	1 1
36	c	142/188 (76%)	130 (92%)	12 (8%)	10 21
37	d	169/181 (93%)	143 (85%)	26 (15%)	2 4
38	e	113/123 (92%)	95 (84%)	18 (16%)	2 4
39	f	83/90 (92%)	69 (83%)	14 (17%)	2 3
40	g	118/127 (93%)	99 (84%)	19 (16%)	2 4
41	h	114/119 (96%)	99 (87%)	15 (13%)	4 7
42	i	90/99 (91%)	76 (84%)	14 (16%)	2 4
43	j	65/92 (71%)	53 (82%)	12 (18%)	1 2
44	k	82/99 (83%)	74 (90%)	8 (10%)	8 15
45	l	97/109 (89%)	85 (88%)	12 (12%)	4 8
46	m	89/101 (88%)	76 (85%)	13 (15%)	3 5
47	n	49/50 (98%)	41 (84%)	8 (16%)	2 3
48	o	78/80 (98%)	71 (91%)	7 (9%)	9 18
49	p	69/74 (93%)	59 (86%)	10 (14%)	3 5
50	q	94/97 (97%)	81 (86%)	13 (14%)	3 6
51	r	59/77 (77%)	50 (85%)	9 (15%)	2 4
52	s	68/80 (85%)	58 (85%)	10 (15%)	3 5
53	t	69/82 (84%)	61 (88%)	8 (12%)	5 10
54	u	18/22 (82%)	16 (89%)	2 (11%)	6 11
59	z	542/560 (97%)	436 (80%)	106 (20%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5236/5760 (91%)	4433 (85%)	803 (15%)	2 4

5 of 803 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	b	212	GLN
42	i	41	VAL
59	z	572	LYS
36	c	192	THR
35	b	208	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
44	k	93	GLN
59	z	275	GLN
46	m	40	ASN
52	s	83	HIS
59	z	538	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2868/2915 (98%)	464 (16%)	42 (1%)
2	B	119/121 (98%)	14 (11%)	0
34	a	1496/1521 (98%)	243 (16%)	0
55	v	12/24 (50%)	1 (8%)	0
56	w	71/76 (93%)	26 (36%)	0
57	x	76/77 (98%)	13 (17%)	0
58	y	71/76 (93%)	28 (39%)	0
All	All	4713/4810 (97%)	789 (16%)	42 (0%)

5 of 789 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	10	G
1	A	14	G
1	A	34	G
1	A	44	C

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1699	G
1	A	2417	U
1	A	2013	G
1	A	2202	G
1	A	2433	A

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

17 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	$\#\|Z\| > 2$
58	PSU	y	39	58	18,21,22	1.47	2 (11%)	22,30,33	1.80	5 (22%)
56	MIA	w	37	56	24,29,32	2.20	3 (12%)	25,41,47	2.83	10 (40%)
56	5MU	w	54	56	19,22,23	1.40	4 (21%)	28,32,35	1.80	7 (25%)
57	PSU	x	55	57	18,21,22	1.42	3 (16%)	22,30,33	1.84	5 (22%)
58	MIA	y	37	58,34	18,24,32	1.26	2 (11%)	18,35,47	1.25	2 (11%)
57	5MU	x	54	60,57	19,22,23	1.30	4 (21%)	28,32,35	2.11	6 (21%)
56	PSU	w	55	56	18,21,22	1.34	2 (11%)	22,30,33	1.76	4 (18%)
56	7MG	w	46	56	22,26,27	1.40	5 (22%)	29,39,42	2.40	7 (24%)
58	4SU	y	8	58	18,21,22	4.60	7 (38%)	26,30,33	11.78	8 (30%)
57	4SU	x	8	57	18,21,22	2.11	6 (33%)	26,30,33	2.02	5 (19%)
56	PSU	w	32	56	18,21,22	1.43	2 (11%)	22,30,33	1.87	5 (22%)
58	PSU	y	32	58	18,21,22	1.40	3 (16%)	22,30,33	1.80	3 (13%)
58	PSU	y	55	58	18,21,22	1.39	2 (11%)	22,30,33	1.89	4 (18%)
57	5MC	x	32	57	18,22,23	0.98	2 (11%)	26,32,35	1.15	2 (7%)
56	4SU	w	8	56	18,21,22	1.81	5 (27%)	26,30,33	1.95	5 (19%)
56	PSU	w	39	56	18,21,22	1.29	2 (11%)	22,30,33	1.90	5 (22%)
58	5MU	y	54	58	19,22,23	1.44	6 (31%)	28,32,35	1.97	8 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PSU	y	39	58	-	0/7/25/26	0/2/2/2
56	MIA	w	37	56	-	6/10/31/34	0/3/3/3
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
57	PSU	x	55	57	-	0/7/25/26	0/2/2/2
58	MIA	y	37	58,34	-	2/3/25/34	0/3/3/3
57	5MU	x	54	60,57	-	0/7/25/26	0/2/2/2
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
56	7MG	w	46	56	-	3/7/37/38	0/3/3/3
58	4SU	y	8	58	-	2/7/25/26	0/2/2/2
57	4SU	x	8	57	-	0/7/25/26	0/2/2/2
56	PSU	w	32	56	-	0/7/25/26	0/2/2/2
58	PSU	y	32	58	-	4/7/25/26	0/2/2/2
58	PSU	y	55	58	-	0/7/25/26	0/2/2/2
57	5MC	x	32	57	-	0/7/25/26	0/2/2/2
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	0/7/25/26	0/2/2/2
58	5MU	y	54	58	-	0/7/25/26	0/2/2/2

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	8	4SU	O2-C2	-12.52	1.00	1.23
58	y	8	4SU	C4-N3	10.94	1.49	1.37
56	w	37	MIA	C2-S10	-7.24	1.69	1.75
56	w	37	MIA	C13-C14	6.90	1.52	1.32
57	x	8	4SU	C4-N3	-5.80	1.31	1.37

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	y	8	4SU	O2-C2-N1	-40.28	69.25	122.79
58	y	8	4SU	O2-C2-N3	-39.78	47.40	121.50
58	y	8	4SU	C6-C5-C4	-12.81	108.86	119.95
58	y	8	4SU	C5-C4-N3	11.26	125.13	114.69
56	w	46	7MG	N9-C4-N3	8.37	137.99	125.47

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	w	37	MIA	C5-C6-N6-C12
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
58	y	32	PSU	C2'-C1'-C5-C4
58	y	32	PSU	C2'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 927 ligands modelled in this entry, 925 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
62	SF4	d	302	37	0,12,12	-	-	-		
63	GCP	z	703	60	27,34,34	2.08	7 (25%)	34,54,54	1.93	8 (23%)

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
62	SF4	d	302	37	-	-	0/6/5/5
63	GCP	z	703	60	-	9/15/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	703	GCP	PB-O2B	-6.34	1.41	1.56
63	z	703	GCP	PG-O3G	-4.32	1.45	1.54
63	z	703	GCP	C2'-C1'	-2.97	1.49	1.53
63	z	703	GCP	PB-O1B	2.77	1.58	1.51
63	z	703	GCP	C5-C6	2.73	1.46	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	z	703	GCP	C2-N3-C4	5.03	121.10	115.36
63	z	703	GCP	C4-C5-C6	-3.70	117.27	120.80
63	z	703	GCP	C2-N1-C6	3.44	121.40	115.93
63	z	703	GCP	C5-C6-N1	-3.24	119.00	123.43
63	z	703	GCP	N3-C2-N1	-3.14	123.04	127.22

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

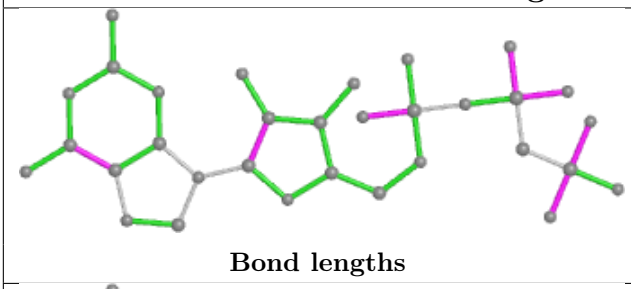
Mol	Chain	Res	Type	Atoms
63	z	703	GCP	PB-C3B-PG-O1G
63	z	703	GCP	PB-C3B-PG-O2G
63	z	703	GCP	PG-C3B-PB-O1B
63	z	703	GCP	C5'-O5'-PA-O3A
63	z	703	GCP	O4'-C4'-C5'-O5'

There are no ring outliers.

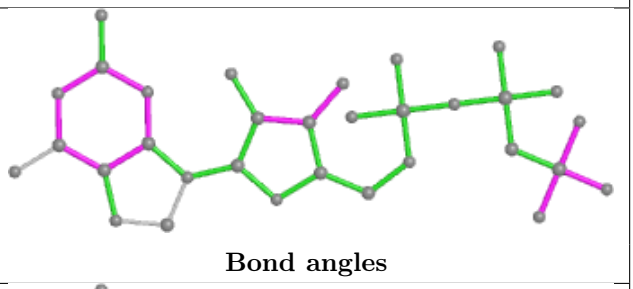
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

