



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:11 AM BST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

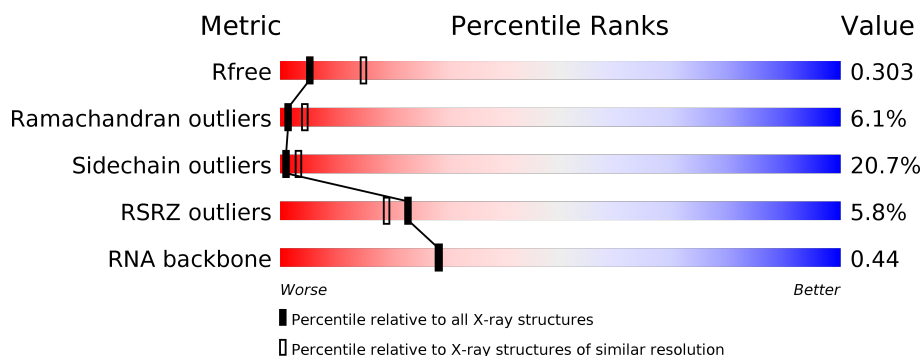
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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








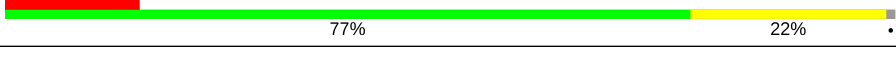

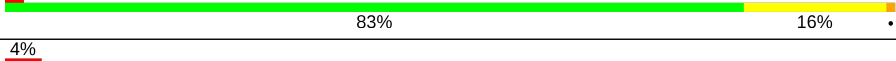

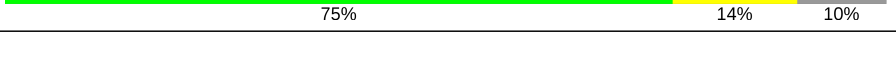
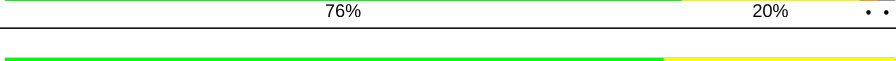
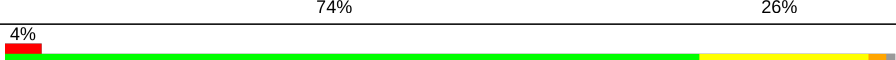
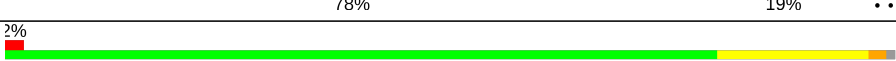

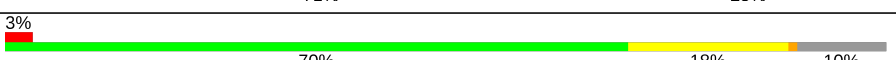


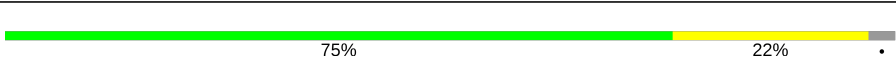



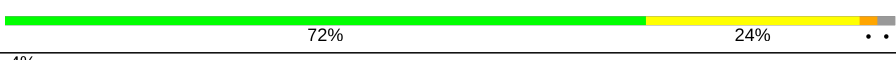
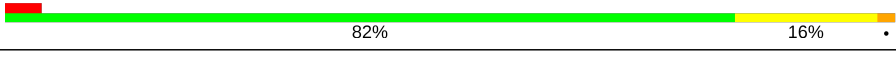


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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

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

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Mol	Chain	Length	Quality of chain
7	H	180	
8	J	173	
9	K	147	
10	N	140	
11	O	122	
12	P	150	
13	Q	141	
14	R	118	
15	S	112	
16	T	146	
17	U	118	
18	V	101	
19	W	113	
20	X	96	
21	Y	110	
22	Z	206	
23	0	85	
24	1	98	
25	2	72	
26	3	60	
27	4	71	
28	5	60	
29	6	54	
30	7	49	
31	8	65	

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Mol	Chain	Length	Quality of chain
32	9	37	
33	x	76	
34	a	1521	
35	b	256	
36	c	239	
37	d	209	
38	e	162	
39	f	101	
40	g	156	
41	h	138	
42	i	128	
43	j	105	
44	k	129	
45	l	132	
46	m	126	
47	n	61	
48	o	89	
49	p	88	
50	q	105	
51	r	88	
52	s	93	
53	t	106	
54	u	27	
55	w	76	
56	v	18	

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Mol	Chain	Length	Quality of chain
57	y	679	

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

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

## 2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2873	Total	C	N	O	P	0	0	0
			61879	27541	11577	19890	2871			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	r	68	Total	C	N	O	S	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	S	0	0	0
			199	122	48	29				

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

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

- Molecule 56 is a RNA chain called mRNA.

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

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

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

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

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

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

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

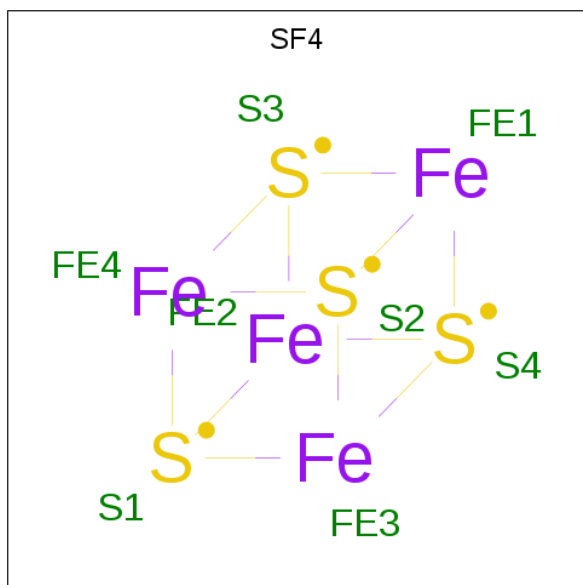
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y	1	Total 1	Zn 1	0	0
59	6	1	Total 1	Zn 1	0	0
59	4	1	Total 1	Zn 1	0	0

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

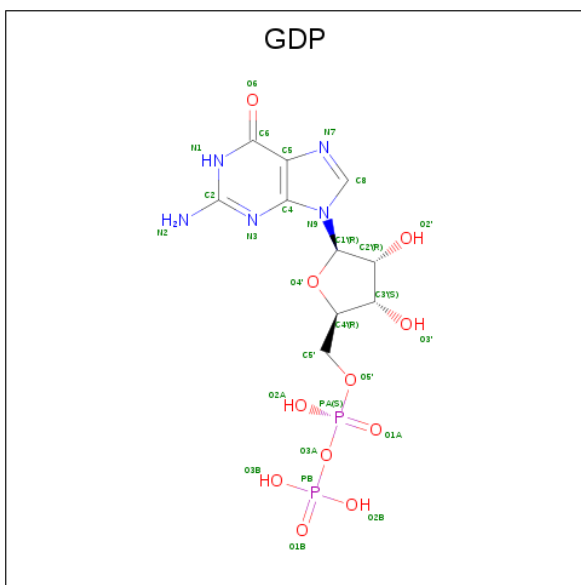
- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

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





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

- Molecule 62 is water.

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

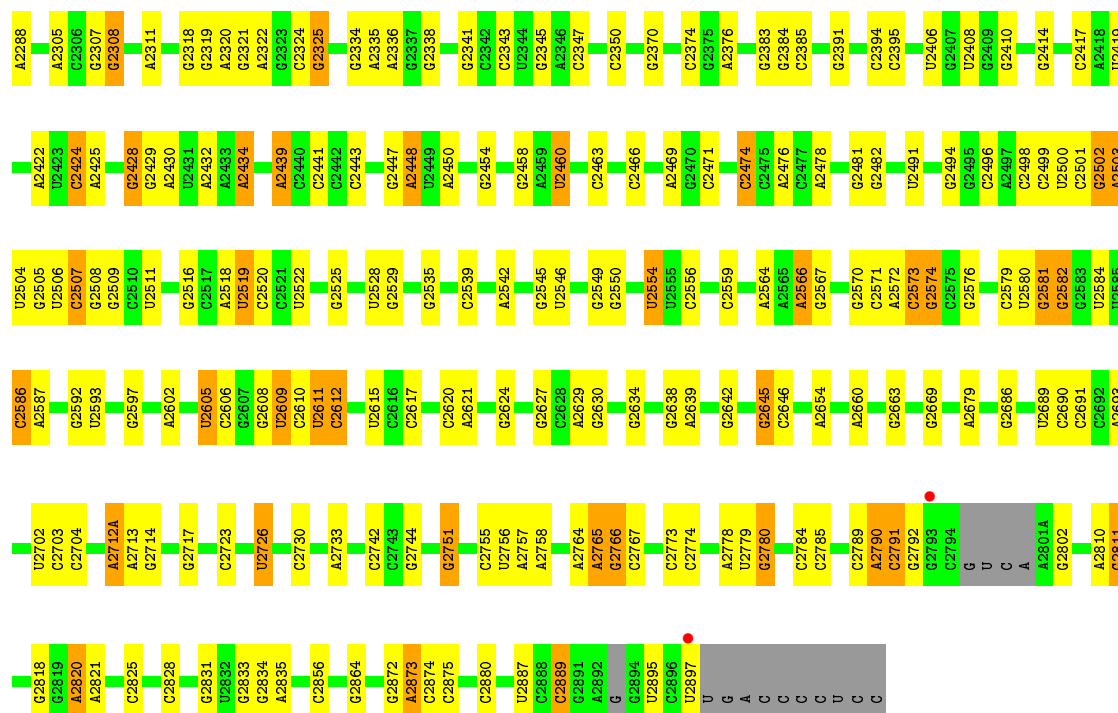
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	R	3	Total 3	O 3	0	0
62	U	2	Total 2	O 2	0	0
62	V	1	Total 1	O 1	0	0
62	W	2	Total 2	O 2	0	0
62	Y	1	Total 1	O 1	0	0
62	0	4	Total 4	O 4	0	0
62	1	2	Total 2	O 2	0	0
62	3	1	Total 1	O 1	0	0
62	5	1	Total 1	O 1	0	0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