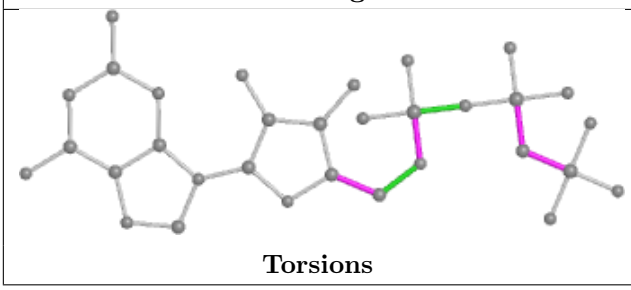
Ligand GCP z 703



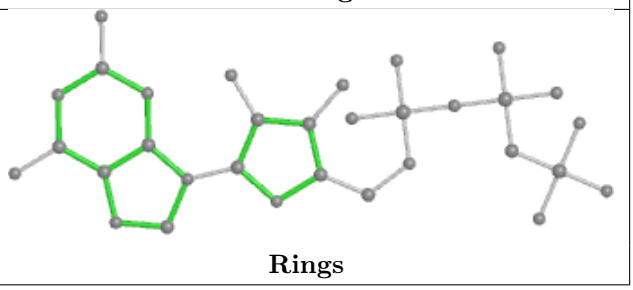
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	2874/2915 (98%)	0.19	151 (5%) 26 20	22, 39, 92, 112	465 (16%)
2	B	120/121 (99%)	0.15	0 100 100	36, 57, 73, 93	18 (15%)
3	C	136/228 (59%)	2.05	60 (44%) 0 0	72, 89, 95, 97	104 (76%)
4	D	275/276 (99%)	-0.01	1 (0%) 92 91	18, 37, 49, 69	42 (15%)
5	E	204/206 (99%)	0.18	5 (2%) 57 51	20, 41, 63, 76	38 (18%)
6	F	203/210 (96%)	0.09	3 (1%) 73 70	22, 50, 75, 90	31 (15%)
7	G	181/182 (99%)	0.35	10 (5%) 25 19	42, 58, 78, 84	38 (20%)
8	H	174/180 (96%)	0.30	8 (4%) 32 26	39, 54, 70, 73	30 (17%)
9	J	130/173 (75%)	3.73	89 (68%) 0 0	84, 138, 186, 214	10 (7%)
10	K	139/147 (94%)	4.74	112 (80%) 0 0	93, 102, 107, 110	115 (82%)
11	N	140/140 (100%)	0.07	3 (2%) 63 58	26, 43, 65, 83	27 (19%)
12	O	122/122 (100%)	-0.06	0 100 100	27, 39, 50, 65	7 (5%)
13	P	149/150 (99%)	0.20	3 (2%) 65 60	21, 48, 65, 83	38 (25%)
14	Q	141/141 (100%)	-0.03	3 (2%) 63 58	27, 42, 59, 87	36 (25%)
15	R	118/118 (100%)	0.10	0 100 100	26, 43, 54, 69	16 (13%)
16	S	110/112 (98%)	0.29	1 (0%) 84 82	40, 52, 65, 75	24 (21%)
17	T	131/146 (89%)	0.23	3 (2%) 60 54	34, 45, 72, 92	22 (16%)
18	U	116/118 (98%)	0.13	0 100 100	26, 40, 49, 53	23 (19%)
19	V	101/101 (100%)	0.07	1 (0%) 82 80	28, 48, 59, 66	12 (11%)
20	W	112/113 (99%)	0.15	1 (0%) 84 82	28, 41, 63, 79	24 (21%)
21	X	95/96 (98%)	0.24	3 (3%) 47 40	39, 50, 72, 84	14 (14%)
22	Y	107/110 (97%)	0.44	8 (7%) 14 10	44, 54, 81, 87	24 (22%)
23	Z	94/206 (45%)	0.48	5 (5%) 26 20	42, 59, 74, 97	15 (15%)
24	0	74/85 (87%)	-0.01	0 100 100	26, 39, 52, 65	16 (21%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	1	97/98 (98%)	0.29	5 (5%) 27 21	24, 39, 70, 81	21 (21%)
26	2	70/72 (97%)	0.51	2 (2%) 51 45	44, 57, 67, 79	13 (18%)
27	3	59/60 (98%)	0.53	5 (8%) 10 7	29, 43, 66, 78	12 (20%)
28	4	69/71 (97%)	1.18	16 (23%) 0 0	52, 73, 94, 99	26 (37%)
29	5	59/60 (98%)	0.04	0 100 100	22, 43, 62, 71	8 (13%)
30	6	53/54 (98%)	0.17	0 100 100	35, 41, 52, 58	11 (20%)
31	7	49/49 (100%)	0.05	2 (4%) 37 30	25, 30, 54, 70	9 (18%)
32	8	64/65 (98%)	0.00	0 100 100	26, 34, 40, 51	7 (10%)
33	9	37/37 (100%)	0.33	2 (5%) 25 20	32, 39, 51, 58	11 (29%)
34	a	1498/1521 (98%)	0.22	73 (4%) 29 23	28, 45, 92, 113	228 (15%)
35	b	231/256 (90%)	0.82	30 (12%) 3 2	51, 71, 92, 100	56 (24%)
36	c	206/239 (86%)	0.24	6 (2%) 51 45	40, 58, 73, 83	19 (9%)
37	d	208/209 (99%)	0.41	7 (3%) 45 38	47, 59, 79, 86	49 (23%)
38	e	148/162 (91%)	0.06	3 (2%) 65 60	33, 48, 60, 78	23 (15%)
39	f	100/101 (99%)	0.40	7 (7%) 16 12	48, 66, 76, 86	17 (17%)
40	g	155/156 (99%)	0.57	13 (8%) 11 7	41, 58, 89, 98	40 (25%)
41	h	137/138 (99%)	0.17	1 (0%) 87 86	39, 48, 57, 65	14 (10%)
42	i	127/128 (99%)	0.36	3 (2%) 59 53	35, 61, 77, 83	15 (11%)
43	j	96/105 (91%)	1.00	18 (18%) 1 0	34, 65, 87, 94	27 (28%)
44	k	114/129 (88%)	0.25	3 (2%) 56 50	32, 54, 67, 72	16 (14%)
45	l	122/132 (92%)	-0.02	1 (0%) 86 84	28, 40, 55, 65	23 (18%)
46	m	119/126 (94%)	0.63	13 (10%) 5 3	32, 57, 77, 82	24 (20%)
47	n	60/61 (98%)	0.22	0 100 100	33, 44, 54, 63	4 (6%)
48	o	88/89 (98%)	0.41	2 (2%) 60 54	37, 50, 65, 74	21 (23%)
49	p	82/88 (93%)	0.59	5 (6%) 21 16	43, 55, 69, 76	14 (17%)
50	q	99/105 (94%)	0.10	0 100 100	41, 49, 61, 65	18 (18%)
51	r	68/88 (77%)	0.56	3 (4%) 34 27	48, 59, 78, 86	14 (20%)
52	s	83/93 (89%)	0.47	7 (8%) 11 7	39, 55, 75, 80	13 (15%)
53	t	96/106 (90%)	0.36	1 (1%) 82 80	40, 49, 59, 71	16 (16%)
54	u	23/27 (85%)	0.44	0 100 100	38, 45, 50, 51	4 (17%)
55	v	13/24 (54%)	0.58	1 (7%) 13 10	36, 48, 70, 81	4 (30%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
56	w	67/76 (88%)	2.16	32 (47%) 0 0	47, 92, 104, 107	54 (80%)
57	x	73/77 (94%)	0.33	4 (5%) 25 19	27, 49, 72, 88	13 (17%)
58	y	68/76 (89%)	1.34	16 (23%) 0 0	29, 84, 103, 108	39 (57%)
59	z	671/679 (98%)	0.52	52 (7%) 13 10	32, 66, 85, 99	164 (24%)
All	All	11355/11953 (94%)	0.40	803 (7%) 16 11	18, 49, 93, 214	2236 (19%)

The worst 5 of 803 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	K	92	GLY	15.0
1	A	934	C	14.8
10	K	122	ALA	14.7
10	K	135	GLY	13.9
10	K	139	VAL	12.3

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	PSU	w	55	20/21	0.67	0.31	96,105,110,111	13
56	5MU	w	54	21/22	0.68	0.48	94,99,101,104	14
58	PSU	y	39	20/21	0.78	0.23	85,93,96,96	8
56	7MG	w	46	24/25	0.79	0.23	91,97,102,104	13
58	PSU	y	32	20/21	0.82	0.20	92,98,106,108	11
58	PSU	y	55	20/21	0.82	0.21	68,75,84,88	11
58	MIA	y	37	22/30	0.83	0.18	75,84,87,89	8
58	4SU	y	8	20/21	0.83	0.20	78,95,101,102	10
56	4SU	w	8	20/21	0.83	0.24	86,92,95,95	12
58	5MU	y	54	21/22	0.87	0.24	67,72,82,83	11
56	PSU	w	32	20/21	0.93	0.15	54,61,66,72	2
56	PSU	w	39	20/21	0.94	0.27	54,63,69,70	7
56	MIA	w	37	27/30	0.94	0.24	42,47,52,52	8
57	5MU	x	54	21/22	0.94	0.20	40,51,55,61	10
57	PSU	x	55	20/21	0.95	0.18	39,51,54,57	7
57	4SU	x	8	20/21	0.96	0.16	41,49,54,54	7
57	5MC	x	32	21/22	0.96	0.18	33,40,44,46	4