A2199	A2134	C2065	C1988	C1914	C1782	G1667	A1572	A1460	A1353	G1245	C1145	G1051	G974
C2200	A2135	G2069	G1989	A1918	A1787	A1668	U1578	G1461	U1357	A1246	G1149	C1052	C975
C2201	C2136	G2070	C1990	A1919	A1787	A1669	U1578	C1467	G1358	A1247	G1149	A1053	G975A
C2202	C2137	G2071	U1991	A1920	G1790	U1673	G1581	C1467	A1359	G1250	C1152	A1054	C976
U2203	C2138	G2072	G1992	G1921	A1791	C1674	A1583	A1471	A1360	C1251	C1153	G1055	G977
C2205	C2139	C2073	U1993	G1924	G1792	G1674	A1583	U1481	C1363	G1252	G1154	G1058	G978
G2206	C2140	C2073	C1996	C1924	G1793	A1677	A1583	U1481	C1363	A1253	A1155	G1059	G979
G2207	G2141	C2073	G1997	U1994	U1794	A1677	A1583	G1482	C1362	G1256	A1156	A980	A981
A2208	C2142	C2073	G1997	U1994	U1794	A1677	A1583	G1482	C1362	C1257	G1157	U1061	A982
G2223	C2143	C2078	G1998	A1927	U1796	U1680	C1584	A1490	C1363	G1271	C1161	G1062	A983
G2224	C2144	U2079	G1999	G1928	U1796	U1680	C1584	A1490	C1363	A1272	C1166	A1067	A984
A2225	C2145	G2080	G2000	G1929	C1797	G1681	C1586	G1492	C1362	U1273	G1171	G1068	C985
C2226	C2146	C2084	A2001	G1930	U1798	G1681	C1586	G1492	A1365	A1276	A1174	A1073	C986
G2227	G2147	C2084	G2001	U1931	G1799	C1691	G1595	C1493	G1368	G1271	C1166	A1067	C985
G2228	G2148	G2087	G2011	A1932	C1800	C1694	C1599	C1493	G1368	A1272	G1166	G1068	C986
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G2230	G2151	G2088	G2018	C1934	A1802	G1695	C1599	G1500	A1373	A1275	G1173	A1070	C991
U2231	G2152	U2091	A2019	G1935	A1812	G1696	A1508	C1501	A1378	A1276	A1174	A1073	A996
G2233	G2153	G2092	A2020	A1936	G1813	G1697	A1509	C1502	A1379	G1277	U1175	C1076	G997
G2234	G2154	G2093	A2021	A1937	G1813	G1698	A1610	C1507	G1380	A1278	A1177	A1077	G1002
G2235	G2155	G2094	U2022	A1938	G1813	G1699	G1613	A1507	A1384	G1285	A1189	U1083	G1005
G2236	G2156	G2095	G2023	U1939	G1816	A1700	A1614	A1508	G1385	G1289	G1190	A1084	G1006
G2238	G2157	U2096	G2024	U1940	G1817	A1701	A1614	A1509	C1386	U1300	G1191	A1085	C1007
G2239	G2158	C2097	C2025	G1941	G1820	G1702	C1617	A1509A	A1395	G1289	U1198	U1088	G1008
G2240	G2159	U2098	C2026	C1942	A1821	G1705	A1618	C1511	A1398	G1299	U1199	U1088	U1012
G2242	G2160	U2098	G2027	U1943	G1822	G1705	A1618	C1511	A1398	A1301	U1199	U1088	U1012
U2243	G2161	U2102	U2028	U1944	G1823	G1721	G1619	G1519	C1398	C1306	G1202	U1088	U1012
G2246	G2162	C2103	G2029	G1950	G1823	A1722	G1620	G1519	A1404	C1307	G1203	A1089	U1014
U2249	C2163	G2104	A2030	U1951	C1827	U1739	U1621	U1523	U1405	A1308	U1205	A1089	G1015
G2250	C2164	G2105	A2031	A1952	G1828	G1740	G1622	G1526	U1406	G1307	A1204	A1089	G1015
G2251	G2165	G2106	G2032	A1953	A1829	C1745	G1628	G1529	G1404	A1308	G1206	U1108	G1016
G2252	U2167	U2107	A2033	G1954	C1837	C1745A	U1629	G1529	U1406	G1309	G1207	A1109	G1017
G2253	G2168	C2108	G2035	U1956	C1838	G1746	A1631A	G1532	G1416	G1310	G1208	A1110	U1019
U2257	A2169	U2109	U2036	C1957	C1838	G1747	A1632	G1532	C1417	U1313	G1209	A1111	A1020
A2170	G2170	G2110	G2038	G1958	G1842	C1751	G1633	G1532	G1417	C1314	A1210	G1112	A1021
A2171	G2171	C2111	C2039	G1959	G1842	C1751	A1634	G1537	U1420	G1320	U1211	G1115	G1022
U2172	U2172	G2112	C2040	A1960	A1847	G1756	A1637	G1537	G1424	A1321	A1213	G1115	U1025
A2173	A2173	U2113	C2043	C1961	A1877	U1757	A1644	G1542	G1424	A1322	A1214	G1119	U1026
C2174	C2174	G2115	U2047	C1962	G1878	G1758	C1645	A1542	A1427	G1325	G1218	C1123	A1027
C2175	C2175	G2116	G2048	U1963	G1878	G1758	C1645	C1543	C1428	G1328	G1219	C1124	G1030
A2176	A2176	G2117	G2049	C1964	A1889	A1762	G1647	C1547	G1429	U1329	A1220	A1127	U1033
C2178	C2178	U2118	G2049	C1966	C1895	G1763	G1648	C1547	C1430	G1332	C1222	A1128	G1034
C2179	C2179	U2118	G2049	C1967	G1896	G1764	G1649	C1547	G1436	G1332	C1224	A1129	U1035
U2180	U2180	A2051	A2051	A1970	G1897	G1767	G1650	A1553	C1437	G1338	G1227	U1130	G1036
G2271	G2181	G2052	G2052	A1971	U1898	C1767	G1651	A1554	G1437	G1338	G1227	G1131	G1037
A2272	G2182	G2053	G2053	A1971	U1898	C1767	G1651	A1554	A1445	G1339	G1227	C1135	G1038
G2273	G2183	G2054	A2054	A1972	G1899	G1772	G1652	A1555	G1450	A1342	C1230	C1135	A1041
C2275	G2184	C2055	C2055	A1973	G1900	A1773	G1653	A1558	C1450A	G1343	C1230	G1137	G1042
G2276	G2185	G2056	G2056	U1977	A1901	C1774	A1654	A1562	G1451	G1347	G1236	G1138	A1045
U2279	G2186	A2057	A2057	A1978	C1902	U1775	A1655	A1562	G1451	G1347	G1236	G1138	A1046
G2283	G2187	G2058	G2058	C1979	G1903	U1776	C1657	A1566	G1451	G1347	G1236	G1138	A1046
G2284	U2188	A2060	A2060	G1980	G1906	U1777	C1662	A1569	G1451	G1347	G1236	G1138	A1046
C2285	G2189	G2061	G2061	A1981	G1906	U1778	C1662	A1569	G1451	G1347	G1236	G1138	A1046
A2287	U2197	C2063	C2063	C1982	U1911	U1779	A1665	A1570	G1451	G1347	G1236	G1138	A1046
	U2197	C2063	C2063	C1982	A1912	U1779	A1665	A1570	G1451	G1347	G1236	G1138	A1046
A2198	A2198	G2133	G2133	G1983	A1913	C1781	G1666	A1571	G1459	C1350	G1244	G1144	G1047



• Molecule 2: 5S Ribosomal RNA

Chain B: 78% 19%



• Molecule 3: 50S ribosomal protein L2

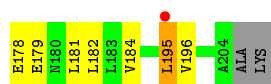
Chain D: 76% 22%



• Molecule 4: 50S ribosomal protein L3

Chain E: 81% 17%





- Molecule 5: 50S ribosomal protein L4

Chain F: 81% 17% ..