6.3 Carbohydrates (i)

There are no monosaccharides 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^{th} 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^2)	Q<0.9
60	MG	a	1614	1/1	0.29	0.67	75,75,75,75	0
60	MG	a	1705	1/1	0.38	0.37	72,72,72,72	0
60	MG	B	206	1/1	0.39	0.37	86,86,86,86	0
60	MG	A	3234	1/1	0.44	0.54	61,61,61,61	0
60	MG	a	1676	1/1	0.46	0.24	58,58,58,58	0
60	MG	A	3208	1/1	0.49	0.34	60,60,60,60	0
60	MG	A	3252	1/1	0.49	0.18	76,76,76,76	0
60	MG	V	202	1/1	0.51	0.55	73,73,73,73	0
60	MG	A	3155	1/1	0.51	0.28	65,65,65,65	0
60	MG	A	3283	1/1	0.53	0.53	41,41,41,41	0
60	MG	A	3057	1/1	0.54	0.38	72,72,72,72	0
60	MG	a	1638	1/1	0.54	0.42	53,53,53,53	0
60	MG	A	3586	1/1	0.55	0.52	75,75,75,75	0
60	MG	a	1661	1/1	0.56	0.19	69,69,69,69	0
60	MG	a	1701	1/1	0.58	0.18	66,66,66,66	0
60	MG	A	3274	1/1	0.59	0.23	66,66,66,66	0
60	MG	A	3169	1/1	0.59	0.45	44,44,44,44	1
60	MG	A	3394	1/1	0.59	0.30	81,81,81,81	0
60	MG	A	3098	1/1	0.60	0.24	61,61,61,61	0
60	MG	A	3267	1/1	0.60	0.45	64,64,64,64	0
60	MG	a	1604	1/1	0.61	0.25	64,64,64,64	0
60	MG	A	3295	1/1	0.62	0.36	58,58,58,58	0
60	MG	a	1689	1/1	0.62	0.24	74,74,74,74	0
60	MG	A	3006	1/1	0.62	0.38	52,52,52,52	1
60	MG	A	3117	1/1	0.62	0.30	48,48,48,48	0
60	MG	x	109	1/1	0.62	0.17	77,77,77,77	0
60	MG	B	204	1/1	0.63	0.24	63,63,63,63	0
60	MG	A	3094	1/1	0.63	0.54	55,55,55,55	0
60	MG	a	1662	1/1	0.64	0.33	53,53,53,53	0
60	MG	B	215	1/1	0.64	0.28	75,75,75,75	1
60	MG	A	3525	1/1	0.64	0.24	37,37,37,37	0
60	MG	A	3092	1/1	0.65	0.27	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3278	1/1	0.65	0.24	56,56,56,56	0
60	MG	A	3236	1/1	0.65	0.63	47,47,47,47	1
60	MG	A	3557	1/1	0.66	0.28	70,70,70,70	0
60	MG	A	3606	1/1	0.66	0.26	56,56,56,56	0
60	MG	A	3066	1/1	0.67	0.32	58,58,58,58	0
60	MG	A	3135	1/1	0.67	0.14	59,59,59,59	0
60	MG	A	3199	1/1	0.67	0.24	45,45,45,45	0
60	MG	A	3585	1/1	0.67	0.25	46,46,46,46	0
60	MG	A	3055	1/1	0.68	0.22	47,47,47,47	0
60	MG	A	3624	1/1	0.68	0.60	63,63,63,63	0
60	MG	A	3265	1/1	0.69	0.24	64,64,64,64	0
60	MG	A	3237	1/1	0.69	0.43	43,43,43,43	1
60	MG	A	3151	1/1	0.69	0.18	72,72,72,72	0
60	MG	R	202	1/1	0.70	0.19	62,62,62,62	0
60	MG	a	1666	1/1	0.70	0.44	68,68,68,68	0
60	MG	A	3014	1/1	0.70	0.32	37,37,37,37	0
60	MG	A	3335	1/1	0.70	0.35	59,59,59,59	1
60	MG	A	3154	1/1	0.70	0.33	67,67,67,67	0
60	MG	B	209	1/1	0.70	0.32	60,60,60,60	0
60	MG	a	1779	1/1	0.70	0.34	55,55,55,55	0
60	MG	A	3050	1/1	0.70	0.42	60,60,60,60	0
60	MG	a	1615	1/1	0.71	0.41	54,54,54,54	0
60	MG	a	1636	1/1	0.71	0.42	59,59,59,59	0
60	MG	a	1698	1/1	0.71	0.22	49,49,49,49	0
60	MG	A	3054	1/1	0.71	0.27	48,48,48,48	0
60	MG	A	3197	1/1	0.71	0.33	48,48,48,48	1
60	MG	B	211	1/1	0.71	0.28	69,69,69,69	0
60	MG	A	3255	1/1	0.71	0.39	94,94,94,94	0
60	MG	A	3022	1/1	0.72	0.29	59,59,59,59	0
60	MG	A	3179	1/1	0.72	0.25	61,61,61,61	0
60	MG	A	3127	1/1	0.72	0.33	24,24,24,24	1
60	MG	A	3602	1/1	0.72	0.34	48,48,48,48	0
60	MG	A	3049	1/1	0.72	0.32	68,68,68,68	0
60	MG	A	3243	1/1	0.72	0.22	52,52,52,52	0
60	MG	x	106	1/1	0.72	0.45	56,56,56,56	1
60	MG	A	3277	1/1	0.72	0.41	47,47,47,47	1
60	MG	a	1641	1/1	0.73	0.34	68,68,68,68	0
60	MG	A	3242	1/1	0.73	0.41	61,61,61,61	0
60	MG	a	1703	1/1	0.73	0.24	57,57,57,57	1
60	MG	A	3577	1/1	0.73	0.42	60,60,60,60	0
60	MG	A	3492	1/1	0.73	0.38	64,64,64,64	1
60	MG	A	3100	1/1	0.73	0.50	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3591	1/1	0.73	0.34	39,39,39,39	1
60	MG	a	1663	1/1	0.74	0.29	60,60,60,60	0
60	MG	A	3607	1/1	0.74	0.15	54,54,54,54	0
60	MG	A	3144	1/1	0.74	0.42	51,51,51,51	0
60	MG	a	1686	1/1	0.74	0.24	61,61,61,61	0
60	MG	A	3630	1/1	0.74	0.38	34,34,34,34	1
60	MG	A	3052	1/1	0.74	0.26	51,51,51,51	1
60	MG	A	3099	1/1	0.74	0.28	51,51,51,51	0
60	MG	A	3223	1/1	0.74	0.42	52,52,52,52	0
60	MG	A	3227	1/1	0.74	0.34	63,63,63,63	0
60	MG	a	1643	1/1	0.74	0.46	58,58,58,58	0
60	MG	A	3228	1/1	0.74	0.31	49,49,49,49	0
60	MG	A	3527	1/1	0.74	0.29	45,45,45,45	0
60	MG	A	3563	1/1	0.75	0.26	46,46,46,46	0
60	MG	A	3371	1/1	0.75	0.24	40,40,40,40	0
60	MG	P	202	1/1	0.75	0.40	59,59,59,59	0
60	MG	A	3097	1/1	0.75	0.29	56,56,56,56	0
60	MG	A	3342	1/1	0.75	0.30	58,58,58,58	0
60	MG	A	3610	1/1	0.75	0.24	62,62,62,62	0
60	MG	a	1660	1/1	0.75	0.36	53,53,53,53	0
60	MG	a	1665	1/1	0.76	0.52	47,47,47,47	1
60	MG	a	1606	1/1	0.76	0.12	48,48,48,48	0
60	MG	A	3521	1/1	0.76	0.23	35,35,35,35	1
60	MG	A	3282	1/1	0.76	0.29	68,68,68,68	0
60	MG	A	3358	1/1	0.76	0.32	46,46,46,46	1
60	MG	a	1691	1/1	0.76	0.29	53,53,53,53	0
60	MG	A	3536	1/1	0.76	0.31	57,57,57,57	0
60	MG	A	3157	1/1	0.76	0.54	40,40,40,40	1
60	MG	A	3064	1/1	0.76	0.14	58,58,58,58	0
60	MG	A	3465	1/1	0.76	0.10	59,59,59,59	0
60	MG	A	3217	1/1	0.76	0.56	56,56,56,56	1
60	MG	0	102	1/1	0.76	0.26	47,47,47,47	0
60	MG	x	108	1/1	0.76	0.26	55,55,55,55	0
60	MG	B	201	1/1	0.76	0.47	53,53,53,53	1
60	MG	a	1772	1/1	0.77	0.35	62,62,62,62	0
60	MG	A	3456	1/1	0.77	0.28	46,46,46,46	1
60	MG	e	201	1/1	0.77	0.15	78,78,78,78	0
60	MG	A	3402	1/1	0.77	0.35	36,36,36,36	0
60	MG	A	3449	1/1	0.77	0.31	29,29,29,29	1
60	MG	A	3517	1/1	0.77	0.21	85,85,85,85	0
60	MG	a	1761	1/1	0.78	0.25	55,55,55,55	1
60	MG	A	3235	1/1	0.78	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3391	1/1	0.78	0.41	56,56,56,56	0
60	MG	A	3060	1/1	0.78	0.13	54,54,54,54	0
60	MG	A	3599	1/1	0.78	0.20	45,45,45,45	0
60	MG	A	3253	1/1	0.78	0.14	67,67,67,67	0
60	MG	A	3579	1/1	0.78	0.25	50,50,50,50	0
60	MG	A	3037	1/1	0.79	0.18	44,44,44,44	0
60	MG	A	3361	1/1	0.79	0.18	64,64,64,64	0
60	MG	A	3142	1/1	0.79	0.23	57,57,57,57	0
60	MG	A	3004	1/1	0.79	0.41	40,40,40,40	1
60	MG	A	3085	1/1	0.79	0.24	70,70,70,70	0
60	MG	A	3121	1/1	0.79	0.34	38,38,38,38	1
60	MG	A	3420	1/1	0.79	0.16	55,55,55,55	0
60	MG	A	3124	1/1	0.79	0.25	32,32,32,32	1
60	MG	A	3087	1/1	0.79	0.14	41,41,41,41	0
60	MG	A	3333	1/1	0.79	0.24	61,61,61,61	1
60	MG	A	3130	1/1	0.79	0.30	55,55,55,55	0
60	MG	x	103	1/1	0.79	0.10	62,62,62,62	0
60	MG	A	3172	1/1	0.79	0.39	49,49,49,49	0
60	MG	A	3518	1/1	0.79	0.19	39,39,39,39	0
60	MG	A	3344	1/1	0.79	0.11	70,70,70,70	0
60	MG	A	3305	1/1	0.80	0.40	38,38,38,38	0
60	MG	F	305	1/1	0.80	0.14	46,46,46,46	0
60	MG	O	201	1/1	0.80	0.23	55,55,55,55	0
60	MG	a	1664	1/1	0.80	0.26	62,62,62,62	0
60	MG	P	201	1/1	0.80	0.36	59,59,59,59	0
60	MG	A	3316	1/1	0.80	0.37	63,63,63,63	0
60	MG	A	3015	1/1	0.80	0.18	45,45,45,45	0
60	MG	a	1679	1/1	0.80	0.21	39,39,39,39	0
60	MG	A	3573	1/1	0.80	0.69	34,34,34,34	1
60	MG	Z	301	1/1	0.80	0.16	61,61,61,61	0
60	MG	A	3611	1/1	0.80	0.20	46,46,46,46	0
60	MG	A	3505	1/1	0.80	0.14	41,41,41,41	0
60	MG	A	3259	1/1	0.80	0.31	60,60,60,60	0
60	MG	a	1611	1/1	0.80	0.18	58,58,58,58	0
60	MG	A	3644	1/1	0.80	0.23	42,42,42,42	0
60	MG	a	1718	1/1	0.80	0.41	55,55,55,55	1
60	MG	A	3581	1/1	0.80	0.10	63,63,63,63	0
60	MG	a	1620	1/1	0.80	0.49	47,47,47,47	0
60	MG	A	3039	1/1	0.80	0.16	63,63,63,63	0
60	MG	a	1785	1/1	0.80	0.47	53,53,53,53	0
60	MG	A	3011	1/1	0.80	0.70	53,53,53,53	0
60	MG	B	207	1/1	0.80	0.15	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3122	1/1	0.80	0.31	51,51,51,51	1
60	MG	a	1648	1/1	0.80	0.27	58,58,58,58	0
60	MG	A	3453	1/1	0.80	0.14	57,57,57,57	0
60	MG	A	3244	1/1	0.81	0.19	53,53,53,53	0
60	MG	A	3438	1/1	0.81	0.13	77,77,77,77	0
60	MG	A	3141	1/1	0.81	0.32	42,42,42,42	1
60	MG	a	1625	1/1	0.81	0.30	60,60,60,60	0
60	MG	a	1629	1/1	0.81	0.15	44,44,44,44	0
60	MG	A	3209	1/1	0.81	0.30	72,72,72,72	0
60	MG	A	3551	1/1	0.81	0.18	71,71,71,71	0
60	MG	a	1704	1/1	0.81	0.22	52,52,52,52	0
60	MG	A	3555	1/1	0.81	0.15	63,63,63,63	0
60	MG	A	3180	1/1	0.81	0.35	44,44,44,44	0
60	MG	A	3257	1/1	0.81	0.16	52,52,52,52	0
60	MG	A	3088	1/1	0.81	0.32	53,53,53,53	0
60	MG	A	3263	1/1	0.81	0.21	67,67,67,67	0
60	MG	A	3510	1/1	0.81	0.33	48,48,48,48	0
60	MG	a	1786	1/1	0.81	0.77	38,38,38,38	1
60	MG	6	101	1/1	0.81	0.35	42,42,42,42	1
60	MG	a	1603	1/1	0.81	0.29	67,67,67,67	0
60	MG	A	3511	1/1	0.81	0.33	50,50,50,50	0
60	MG	A	3068	1/1	0.81	0.38	69,69,69,69	0
60	MG	A	3200	1/1	0.81	0.18	39,39,39,39	0
60	MG	A	3249	1/1	0.82	0.41	72,72,72,72	0
60	MG	A	3212	1/1	0.82	0.13	46,46,46,46	0
60	MG	A	3270	1/1	0.82	0.19	51,51,51,51	0
60	MG	A	3597	1/1	0.82	0.34	47,47,47,47	0
60	MG	A	3132	1/1	0.82	0.42	43,43,43,43	1
60	MG	A	3556	1/1	0.82	0.29	35,35,35,35	1
60	MG	a	1725	1/1	0.82	0.30	51,51,51,51	0
60	MG	A	3604	1/1	0.82	0.17	64,64,64,64	0
60	MG	A	3170	1/1	0.82	0.25	33,33,33,33	0
60	MG	A	3150	1/1	0.82	0.17	54,54,54,54	0
60	MG	a	1782	1/1	0.82	0.58	62,62,62,62	0
60	MG	a	1616	1/1	0.82	0.21	54,54,54,54	0
60	MG	a	1675	1/1	0.82	0.60	61,61,61,61	0
60	MG	A	3029	1/1	0.82	0.30	48,48,48,48	0
60	MG	A	3519	1/1	0.82	0.17	48,48,48,48	0
60	MG	A	3167	1/1	0.82	0.37	51,51,51,51	0
60	MG	A	3284	1/1	0.82	0.28	39,39,39,39	1
60	MG	A	3639	1/1	0.82	0.29	36,36,36,36	0
60	MG	z	702	1/1	0.82	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3262	1/1	0.83	0.12	50,50,50,50	1
60	MG	A	3281	1/1	0.83	0.23	43,43,43,43	0
60	MG	a	1715	1/1	0.83	0.31	58,58,58,58	0
60	MG	A	3158	1/1	0.83	0.34	38,38,38,38	1
60	MG	A	3603	1/1	0.83	0.37	50,50,50,50	0
60	MG	a	1731	1/1	0.83	0.20	49,49,49,49	0
60	MG	a	1741	1/1	0.83	0.18	63,63,63,63	0
60	MG	A	3008	1/1	0.83	0.17	42,42,42,42	0
60	MG	A	3362	1/1	0.83	0.28	47,47,47,47	0
60	MG	A	3266	1/1	0.83	0.55	67,67,67,67	0
60	MG	A	3387	1/1	0.83	0.24	26,26,26,26	0
60	MG	a	1784	1/1	0.83	0.41	52,52,52,52	0
60	MG	A	3080	1/1	0.83	0.43	48,48,48,48	0
60	MG	A	3056	1/1	0.83	0.24	39,39,39,39	0
60	MG	A	3627	1/1	0.83	0.22	25,25,25,25	0
60	MG	n	101	1/1	0.83	0.66	64,64,64,64	0
60	MG	A	3106	1/1	0.83	0.28	46,46,46,46	1
60	MG	A	3275	1/1	0.83	0.29	55,55,55,55	1
60	MG	a	1642	1/1	0.83	0.38	70,70,70,70	0
60	MG	A	3040	1/1	0.83	0.36	31,31,31,31	1
60	MG	z	701	1/1	0.83	0.28	59,59,59,59	0
60	MG	A	3341	1/1	0.83	0.27	30,30,30,30	0
60	MG	A	3026	1/1	0.84	0.25	43,43,43,43	0
60	MG	A	3188	1/1	0.84	0.29	39,39,39,39	0
60	MG	A	3044	1/1	0.84	0.30	25,25,25,25	1
60	MG	A	3588	1/1	0.84	0.29	60,60,60,60	0
60	MG	A	3462	1/1	0.84	0.13	58,58,58,58	0
60	MG	a	1612	1/1	0.84	0.13	57,57,57,57	0
60	MG	A	3541	1/1	0.84	0.08	63,63,63,63	0
60	MG	A	3542	1/1	0.84	0.25	63,63,63,63	0
60	MG	A	3549	1/1	0.84	0.09	47,47,47,47	0
60	MG	A	3272	1/1	0.84	0.31	55,55,55,55	0
60	MG	A	3137	1/1	0.84	0.28	35,35,35,35	0
60	MG	d	301	1/1	0.84	0.56	59,59,59,59	0
60	MG	A	3260	1/1	0.84	0.32	44,44,44,44	1
60	MG	a	1635	1/1	0.84	0.26	55,55,55,55	0
60	MG	A	3089	1/1	0.84	0.15	58,58,58,58	0
60	MG	A	3002	1/1	0.84	0.09	58,58,58,58	0
60	MG	A	3572	1/1	0.84	0.21	58,58,58,58	0
60	MG	A	3418	1/1	0.84	0.34	48,48,48,48	0
60	MG	A	3264	1/1	0.84	0.28	23,23,23,23	1
60	MG	A	3143	1/1	0.84	0.22	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	a	1669	1/1	0.85	0.27	60,60,60,60	0
60	MG	a	1674	1/1	0.85	0.43	50,50,50,50	0
60	MG	A	3081	1/1	0.85	0.35	56,56,56,56	0
60	MG	A	3206	1/1	0.85	0.31	50,50,50,50	0
60	MG	A	3546	1/1	0.85	0.13	53,53,53,53	0
60	MG	a	1601	1/1	0.85	0.53	68,68,68,68	0
60	MG	A	3353	1/1	0.85	0.22	60,60,60,60	0
60	MG	a	1690	1/1	0.85	0.14	69,69,69,69	0
60	MG	A	3458	1/1	0.85	0.24	38,38,38,38	0
60	MG	a	1693	1/1	0.85	0.32	39,39,39,39	0
60	MG	A	3552	1/1	0.85	0.12	48,48,48,48	0
60	MG	a	1609	1/1	0.85	0.55	51,51,51,51	0
60	MG	A	3280	1/1	0.85	0.33	46,46,46,46	0
60	MG	A	3082	1/1	0.85	0.31	43,43,43,43	1
60	MG	A	3084	1/1	0.85	0.11	56,56,56,56	0
60	MG	A	3072	1/1	0.85	0.17	46,46,46,46	0
60	MG	A	3568	1/1	0.85	0.24	61,61,61,61	0
60	MG	A	3059	1/1	0.85	0.22	37,37,37,37	1
60	MG	A	3183	1/1	0.85	0.25	21,21,21,21	0
60	MG	A	3574	1/1	0.85	0.18	39,39,39,39	0
60	MG	A	3250	1/1	0.85	0.28	64,64,64,64	0
60	MG	a	1763	1/1	0.85	0.27	34,34,34,34	1
60	MG	a	1767	1/1	0.85	0.12	45,45,45,45	0
60	MG	A	3225	1/1	0.85	0.29	54,54,54,54	0
60	MG	A	3118	1/1	0.85	0.23	64,64,64,64	0
60	MG	B	212	1/1	0.85	0.18	52,52,52,52	0
60	MG	A	3520	1/1	0.85	0.36	55,55,55,55	0
60	MG	A	3161	1/1	0.85	0.29	34,34,34,34	1
60	MG	a	1644	1/1	0.85	0.17	46,46,46,46	0
60	MG	F	306	1/1	0.85	0.33	46,46,46,46	0
60	MG	G	202	1/1	0.85	0.10	48,48,48,48	0
60	MG	A	3423	1/1	0.85	0.20	73,73,73,73	0
60	MG	A	3433	1/1	0.85	0.20	27,27,27,27	1
60	MG	A	3528	1/1	0.85	0.51	51,51,51,51	0
60	MG	A	3531	1/1	0.85	0.41	55,55,55,55	0
60	MG	A	3148	1/1	0.85	0.30	47,47,47,47	0
60	MG	W	201	1/1	0.85	0.29	59,59,59,59	0
60	MG	a	1667	1/1	0.85	0.21	55,55,55,55	0
60	MG	A	3350	1/1	0.86	0.12	59,59,59,59	0
60	MG	A	3043	1/1	0.86	0.24	39,39,39,39	0
60	MG	A	3356	1/1	0.86	0.40	50,50,50,50	0
60	MG	a	1640	1/1	0.86	0.62	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3429	1/1	0.86	0.29	45,45,45,45	0
60	MG	A	3067	1/1	0.86	0.18	34,34,34,34	0
60	MG	A	3182	1/1	0.86	0.41	43,43,43,43	0
60	MG	a	1721	1/1	0.86	0.08	41,41,41,41	0
60	MG	A	3441	1/1	0.86	0.56	52,52,52,52	0
60	MG	A	3443	1/1	0.86	0.28	41,41,41,41	0
60	MG	A	3448	1/1	0.86	0.43	60,60,60,60	0
60	MG	a	1752	1/1	0.86	0.35	43,43,43,43	0
60	MG	A	3633	1/1	0.86	0.31	30,30,30,30	0
60	MG	A	3576	1/1	0.86	0.12	59,59,59,59	0
60	MG	A	3063	1/1	0.86	0.29	49,49,49,49	0
60	MG	A	3530	1/1	0.86	0.42	38,38,38,38	1
60	MG	A	3111	1/1	0.86	0.23	46,46,46,46	0
60	MG	A	3384	1/1	0.86	0.23	39,39,39,39	0
60	MG	A	3540	1/1	0.86	0.10	57,57,57,57	0
60	MG	A	3024	1/1	0.86	0.28	40,40,40,40	0
60	MG	A	3258	1/1	0.86	0.41	41,41,41,41	0
60	MG	A	3247	1/1	0.86	0.23	46,46,46,46	1
60	MG	A	3271	1/1	0.86	0.48	71,71,71,71	0
60	MG	f	201	1/1	0.86	0.19	53,53,53,53	0
60	MG	B	216	1/1	0.86	0.11	53,53,53,53	0
60	MG	a	1681	1/1	0.86	0.16	55,55,55,55	0
60	MG	D	304	1/1	0.86	0.32	36,36,36,36	1
60	MG	F	302	1/1	0.86	0.27	32,32,32,32	1
60	MG	a	1627	1/1	0.86	0.28	47,47,47,47	0
60	MG	A	3404	1/1	0.86	0.27	35,35,35,35	0
60	MG	a	1631	1/1	0.86	0.43	42,42,42,42	0
60	MG	A	3450	1/1	0.87	0.33	58,58,58,58	0
60	MG	U	201	1/1	0.87	0.33	30,30,30,30	1
60	MG	A	3110	1/1	0.87	0.27	25,25,25,25	1
60	MG	A	3343	1/1	0.87	0.09	64,64,64,64	0
60	MG	a	1672	1/1	0.87	0.23	41,41,41,41	0
60	MG	A	3133	1/1	0.87	0.26	36,36,36,36	1
60	MG	a	1632	1/1	0.87	0.36	42,42,42,42	0
60	MG	A	3075	1/1	0.87	0.14	60,60,60,60	1
60	MG	A	3436	1/1	0.87	0.21	43,43,43,43	0
60	MG	a	1775	1/1	0.87	0.18	53,53,53,53	1
60	MG	7	101	1/1	0.87	0.14	63,63,63,63	0
60	MG	A	3580	1/1	0.87	0.35	43,43,43,43	0
60	MG	a	1602	1/1	0.87	0.28	57,57,57,57	0
60	MG	A	3612	1/1	0.87	0.10	62,62,62,62	0
60	MG	A	3320	1/1	0.87	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3354	1/1	0.87	0.30	53,53,53,53	0
60	MG	a	1694	1/1	0.87	0.15	41,41,41,41	0
60	MG	A	3153	1/1	0.87	0.24	45,45,45,45	0
60	MG	a	1653	1/1	0.87	0.42	61,61,61,61	0
60	MG	A	3559	1/1	0.87	0.27	38,38,38,38	1
60	MG	A	3073	1/1	0.87	0.21	32,32,32,32	0
60	MG	A	3642	1/1	0.87	0.21	38,38,38,38	1
60	MG	a	1709	1/1	0.87	0.12	36,36,36,36	0
60	MG	A	3291	1/1	0.87	0.40	55,55,55,55	0
60	MG	A	3571	1/1	0.87	0.30	38,38,38,38	1
60	MG	A	3339	1/1	0.88	0.12	54,54,54,54	0
60	MG	A	3001	1/1	0.88	0.20	51,51,51,51	0
60	MG	A	3224	1/1	0.88	0.20	34,34,34,34	0
60	MG	A	3012	1/1	0.88	0.30	60,60,60,60	0
60	MG	A	3246	1/1	0.88	0.29	66,66,66,66	0
60	MG	A	3152	1/1	0.88	0.10	48,48,48,48	0
60	MG	A	3351	1/1	0.88	0.37	33,33,33,33	0
60	MG	A	3164	1/1	0.88	0.32	31,31,31,31	0
60	MG	A	3229	1/1	0.88	0.26	39,39,39,39	0
60	MG	A	3532	1/1	0.88	0.20	41,41,41,41	0
60	MG	a	1713	1/1	0.88	0.45	43,43,43,43	0
60	MG	F	303	1/1	0.88	0.20	53,53,53,53	0
60	MG	F	304	1/1	0.88	0.70	28,28,28,28	1
60	MG	A	3025	1/1	0.88	0.28	51,51,51,51	1
60	MG	A	3592	1/1	0.88	0.48	41,41,41,41	1
60	MG	A	3038	1/1	0.88	0.21	29,29,29,29	0
60	MG	A	3297	1/1	0.88	0.28	35,35,35,35	1
60	MG	a	1742	1/1	0.88	0.18	58,58,58,58	0
60	MG	A	3299	1/1	0.88	0.32	35,35,35,35	0
60	MG	a	1759	1/1	0.88	0.13	53,53,53,53	0
60	MG	A	3544	1/1	0.88	0.33	53,53,53,53	0
60	MG	a	1654	1/1	0.88	0.16	50,50,50,50	0
60	MG	a	1657	1/1	0.88	0.14	57,57,57,57	0
60	MG	A	3254	1/1	0.88	0.30	62,62,62,62	0
60	MG	A	3548	1/1	0.88	0.38	65,65,65,65	0
60	MG	A	3375	1/1	0.88	0.20	35,35,35,35	0
60	MG	A	3382	1/1	0.88	0.27	30,30,30,30	0