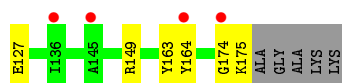
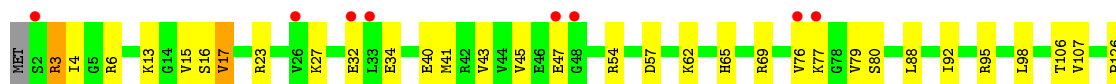
- Molecule 6: 50S ribosomal protein L5

Chain G: 3% 74% 24% ..



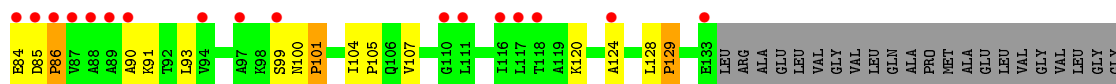
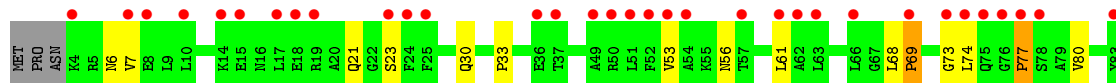
- Molecule 7: 50S ribosomal protein L6

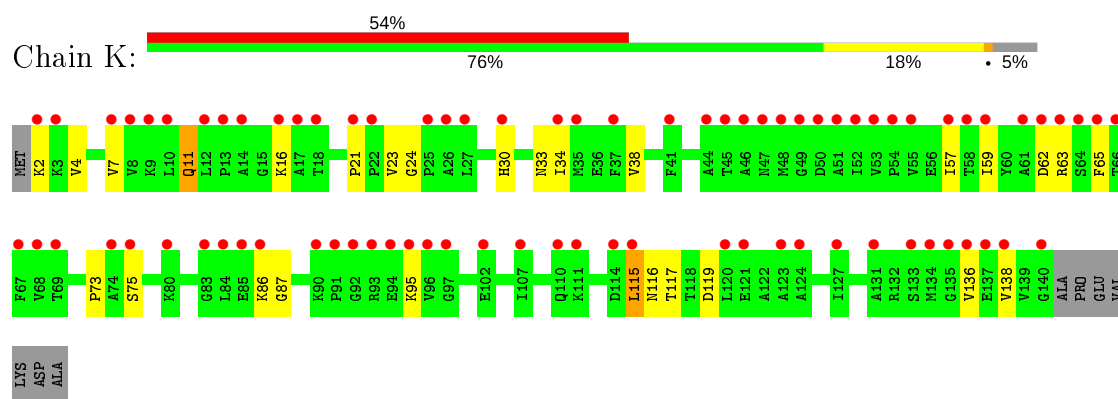
Chain H: 7% 76% 20% ..



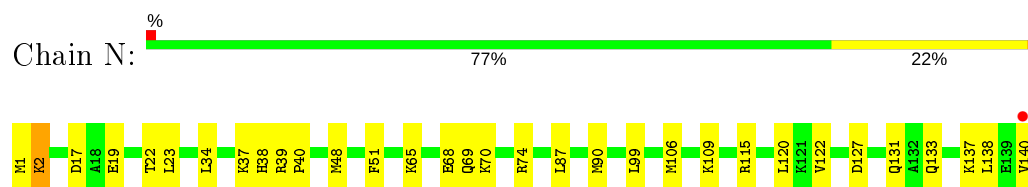
- Molecule 8: 50S ribosomal protein L10

Chain J: 29% 57% 15% 25%

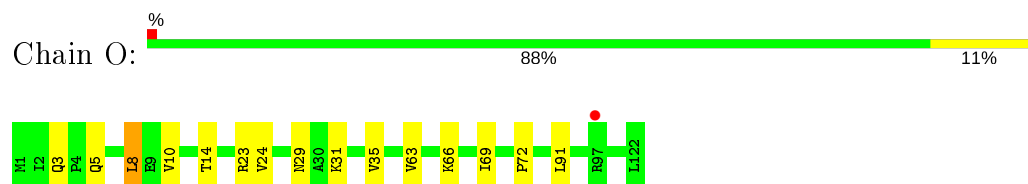




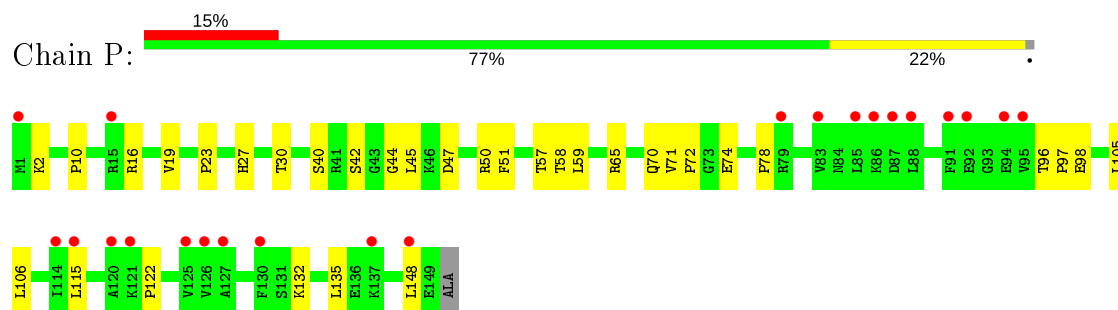
- Molecule 10: 50S ribosomal protein L13