60	MG	A	3310	1/1	0.88	0.16	37,37,37,37	0
60	MG	A	3129	1/1	0.88	0.19	35,35,35,35	1
60	MG	A	3617	1/1	0.88	0.16	45,45,45,45	0
60	MG	A	3618	1/1	0.88	0.17	57,57,57,57	0
60	MG	A	3620	1/1	0.88	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3496	1/1	0.88	0.31	33,33,33,33	1
60	MG	A	3502	1/1	0.88	0.14	44,44,44,44	0
60	MG	A	3221	1/1	0.88	0.30	49,49,49,49	0
60	MG	A	3560	1/1	0.88	0.20	58,58,58,58	0
60	MG	A	3328	1/1	0.88	0.17	62,62,62,62	0
60	MG	A	3239	1/1	0.88	0.49	51,51,51,51	0
60	MG	A	3514	1/1	0.88	0.15	69,69,69,69	0
60	MG	A	3276	1/1	0.88	0.20	51,51,51,51	1
60	MG	A	3041	1/1	0.89	0.26	38,38,38,38	0
60	MG	A	3251	1/1	0.89	0.15	46,46,46,46	0
60	MG	A	3160	1/1	0.89	0.45	57,57,57,57	0
60	MG	A	3226	1/1	0.89	0.29	45,45,45,45	0
60	MG	A	3190	1/1	0.89	0.49	58,58,58,58	0
60	MG	A	3191	1/1	0.89	0.22	51,51,51,51	0
60	MG	A	3196	1/1	0.89	0.20	51,51,51,51	0
60	MG	A	3537	1/1	0.89	0.16	45,45,45,45	0
60	MG	D	303	1/1	0.89	0.24	24,24,24,24	1
60	MG	A	3231	1/1	0.89	0.24	68,68,68,68	0
60	MG	A	3146	1/1	0.89	0.09	72,72,72,72	0
60	MG	A	3593	1/1	0.89	0.08	70,70,70,70	0
60	MG	A	3016	1/1	0.89	0.38	59,59,59,59	0
60	MG	A	3289	1/1	0.89	0.19	59,59,59,59	0
60	MG	A	3545	1/1	0.89	0.42	42,42,42,42	0
60	MG	A	3290	1/1	0.89	0.20	56,56,56,56	0
60	MG	H	201	1/1	0.89	0.18	62,62,62,62	0
60	MG	a	1732	1/1	0.89	0.17	54,54,54,54	0
60	MG	A	3112	1/1	0.89	0.27	44,44,44,44	0
60	MG	A	3201	1/1	0.89	0.48	45,45,45,45	0
60	MG	A	3550	1/1	0.89	0.39	65,65,65,65	0
60	MG	a	1758	1/1	0.89	0.49	72,72,72,72	0
60	MG	a	1656	1/1	0.89	0.10	60,60,60,60	0
60	MG	A	3474	1/1	0.89	0.34	44,44,44,44	0
60	MG	a	1659	1/1	0.89	0.27	55,55,55,55	0
60	MG	a	1765	1/1	0.89	0.13	55,55,55,55	0
60	MG	A	3374	1/1	0.89	0.22	54,54,54,54	0
60	MG	V	201	1/1	0.89	0.40	55,55,55,55	0
60	MG	A	3554	1/1	0.89	0.16	67,67,67,67	0
60	MG	A	3296	1/1	0.89	0.20	31,31,31,31	0
60	MG	A	3083	1/1	0.89	0.18	51,51,51,51	0
60	MG	A	3065	1/1	0.89	0.29	64,64,64,64	0
60	MG	A	3101	1/1	0.89	0.23	47,47,47,47	0
60	MG	A	3625	1/1	0.89	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3102	1/1	0.89	0.31	55,55,55,55	0
60	MG	A	3268	1/1	0.89	0.27	52,52,52,52	0
60	MG	a	1673	1/1	0.89	0.24	60,60,60,60	0
60	MG	A	3319	1/1	0.89	0.21	43,43,43,43	0
60	MG	A	3636	1/1	0.89	0.32	37,37,37,37	1
60	MG	A	3269	1/1	0.89	0.20	64,64,64,64	0
60	MG	a	1677	1/1	0.89	0.20	63,63,63,63	0
60	MG	A	3071	1/1	0.89	0.15	61,61,61,61	0
60	MG	A	3181	1/1	0.89	0.40	49,49,49,49	0
60	MG	A	3109	1/1	0.89	0.30	25,25,25,25	1
60	MG	A	3589	1/1	0.90	0.14	42,42,42,42	0
60	MG	A	3047	1/1	0.90	0.18	29,29,29,29	0
60	MG	a	1650	1/1	0.90	0.47	47,47,47,47	0
60	MG	0	101	1/1	0.90	0.23	39,39,39,39	0
60	MG	A	3220	1/1	0.90	0.29	45,45,45,45	0
60	MG	a	1717	1/1	0.90	0.63	54,54,54,54	0
60	MG	5	102	1/1	0.90	0.39	58,58,58,58	0
60	MG	A	3240	1/1	0.90	0.08	56,56,56,56	0
60	MG	A	3163	1/1	0.90	0.11	26,26,26,26	0
60	MG	A	3042	1/1	0.90	0.38	40,40,40,40	0
60	MG	A	3332	1/1	0.90	0.13	53,53,53,53	0
60	MG	A	3119	1/1	0.90	0.18	68,68,68,68	0
60	MG	A	3107	1/1	0.90	0.21	55,55,55,55	0
60	MG	A	3336	1/1	0.90	0.10	52,52,52,52	0
60	MG	A	3338	1/1	0.90	0.29	20,20,20,20	0
60	MG	A	3609	1/1	0.90	0.21	31,31,31,31	0
60	MG	A	3010	1/1	0.90	0.36	32,32,32,32	1
60	MG	E	304	1/1	0.90	0.20	35,35,35,35	0
60	MG	A	3003	1/1	0.90	0.24	32,32,32,32	0
60	MG	A	3535	1/1	0.90	0.26	55,55,55,55	0
60	MG	a	1770	1/1	0.90	0.35	56,56,56,56	0
60	MG	A	3613	1/1	0.90	0.31	67,67,67,67	0
60	MG	a	1622	1/1	0.90	0.21	36,36,36,36	0
60	MG	A	3468	1/1	0.90	0.18	37,37,37,37	1
60	MG	a	1626	1/1	0.90	0.42	52,52,52,52	0
60	MG	A	3471	1/1	0.90	0.13	65,65,65,65	0
60	MG	A	3090	1/1	0.90	0.21	43,43,43,43	0
60	MG	a	1683	1/1	0.90	0.40	58,58,58,58	0
60	MG	A	3480	1/1	0.90	0.34	41,41,41,41	0
60	MG	A	3202	1/1	0.90	0.09	36,36,36,36	0
60	MG	A	3079	1/1	0.90	0.17	18,18,18,18	0
60	MG	A	3232	1/1	0.90	0.20	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	R	201	1/1	0.90	0.45	50,50,50,50	0
60	MG	A	3114	1/1	0.90	0.39	42,42,42,42	0
60	MG	a	1697	1/1	0.90	0.21	34,34,34,34	0
60	MG	A	3159	1/1	0.90	0.18	45,45,45,45	1
60	MG	A	3638	1/1	0.90	0.23	38,38,38,38	0
60	MG	A	3147	1/1	0.90	0.24	50,50,50,50	0
60	MG	E	301	1/1	0.91	0.17	33,33,33,33	0
60	MG	a	1687	1/1	0.91	0.29	29,29,29,29	0
60	MG	E	303	1/1	0.91	0.31	32,32,32,32	1
60	MG	A	3406	1/1	0.91	0.06	74,74,74,74	0
60	MG	F	301	1/1	0.91	0.20	44,44,44,44	0
60	MG	A	3499	1/1	0.91	0.19	36,36,36,36	0
60	MG	a	1628	1/1	0.91	0.20	45,45,45,45	0
60	MG	A	3321	1/1	0.91	0.17	49,49,49,49	0
60	MG	a	1630	1/1	0.91	0.31	44,44,44,44	0
60	MG	A	3045	1/1	0.91	0.35	20,20,20,20	0
60	MG	A	3245	1/1	0.91	0.18	45,45,45,45	0
60	MG	A	3256	1/1	0.91	0.50	62,62,62,62	0
60	MG	A	3334	1/1	0.91	0.37	57,57,57,57	0
60	MG	a	1706	1/1	0.91	0.11	48,48,48,48	0
60	MG	A	3435	1/1	0.91	0.33	51,51,51,51	0
60	MG	a	1712	1/1	0.91	0.25	54,54,54,54	0
60	MG	N	201	1/1	0.91	0.24	42,42,42,42	0
60	MG	A	3091	1/1	0.91	0.21	49,49,49,49	0
60	MG	A	3562	1/1	0.91	0.16	67,67,67,67	0
60	MG	A	3437	1/1	0.91	0.21	30,30,30,30	1
60	MG	Q	202	1/1	0.91	0.21	33,33,33,33	0
60	MG	a	1647	1/1	0.91	0.10	35,35,35,35	0
60	MG	a	1730	1/1	0.91	0.45	53,53,53,53	0
60	MG	A	3365	1/1	0.91	0.16	35,35,35,35	0
60	MG	A	3370	1/1	0.91	0.38	39,39,39,39	0
60	MG	a	1736	1/1	0.91	0.07	46,46,46,46	0
60	MG	a	1740	1/1	0.91	0.24	58,58,58,58	0
60	MG	a	1651	1/1	0.91	0.13	64,64,64,64	0
60	MG	A	3524	1/1	0.91	0.19	49,49,49,49	1
60	MG	a	1747	1/1	0.91	0.11	38,38,38,38	0
60	MG	a	1751	1/1	0.91	0.14	59,59,59,59	0
60	MG	A	3176	1/1	0.91	0.13	37,37,37,37	0
60	MG	A	3165	1/1	0.91	0.34	42,42,42,42	0
60	MG	A	3218	1/1	0.91	0.65	52,52,52,52	0
60	MG	A	3311	1/1	0.91	0.20	41,41,41,41	0
60	MG	a	1762	1/1	0.91	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3578	1/1	0.91	0.18	60,60,60,60	0
60	MG	A	3312	1/1	0.91	0.18	40,40,40,40	0
60	MG	A	3385	1/1	0.91	0.16	35,35,35,35	0
60	MG	a	1769	1/1	0.91	0.12	58,58,58,58	0
60	MG	A	3315	1/1	0.91	0.16	37,37,37,37	0
60	MG	A	3460	1/1	0.91	0.13	41,41,41,41	0
60	MG	8	101	1/1	0.91	0.21	35,35,35,35	0
60	MG	9	101	1/1	0.91	0.31	50,50,50,50	0
60	MG	A	3461	1/1	0.91	0.22	40,40,40,40	0
60	MG	a	1783	1/1	0.91	0.39	60,60,60,60	0
60	MG	B	205	1/1	0.91	0.15	52,52,52,52	0
60	MG	A	3058	1/1	0.91	0.21	59,59,59,59	0
60	MG	A	3392	1/1	0.91	0.17	42,42,42,42	0
60	MG	a	1787	1/1	0.91	0.90	40,40,40,40	1
60	MG	A	3346	1/1	0.91	0.21	57,57,57,57	0
60	MG	A	3400	1/1	0.91	0.35	42,42,42,42	0
60	MG	A	3203	1/1	0.91	0.26	52,52,52,52	0
60	MG	A	3403	1/1	0.91	0.20	37,37,37,37	0
60	MG	n	102	1/1	0.91	0.32	28,28,28,28	0
60	MG	v	101	1/1	0.91	0.36	35,35,35,35	1
60	MG	A	3598	1/1	0.91	0.18	29,29,29,29	0
60	MG	a	1680	1/1	0.91	0.33	60,60,60,60	0
60	MG	A	3035	1/1	0.91	0.40	30,30,30,30	1
60	MG	a	1682	1/1	0.91	0.20	45,45,45,45	0
60	MG	A	3493	1/1	0.91	0.25	48,48,48,48	1
60	MG	a	1685	1/1	0.91	0.16	46,46,46,46	0
60	MG	a	1695	1/1	0.92	0.41	40,40,40,40	0
60	MG	D	302	1/1	0.92	0.19	43,43,43,43	0
60	MG	A	3095	1/1	0.92	0.10	32,32,32,32	0
60	MG	A	3359	1/1	0.92	0.16	63,63,63,63	0
60	MG	A	3442	1/1	0.92	0.44	60,60,60,60	0
60	MG	A	3233	1/1	0.92	0.12	56,56,56,56	0
60	MG	A	3103	1/1	0.92	0.17	44,44,44,44	0
60	MG	A	3115	1/1	0.92	0.33	27,27,27,27	1
60	MG	a	1637	1/1	0.92	0.41	54,54,54,54	0
60	MG	A	3538	1/1	0.92	0.27	39,39,39,39	0
60	MG	a	1639	1/1	0.92	0.15	48,48,48,48	0
60	MG	A	3367	1/1	0.92	0.15	40,40,40,40	0
60	MG	A	3317	1/1	0.92	0.09	52,52,52,52	0
60	MG	A	3104	1/1	0.92	0.17	25,25,25,25	0
60	MG	a	1719	1/1	0.92	0.20	48,48,48,48	0
60	MG	A	3543	1/1	0.92	0.26	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3166	1/1	0.92	0.17	40,40,40,40	0
60	MG	A	3219	1/1	0.92	0.20	50,50,50,50	0
60	MG	A	3377	1/1	0.92	0.29	26,26,26,26	0
60	MG	A	3379	1/1	0.92	0.15	36,36,36,36	0
60	MG	A	3326	1/1	0.92	0.17	32,32,32,32	0
60	MG	A	3194	1/1	0.92	0.12	63,63,63,63	0
60	MG	A	3329	1/1	0.92	0.21	33,33,33,33	1
60	MG	A	3614	1/1	0.92	0.19	39,39,39,39	0
60	MG	A	3076	1/1	0.92	0.27	33,33,33,33	1
60	MG	A	3388	1/1	0.92	0.19	31,31,31,31	0
60	MG	A	3488	1/1	0.92	0.24	41,41,41,41	0