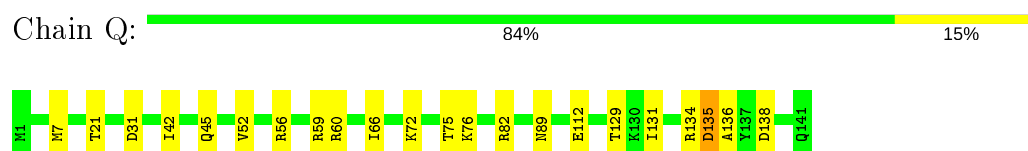
- Molecule 11: 50S ribosomal protein L14



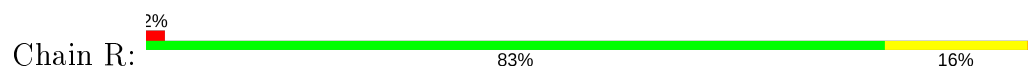
- Molecule 12: 50S ribosomal protein L15

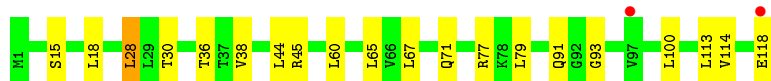


- Molecule 13: 50S ribosomal protein L16

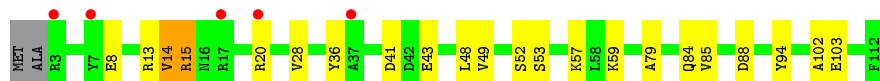
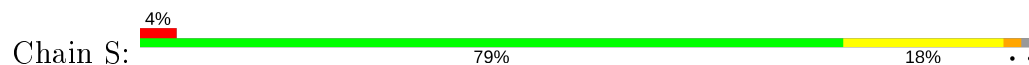


- Molecule 14: 50S ribosomal protein L17

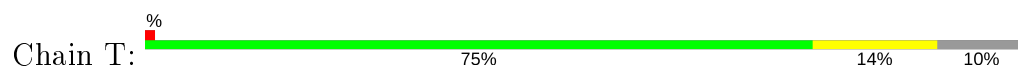




- Molecule 15: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L19



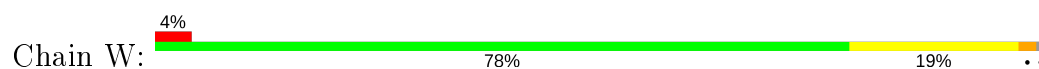
- Molecule 17: 50S ribosomal protein L20



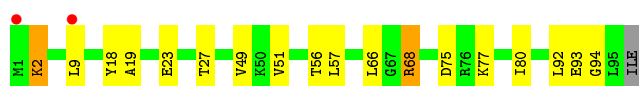
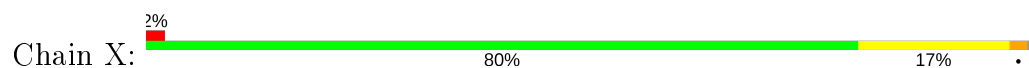
- Molecule 18: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L22

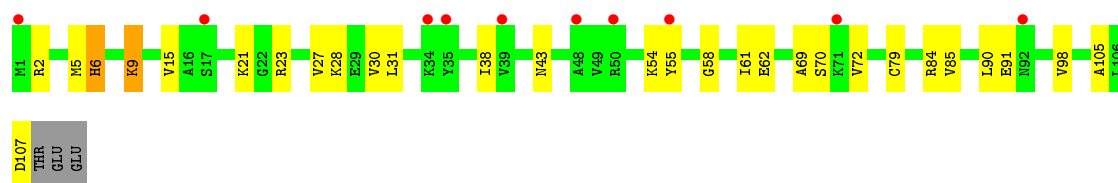


- Molecule 20: 50S ribosomal protein L23

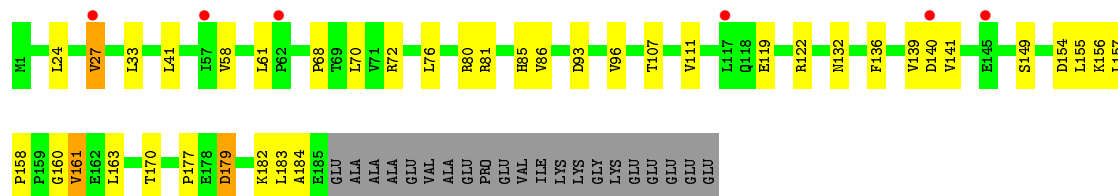


- Molecule 21: 50S ribosomal protein L24





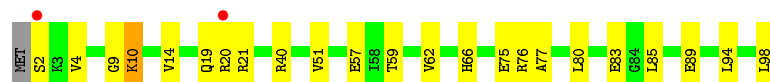
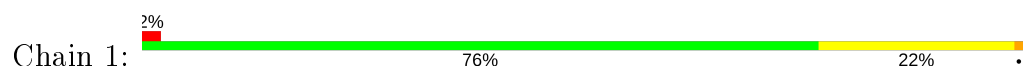
- Molecule 22: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L27



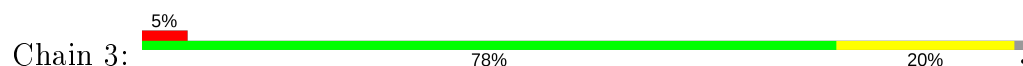
- Molecule 24: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L29



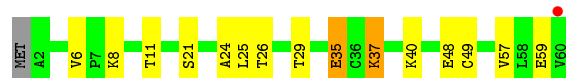
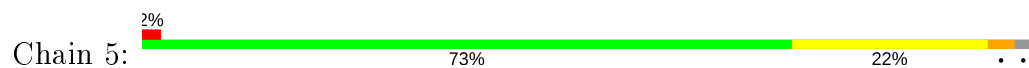
- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L31



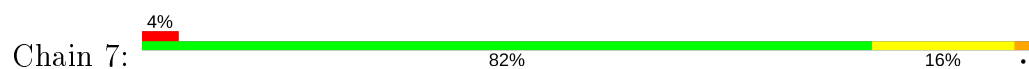
- Molecule 28: 50S ribosomal protein L32



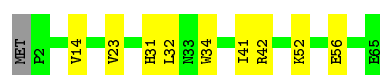
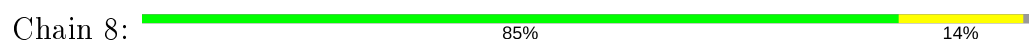
- Molecule 29: 50S ribosomal protein L33



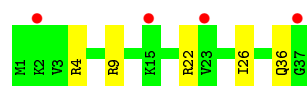
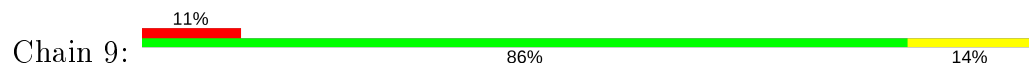
- Molecule 30: 50S ribosomal protein L34



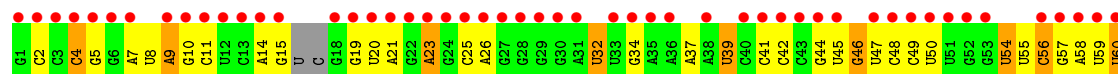
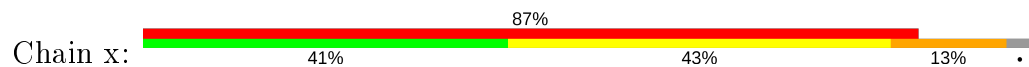
- Molecule 31: 50S ribosomal protein L35