60	MG	A	3623	1/1	0.92	0.35	57,57,57,57	0
60	MG	A	3390	1/1	0.92	0.13	36,36,36,36	0
60	MG	A	3222	1/1	0.92	0.15	39,39,39,39	0
60	MG	A	3626	1/1	0.92	0.26	30,30,30,30	1
60	MG	A	3288	1/1	0.92	0.24	45,45,45,45	0
60	MG	A	3136	1/1	0.92	0.27	32,32,32,32	0
60	MG	A	3631	1/1	0.92	0.42	24,24,24,24	1
60	MG	a	1768	1/1	0.92	0.36	43,43,43,43	0
60	MG	A	3632	1/1	0.92	0.26	35,35,35,35	1
60	MG	a	1670	1/1	0.92	0.10	57,57,57,57	0
60	MG	a	1671	1/1	0.92	0.22	48,48,48,48	0
60	MG	a	1773	1/1	0.92	0.14	58,58,58,58	0
60	MG	A	3034	1/1	0.92	0.43	59,59,59,59	0
60	MG	A	3634	1/1	0.92	0.14	42,42,42,42	1
60	MG	A	3635	1/1	0.92	0.35	29,29,29,29	1
60	MG	A	3504	1/1	0.92	0.21	25,25,25,25	0
60	MG	A	3108	1/1	0.92	0.36	60,60,60,60	0
60	MG	A	3569	1/1	0.92	0.18	41,41,41,41	0
60	MG	a	1678	1/1	0.92	0.23	36,36,36,36	0
60	MG	a	1605	1/1	0.92	0.27	54,54,54,54	0
60	MG	A	3292	1/1	0.92	0.42	47,47,47,47	0
60	MG	A	3293	1/1	0.92	0.26	48,48,48,48	0
60	MG	A	3021	1/1	0.92	0.19	34,34,34,34	0
60	MG	A	3414	1/1	0.92	0.09	47,47,47,47	0
60	MG	A	3248	1/1	0.92	0.34	48,48,48,48	1
60	MG	A	3028	1/1	0.92	0.11	57,57,57,57	0
60	MG	A	3125	1/1	0.92	0.30	22,22,22,22	1
60	MG	A	3300	1/1	0.92	0.28	42,42,42,42	0
60	MG	A	3204	1/1	0.92	0.35	39,39,39,39	0
60	MG	A	3306	1/1	0.92	0.28	33,33,33,33	0
60	MG	A	3307	1/1	0.92	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3009	1/1	0.92	0.14	52,52,52,52	0
60	MG	A	3466	1/1	0.93	0.22	49,49,49,49	0
60	MG	A	3409	1/1	0.93	0.16	35,35,35,35	0
60	MG	A	3048	1/1	0.93	0.15	35,35,35,35	0
60	MG	A	3189	1/1	0.93	0.31	50,50,50,50	0
60	MG	A	3476	1/1	0.93	0.09	58,58,58,58	0
60	MG	A	3019	1/1	0.93	0.31	20,20,20,20	0
60	MG	A	3482	1/1	0.93	0.25	38,38,38,38	0
60	MG	G	201	1/1	0.93	0.21	48,48,48,48	0
60	MG	A	3285	1/1	0.93	0.31	31,31,31,31	0
60	MG	a	1714	1/1	0.93	0.44	54,54,54,54	0
60	MG	A	3427	1/1	0.93	0.20	49,49,49,49	0
60	MG	A	3428	1/1	0.93	0.19	56,56,56,56	0
60	MG	A	3494	1/1	0.93	0.20	35,35,35,35	0
60	MG	A	3553	1/1	0.93	0.25	51,51,51,51	1
60	MG	A	3287	1/1	0.93	0.20	35,35,35,35	0
60	MG	a	1649	1/1	0.93	0.43	67,67,67,67	0
60	MG	A	3431	1/1	0.93	0.31	52,52,52,52	0
60	MG	A	3500	1/1	0.93	0.20	30,30,30,30	0
60	MG	A	3020	1/1	0.93	0.18	26,26,26,26	0
60	MG	A	3313	1/1	0.93	0.17	29,29,29,29	0
60	MG	A	3193	1/1	0.93	0.22	27,27,27,27	0
60	MG	A	3561	1/1	0.93	0.20	60,60,60,60	0
60	MG	a	1658	1/1	0.93	0.12	30,30,30,30	0
60	MG	A	3507	1/1	0.93	0.13	42,42,42,42	0
60	MG	X	101	1/1	0.93	0.25	50,50,50,50	0
60	MG	A	3508	1/1	0.93	0.11	68,68,68,68	0
60	MG	a	1753	1/1	0.93	0.32	46,46,46,46	0
60	MG	a	1754	1/1	0.93	0.12	42,42,42,42	0
60	MG	a	1755	1/1	0.93	0.08	40,40,40,40	0
60	MG	A	3566	1/1	0.93	0.44	55,55,55,55	0
60	MG	A	3381	1/1	0.93	0.16	56,56,56,56	0
60	MG	5	101	1/1	0.93	0.30	44,44,44,44	1
60	MG	A	3207	1/1	0.93	0.32	61,61,61,61	0
60	MG	A	3345	1/1	0.93	0.26	48,48,48,48	0
60	MG	A	3093	1/1	0.93	0.30	50,50,50,50	0
60	MG	A	3347	1/1	0.93	0.27	37,37,37,37	1
60	MG	A	3349	1/1	0.93	0.18	42,42,42,42	0
60	MG	A	3575	1/1	0.93	0.29	39,39,39,39	1
60	MG	A	3641	1/1	0.93	0.17	32,32,32,32	1
60	MG	A	3195	1/1	0.93	0.47	55,55,55,55	0
60	MG	A	3210	1/1	0.93	0.56	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3452	1/1	0.93	0.07	69,69,69,69	0
60	MG	a	1777	1/1	0.93	0.28	32,32,32,32	1
60	MG	a	1778	1/1	0.93	0.26	53,53,53,53	0
60	MG	A	3211	1/1	0.93	0.23	50,50,50,50	0
60	MG	A	3455	1/1	0.93	0.27	28,28,28,28	0
60	MG	A	3325	1/1	0.93	0.14	23,23,23,23	0
60	MG	A	3583	1/1	0.93	0.21	46,46,46,46	0
60	MG	A	3457	1/1	0.93	0.18	24,24,24,24	0
60	MG	A	3156	1/1	0.93	0.19	26,26,26,26	0
60	MG	A	3149	1/1	0.93	0.08	54,54,54,54	0
60	MG	a	1617	1/1	0.93	0.38	47,47,47,47	0
60	MG	a	1619	1/1	0.93	0.27	32,32,32,32	0
60	MG	A	3007	1/1	0.93	0.21	35,35,35,35	0
60	MG	A	3134	1/1	0.93	0.19	25,25,25,25	0
60	MG	a	1623	1/1	0.93	0.22	46,46,46,46	1
60	MG	A	3463	1/1	0.93	0.68	48,48,48,48	0
60	MG	x	101	1/1	0.93	0.33	29,29,29,29	1
60	MG	A	3464	1/1	0.93	0.13	56,56,56,56	0
60	MG	A	3596	1/1	0.93	0.25	44,44,44,44	1
60	MG	x	107	1/1	0.93	0.09	69,69,69,69	0
60	MG	D	306	1/1	0.93	0.16	25,25,25,25	0
60	MG	A	3539	1/1	0.93	0.17	21,21,21,21	0
60	MG	a	1696	1/1	0.93	0.49	52,52,52,52	0
60	MG	A	3303	1/1	0.93	0.17	57,57,57,57	0
60	MG	A	3364	1/1	0.94	0.10	45,45,45,45	0
60	MG	A	3621	1/1	0.94	0.31	48,48,48,48	0
60	MG	A	3078	1/1	0.94	0.33	27,27,27,27	1
60	MG	a	1737	1/1	0.94	0.35	46,46,46,46	0
60	MG	a	1739	1/1	0.94	0.17	42,42,42,42	0
60	MG	a	1618	1/1	0.94	0.54	54,54,54,54	0
60	MG	A	3498	1/1	0.94	0.15	68,68,68,68	0
60	MG	A	3185	1/1	0.94	0.22	32,32,32,32	0
60	MG	a	1745	1/1	0.94	0.21	40,40,40,40	0
60	MG	A	3304	1/1	0.94	0.13	53,53,53,53	0
60	MG	A	3126	1/1	0.94	0.28	28,28,28,28	1
60	MG	a	1624	1/1	0.94	0.14	39,39,39,39	0
60	MG	A	3372	1/1	0.94	0.20	41,41,41,41	0
60	MG	A	3327	1/1	0.94	0.23	30,30,30,30	0
60	MG	A	3214	1/1	0.94	0.52	44,44,44,44	1
60	MG	A	3584	1/1	0.94	0.13	39,39,39,39	0
60	MG	A	3131	1/1	0.94	0.20	57,57,57,57	0
60	MG	A	3547	1/1	0.94	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3331	1/1	0.94	0.21	31,31,31,31	0
60	MG	A	3637	1/1	0.94	0.45	37,37,37,37	0
60	MG	a	1634	1/1	0.94	0.35	53,53,53,53	0
60	MG	a	1766	1/1	0.94	0.24	49,49,49,49	0
60	MG	A	3175	1/1	0.94	0.19	62,62,62,62	0
60	MG	A	3352	1/1	0.94	0.36	39,39,39,39	0
60	MG	A	3516	1/1	0.94	0.19	25,25,25,25	1
60	MG	A	3053	1/1	0.94	0.27	35,35,35,35	0
60	MG	A	3643	1/1	0.94	0.29	34,34,34,34	0
60	MG	A	3192	1/1	0.94	0.18	26,26,26,26	0
60	MG	a	1774	1/1	0.94	0.14	29,29,29,29	0
60	MG	A	3432	1/1	0.94	0.16	54,54,54,54	0
60	MG	A	3386	1/1	0.94	0.24	33,33,33,33	0
60	MG	0	103	1/1	0.94	0.08	53,53,53,53	0
60	MG	A	3469	1/1	0.94	0.12	48,48,48,48	0
60	MG	A	3523	1/1	0.94	0.28	31,31,31,31	0
60	MG	A	3205	1/1	0.94	0.17	53,53,53,53	0
60	MG	6	103	1/1	0.94	0.17	41,41,41,41	0
60	MG	A	3138	1/1	0.94	0.12	31,31,31,31	0
60	MG	A	3605	1/1	0.94	0.36	50,50,50,50	0
60	MG	A	3526	1/1	0.94	0.20	29,29,29,29	0
60	MG	a	1707	1/1	0.94	0.16	34,34,34,34	0
60	MG	A	3139	1/1	0.94	0.30	37,37,37,37	0
60	MG	a	1710	1/1	0.94	0.34	53,53,53,53	1
60	MG	a	1711	1/1	0.94	0.18	48,48,48,48	0
60	MG	A	3608	1/1	0.94	0.23	32,32,32,32	0
60	MG	n	103	1/1	0.94	0.31	55,55,55,55	0
60	MG	A	3478	1/1	0.94	0.34	50,50,50,50	0
60	MG	v	102	1/1	0.94	0.30	42,42,42,42	0
60	MG	A	3564	1/1	0.94	0.13	52,52,52,52	0
60	MG	x	102	1/1	0.94	0.07	77,77,77,77	0
60	MG	A	3140	1/1	0.94	0.19	48,48,48,48	0
60	MG	x	105	1/1	0.94	0.12	51,51,51,51	0
60	MG	A	3128	1/1	0.94	0.26	37,37,37,37	0
60	MG	A	3393	1/1	0.94	0.28	41,41,41,41	0
60	MG	A	3533	1/1	0.94	0.41	52,52,52,52	0
60	MG	A	3363	1/1	0.94	0.21	35,35,35,35	0
60	MG	a	1613	1/1	0.94	0.26	29,29,29,29	0
60	MG	A	3398	1/1	0.94	0.10	37,37,37,37	0
60	MG	A	3074	1/1	0.95	0.15	29,29,29,29	0
60	MG	B	218	1/1	0.95	0.27	49,49,49,49	0
60	MG	A	3426	1/1	0.95	0.15	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	a	1668	1/1	0.95	0.18	30,30,30,30	0
60	MG	A	3357	1/1	0.95	0.48	36,36,36,36	0
60	MG	A	3522	1/1	0.95	0.21	28,28,28,28	0
60	MG	D	305	1/1	0.95	0.43	43,43,43,43	0
60	MG	a	1749	1/1	0.95	0.33	54,54,54,54	0
60	MG	a	1750	1/1	0.95	0.22	41,41,41,41	0
60	MG	A	3467	1/1	0.95	0.21	37,37,37,37	0
60	MG	A	3069	1/1	0.95	0.24	30,30,30,30	0
60	MG	A	3027	1/1	0.95	0.14	62,62,62,62	0
60	MG	A	3567	1/1	0.95	0.15	38,38,38,38	1
60	MG	A	3186	1/1	0.95	0.13	33,33,33,33	0
60	MG	a	1757	1/1	0.95	0.24	46,46,46,46	0
60	MG	A	3616	1/1	0.95	0.18	45,45,45,45	0
60	MG	A	3473	1/1	0.95	0.18	27,27,27,27	0
60	MG	a	1760	1/1	0.95	0.17	38,38,38,38	0
60	MG	A	3570	1/1	0.95	0.17	54,54,54,54	0
60	MG	A	3389	1/1	0.95	0.10	33,33,33,33	0
60	MG	A	3294	1/1	0.95	0.18	25,25,25,25	1
60	MG	A	3622	1/1	0.95	0.35	57,57,57,57	0
60	MG	A	3434	1/1	0.95	0.23	41,41,41,41	0
60	MG	a	1684	1/1	0.95	0.14	31,31,31,31	0
60	MG	A	3279	1/1	0.95	0.29	30,30,30,30	1
60	MG	A	3481	1/1	0.95	0.13	46,46,46,46	0
60	MG	A	3187	1/1	0.95	0.40	31,31,31,31	0
60	MG	a	1771	1/1	0.95	0.13	67,67,67,67	0
60	MG	A	3485	1/1	0.95	0.16	59,59,59,59	0
60	MG	A	3628	1/1	0.95	0.30	35,35,35,35	0