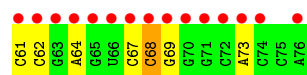


- Molecule 32: 50S ribosomal protein L36



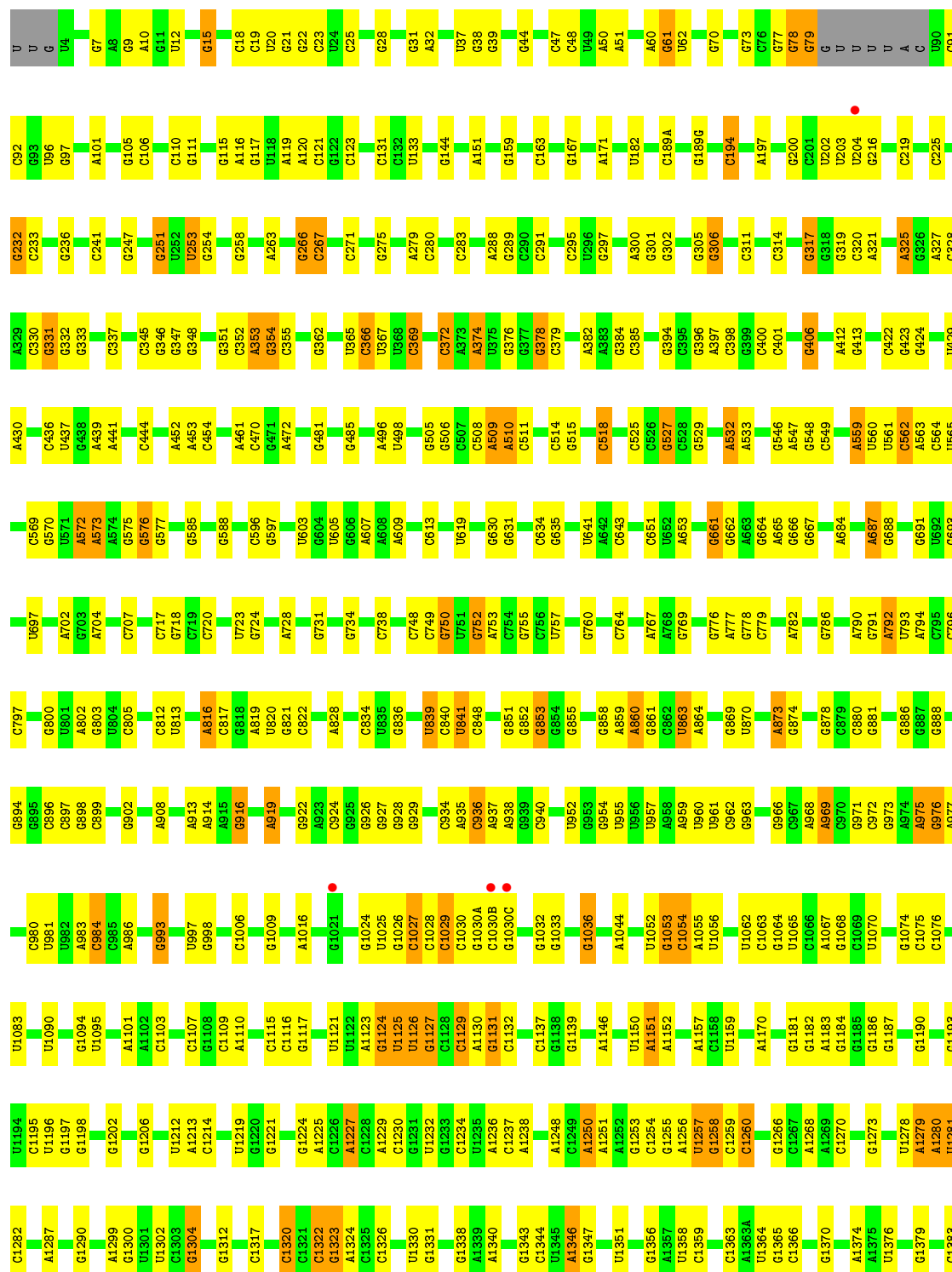
- Molecule 33: E-site tRNA

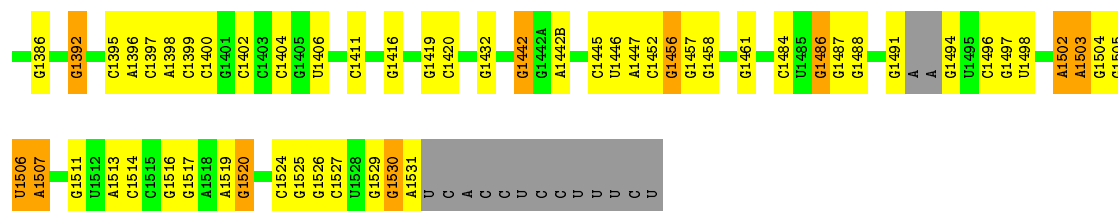




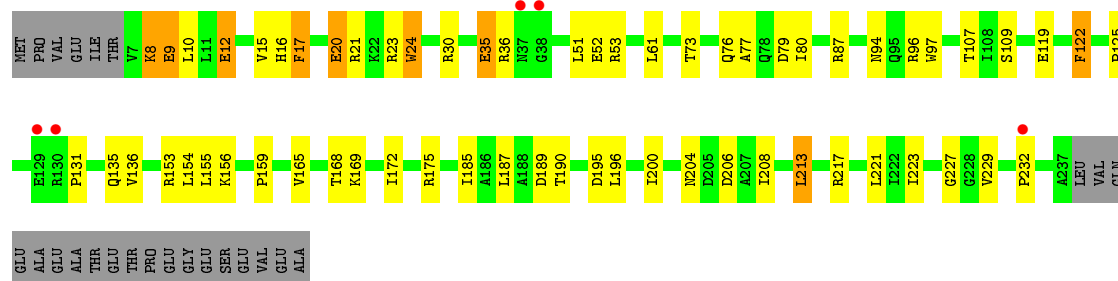
- Molecule 34: 16S Ribosomal RNA

Chain a:  63% 30% 6%

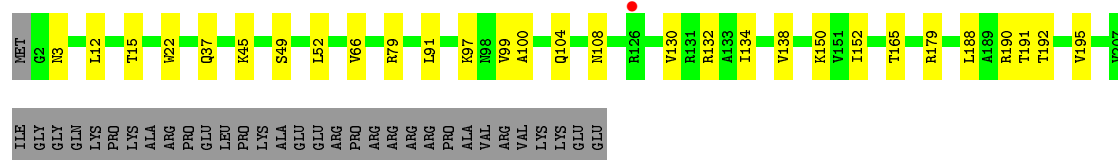




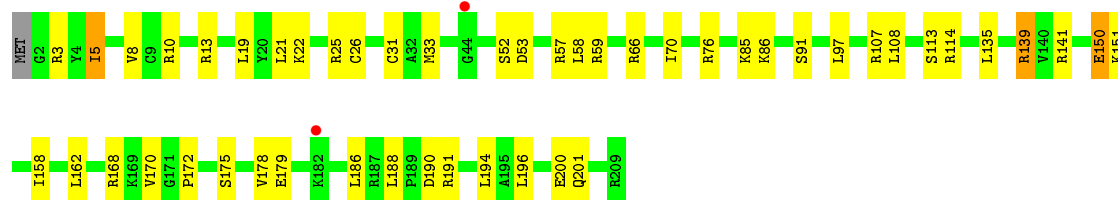
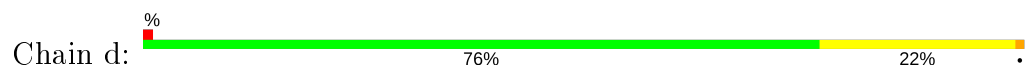
• Molecule 35: 30S ribosomal protein S2



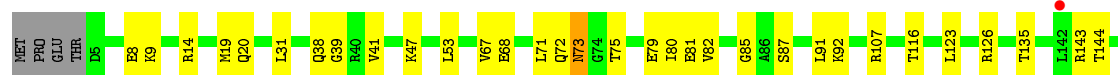
• Molecule 36: 30S ribosomal protein S3

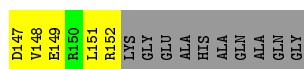


• Molecule 37: 30S ribosomal protein S4

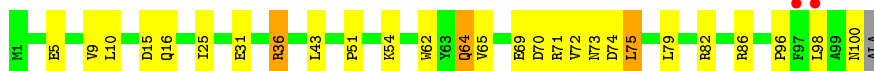


• Molecule 38: 30S ribosomal protein S5

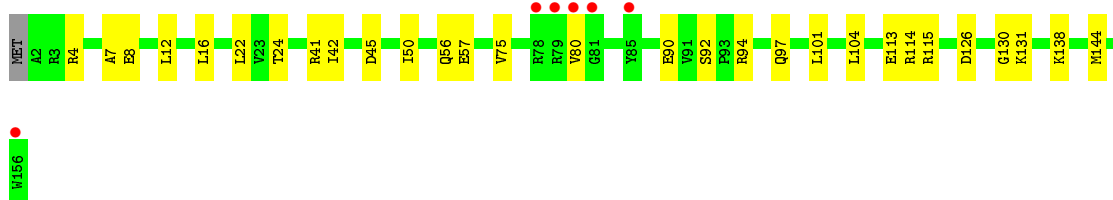
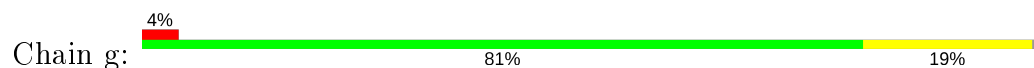




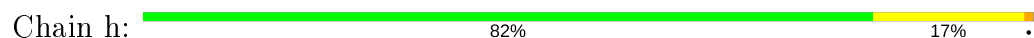
- Molecule 39: 30S ribosomal protein S6



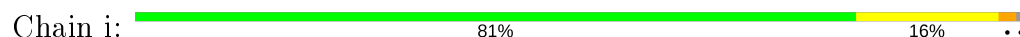
- Molecule 40: 30S ribosomal protein S7



- Molecule 41: 30S ribosomal protein S8



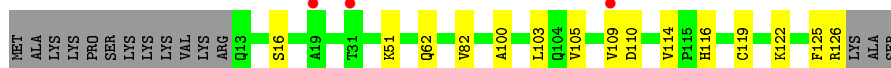
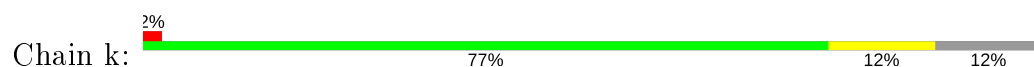
- Molecule 42: 30S ribosomal protein S9