60	MG	A	3629	1/1	0.95	0.17	21,21,21,21	0
60	MG	A	3174	1/1	0.95	0.26	25,25,25,25	0
60	MG	A	3105	1/1	0.95	0.25	28,28,28,28	1
60	MG	A	3397	1/1	0.95	0.27	38,38,38,38	0
60	MG	A	3368	1/1	0.95	0.21	36,36,36,36	0
60	MG	A	3323	1/1	0.95	0.15	72,72,72,72	0
60	MG	A	3241	1/1	0.95	0.22	20,20,20,20	0
60	MG	A	3301	1/1	0.95	0.29	54,54,54,54	0
60	MG	A	3033	1/1	0.95	0.26	59,59,59,59	1
60	MG	A	3405	1/1	0.95	0.29	32,32,32,32	0
60	MG	a	1646	1/1	0.95	0.20	52,52,52,52	0
60	MG	A	3215	1/1	0.95	0.42	44,44,44,44	0
60	MG	A	3454	1/1	0.95	0.42	44,44,44,44	0
60	MG	0	104	1/1	0.95	0.40	36,36,36,36	1
60	MG	l	201	1/1	0.95	0.22	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3408	1/1	0.95	0.27	33,33,33,33	0
60	MG	A	3286	1/1	0.95	0.49	48,48,48,48	0
60	MG	a	1652	1/1	0.95	0.18	20,20,20,20	0
60	MG	A	3595	1/1	0.95	0.27	27,27,27,27	0
60	MG	A	3410	1/1	0.95	0.23	44,44,44,44	0
60	MG	a	1655	1/1	0.95	0.40	47,47,47,47	0
60	MG	A	3061	1/1	0.95	0.28	43,43,43,43	0
60	MG	A	3513	1/1	0.95	0.18	58,58,58,58	0
60	MG	A	3416	1/1	0.95	0.17	31,31,31,31	0
60	MG	A	3601	1/1	0.95	0.24	33,33,33,33	0
60	MG	B	208	1/1	0.95	0.08	64,64,64,64	0
60	MG	A	3515	1/1	0.95	0.28	47,47,47,47	0
60	MG	A	3417	1/1	0.95	0.28	43,43,43,43	0
60	MG	A	3123	1/1	0.95	0.22	30,30,30,30	1
60	MG	A	3168	1/1	0.95	0.22	23,23,23,23	0
61	ZN	4	501	1/1	0.95	0.06	79,79,79,79	0
61	ZN	6	102	1/1	0.95	0.25	72,72,72,72	0
62	SF4	d	302	8/8	0.95	0.05	60,65,70,71	2
60	MG	E	302	1/1	0.96	0.29	32,32,32,32	0
60	MG	A	3230	1/1	0.96	0.26	40,40,40,40	0
60	MG	a	1756	1/1	0.96	0.15	52,52,52,52	0
60	MG	a	1692	1/1	0.96	0.25	41,41,41,41	0
60	MG	A	3529	1/1	0.96	0.12	59,59,59,59	0
60	MG	A	3495	1/1	0.96	0.16	35,35,35,35	0
60	MG	A	3030	1/1	0.96	0.18	33,33,33,33	0
60	MG	A	3298	1/1	0.96	0.20	34,34,34,34	0
60	MG	A	3366	1/1	0.96	0.15	19,19,19,19	1
60	MG	A	3337	1/1	0.96	0.29	48,48,48,48	0
60	MG	a	1700	1/1	0.96	0.25	50,50,50,50	0
60	MG	A	3077	1/1	0.96	0.31	24,24,24,24	1
60	MG	A	3412	1/1	0.96	0.21	44,44,44,44	0
60	MG	A	3440	1/1	0.96	0.13	45,45,45,45	0
60	MG	A	3640	1/1	0.96	0.14	30,30,30,30	1
60	MG	A	3506	1/1	0.96	0.33	41,41,41,41	0
60	MG	A	3116	1/1	0.96	0.24	47,47,47,47	0
60	MG	O	202	1/1	0.96	0.16	50,50,50,50	0
60	MG	A	3340	1/1	0.96	0.24	45,45,45,45	0
60	MG	a	1621	1/1	0.96	0.10	64,64,64,64	0
60	MG	A	3470	1/1	0.96	0.22	51,51,51,51	0
60	MG	Q	201	1/1	0.96	0.45	47,47,47,47	0
60	MG	A	3046	1/1	0.96	0.15	29,29,29,29	0
60	MG	B	203	1/1	0.96	0.07	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	a	1780	1/1	0.96	0.23	54,54,54,54	0
60	MG	a	1716	1/1	0.96	0.16	36,36,36,36	0
60	MG	A	3472	1/1	0.96	0.47	25,25,25,25	0
60	MG	A	3373	1/1	0.96	0.25	34,34,34,34	0
60	MG	A	3419	1/1	0.96	0.26	30,30,30,30	1
60	MG	A	3162	1/1	0.96	0.19	29,29,29,29	0
60	MG	a	1722	1/1	0.96	0.15	51,51,51,51	0
60	MG	a	1723	1/1	0.96	0.27	48,48,48,48	0
60	MG	A	3422	1/1	0.96	0.20	52,52,52,52	0
60	MG	a	1729	1/1	0.96	0.35	50,50,50,50	0
60	MG	A	3479	1/1	0.96	0.10	41,41,41,41	0
60	MG	m	201	1/1	0.96	0.22	38,38,38,38	1
60	MG	A	3619	1/1	0.96	0.30	16,16,16,16	0
60	MG	a	1633	1/1	0.96	0.21	32,32,32,32	0
60	MG	a	1735	1/1	0.96	0.15	37,37,37,37	0
60	MG	A	3395	1/1	0.96	0.29	51,51,51,51	0
60	MG	B	213	1/1	0.96	0.17	52,52,52,52	0
60	MG	B	214	1/1	0.96	0.07	59,59,59,59	0
60	MG	A	3330	1/1	0.96	0.34	37,37,37,37	1
60	MG	A	3005	1/1	0.96	0.17	31,31,31,31	1
60	MG	A	3360	1/1	0.96	0.19	54,54,54,54	0
60	MG	a	1743	1/1	0.96	0.31	45,45,45,45	0
60	MG	A	3023	1/1	0.96	0.17	34,34,34,34	0
60	MG	a	1746	1/1	0.96	0.09	49,49,49,49	0
60	MG	A	3489	1/1	0.96	0.26	27,27,27,27	0
60	MG	A	3490	1/1	0.96	0.12	40,40,40,40	0
60	MG	A	3113	1/1	0.96	0.25	29,29,29,29	1
61	ZN	Y	501	1/1	0.96	0.05	63,63,63,63	0
60	MG	A	3558	1/1	0.96	0.24	53,53,53,53	0
60	MG	a	1645	1/1	0.96	0.20	42,42,42,42	0
60	MG	A	3459	1/1	0.96	0.24	33,33,33,33	0
63	GCP	z	703	32/32	0.96	0.15	47,57,62,63	13
60	MG	A	3376	1/1	0.97	0.14	31,31,31,31	0
60	MG	A	3173	1/1	0.97	0.65	37,37,37,37	0
60	MG	A	3378	1/1	0.97	0.31	41,41,41,41	0
60	MG	A	3062	1/1	0.97	0.16	41,41,41,41	0
60	MG	P	203	1/1	0.97	0.28	45,45,45,45	1
60	MG	B	202	1/1	0.97	0.14	52,52,52,52	0
60	MG	A	3380	1/1	0.97	0.18	45,45,45,45	0
60	MG	A	3017	1/1	0.97	0.28	41,41,41,41	0
60	MG	A	3261	1/1	0.97	0.19	46,46,46,46	0
60	MG	A	3383	1/1	0.97	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3216	1/1	0.97	0.38	31,31,31,31	0
60	MG	A	3031	1/1	0.97	0.20	33,33,33,33	0
60	MG	A	3177	1/1	0.97	0.37	39,39,39,39	0
60	MG	B	210	1/1	0.97	0.13	44,44,44,44	0
60	MG	a	1776	1/1	0.97	0.25	52,52,52,52	0
60	MG	A	3411	1/1	0.97	0.15	39,39,39,39	0
60	MG	A	3439	1/1	0.97	0.25	50,50,50,50	0
60	MG	a	1726	1/1	0.97	0.10	43,43,43,43	0
60	MG	a	1728	1/1	0.97	0.13	33,33,33,33	0
60	MG	a	1781	1/1	0.97	0.23	46,46,46,46	0
60	MG	A	3302	1/1	0.97	0.15	22,22,22,22	0
60	MG	A	3413	1/1	0.97	0.13	35,35,35,35	0
60	MG	A	3178	1/1	0.97	0.40	56,56,56,56	0
60	MG	A	3582	1/1	0.97	0.19	21,21,21,21	1
60	MG	a	1733	1/1	0.97	0.28	51,51,51,51	0
60	MG	B	217	1/1	0.97	0.13	40,40,40,40	0
60	MG	A	3415	1/1	0.97	0.11	34,34,34,34	0
60	MG	D	301	1/1	0.97	0.26	21,21,21,21	0
60	MG	a	1738	1/1	0.97	0.17	35,35,35,35	0
60	MG	A	3445	1/1	0.97	0.26	42,42,42,42	1
60	MG	A	3475	1/1	0.97	0.15	41,41,41,41	0
60	MG	m	202	1/1	0.97	0.31	56,56,56,56	0
60	MG	A	3446	1/1	0.97	0.24	26,26,26,26	0
60	MG	A	3477	1/1	0.97	0.22	21,21,21,21	0
60	MG	A	3447	1/1	0.97	0.21	47,47,47,47	0
60	MG	a	1744	1/1	0.97	0.16	46,46,46,46	0
60	MG	A	3590	1/1	0.97	0.29	63,63,63,63	0
60	MG	A	3198	1/1	0.97	0.10	20,20,20,20	0
60	MG	A	3322	1/1	0.97	0.18	42,42,42,42	1
60	MG	a	1748	1/1	0.97	0.07	46,46,46,46	0
60	MG	A	3145	1/1	0.97	0.41	61,61,61,61	0
60	MG	A	3594	1/1	0.97	0.34	85,85,85,85	0
60	MG	A	3451	1/1	0.97	0.29	45,45,45,45	0
60	MG	A	3355	1/1	0.97	0.17	61,61,61,61	0
60	MG	A	3487	1/1	0.97	0.21	35,35,35,35	0
60	MG	A	3324	1/1	0.97	0.11	38,38,38,38	0
60	MG	A	3421	1/1	0.97	0.14	57,57,57,57	0
60	MG	a	1702	1/1	0.97	0.48	42,42,42,42	0
60	MG	A	3600	1/1	0.97	0.08	53,53,53,53	0
61	ZN	5	103	1/1	0.97	0.08	54,54,54,54	0
60	MG	A	3120	1/1	0.97	0.33	26,26,26,26	0
61	ZN	9	102	1/1	0.97	0.19	49,49,49,49	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3491	1/1	0.97	0.34	39,39,39,39	0
60	MG	A	3032	1/1	0.97	0.27	50,50,50,50	0
60	MG	a	1734	1/1	0.98	0.09	33,33,33,33	0
60	MG	A	3503	1/1	0.98	0.21	53,53,53,53	0
60	MG	A	3565	1/1	0.98	0.12	35,35,35,35	0
60	MG	A	3534	1/1	0.98	0.23	35,35,35,35	0
60	MG	A	3051	1/1	0.98	0.31	54,54,54,54	0
60	MG	A	3036	1/1	0.98	0.25	25,25,25,25	1
60	MG	a	1699	1/1	0.98	0.26	56,56,56,56	0
60	MG	A	3318	1/1	0.98	0.17	42,42,42,42	1
60	MG	A	3096	1/1	0.98	0.14	27,27,27,27	0
60	MG	A	3348	1/1	0.98	0.24	30,30,30,30	0
60	MG	A	3509	1/1	0.98	0.37	45,45,45,45	0
60	MG	A	3018	1/1	0.98	0.25	27,27,27,27	0
60	MG	A	3070	1/1	0.98	0.27	10,10,10,10	0
60	MG	a	1788	1/1	0.98	0.10	43,43,43,43	1
60	MG	A	3512	1/1	0.98	0.22	44,44,44,44	0
60	MG	A	3483	1/1	0.98	0.21	31,31,31,31	0
60	MG	a	1708	1/1	0.98	0.11	40,40,40,40	0
60	MG	A	3484	1/1	0.98	0.40	41,41,41,41	0
60	MG	A	3308	1/1	0.98	0.23	14,14,14,14	0
60	MG	A	3486	1/1	0.98	0.17	44,44,44,44	0
60	MG	A	3401	1/1	0.98	0.37	36,36,36,36	0
60	MG	A	3309	1/1	0.98	0.20	49,49,49,49	0
60	MG	A	3086	1/1	0.98	0.31	21,21,21,21	0
60	MG	a	1610	1/1	0.98	0.29	32,32,32,32	1
60	MG	A	3369	1/1	0.98	0.14	31,31,31,31	0
60	MG	A	3444	1/1	0.98	0.31	39,39,39,39	0
60	MG	A	3238	1/1	0.98	0.31	38,38,38,38	0
60	MG	A	3424	1/1	0.98	0.33	20,20,20,20	0
60	MG	x	104	1/1	0.98	0.30	43,43,43,43	0
60	MG	a	1720	1/1	0.98	0.22	48,48,48,48	0
60	MG	A	3587	1/1	0.98	0.28	23,23,23,23	1
60	MG	A	3425	1/1	0.98	0.28	54,54,54,54	0
60	MG	a	1764	1/1	0.98	0.49	37,37,37,37	0
60	MG	A	3013	1/1	0.98	0.23	24,24,24,24	0
60	MG	A	3407	1/1	0.98	0.17	30,30,30,30	0
60	MG	A	3497	1/1	0.98	0.25	38,38,38,38	1
60	MG	a	1727	1/1	0.98	0.13	49,49,49,49	0
60	MG	a	1688	1/1	0.98	0.22	32,32,32,32	0
60	MG	A	3171	1/1	0.98	0.19	31,31,31,31	0
60	MG	A	3314	1/1	0.98	0.09	48,48,48,48	0

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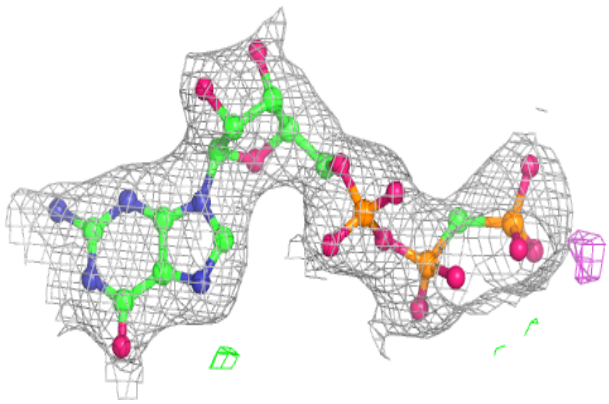
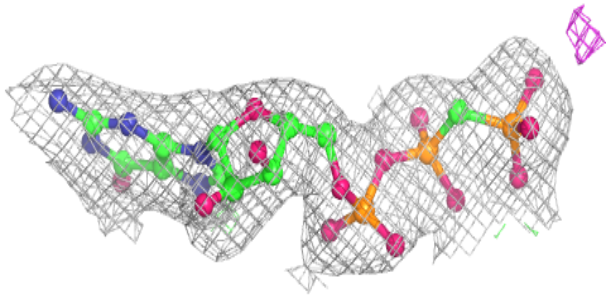
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	A	3430	1/1	0.98	0.22	43,43,43,43	0
60	MG	A	3501	1/1	0.98	0.15	24,24,24,24	0
60	MG	A	3213	1/1	0.98	0.10	34,34,34,34	1
60	MG	a	1607	1/1	0.99	0.35	42,42,42,42	1
60	MG	a	1608	1/1	0.99	0.29	23,23,23,23	0
60	MG	A	3184	1/1	0.99	0.42	30,30,30,30	0
60	MG	A	3273	1/1	0.99	0.34	37,37,37,37	1
60	MG	A	3615	1/1	0.99	0.14	34,34,34,34	0
60	MG	a	1724	1/1	0.99	0.34	42,42,42,42	0
60	MG	A	3399	1/1	0.99	0.28	44,44,44,44	0
61	ZN	n	104	1/1	0.99	0.15	44,44,44,44	0
60	MG	A	3396	1/1	0.99	0.18	26,26,26,26	0
60	MG	E	305	1/1	0.99	0.16	23,23,23,23	1

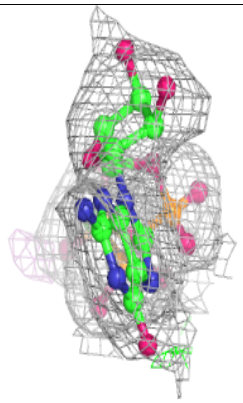
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GCP z 703:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.