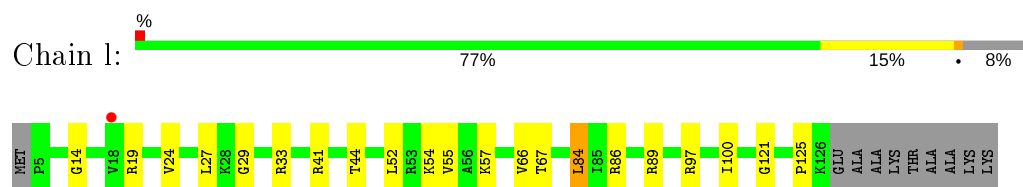
- Molecule 43: 30S ribosomal protein S10



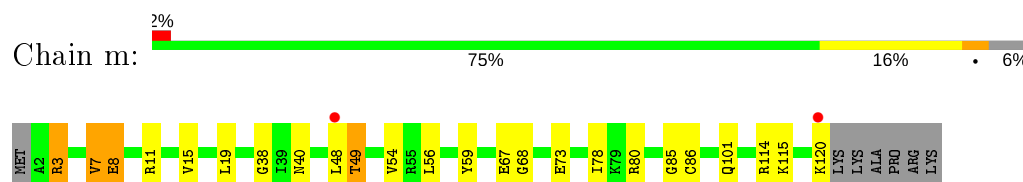
- Molecule 44: 30S ribosomal protein S11



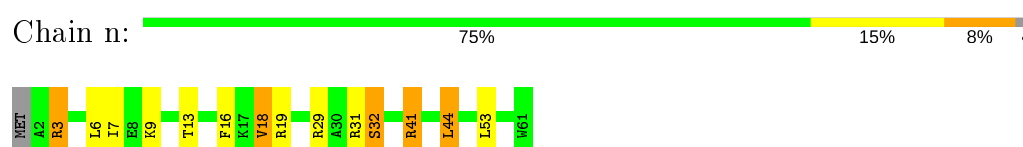
- Molecule 45: 30S ribosomal protein S12



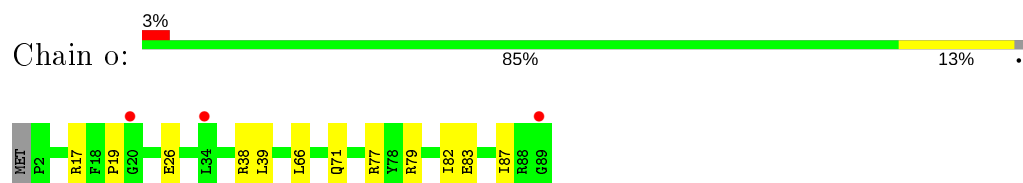
- Molecule 46: 30S ribosomal protein S13



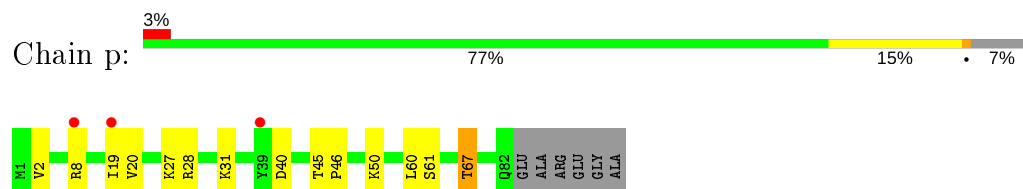
- Molecule 47: 30S ribosomal protein S14 type Z



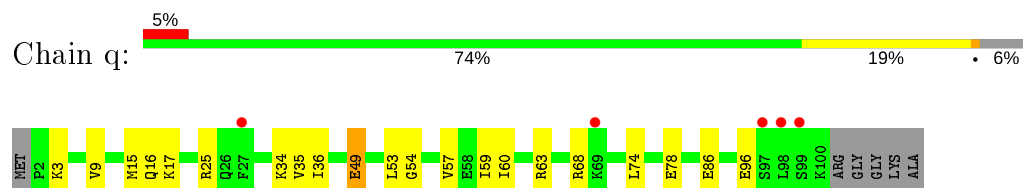
- Molecule 48: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S16

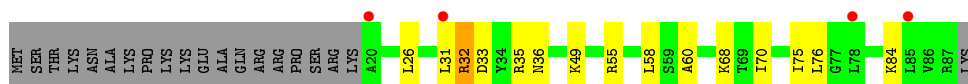


- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18





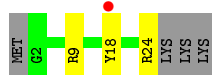
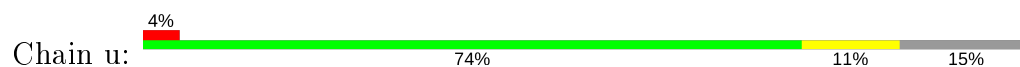
- Molecule 52: 30S ribosomal protein S19



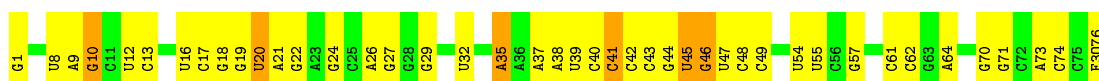
- Molecule 53: 30S ribosomal protein S20



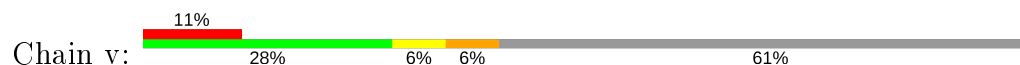
- Molecule 54: 30S ribosomal protein Thx



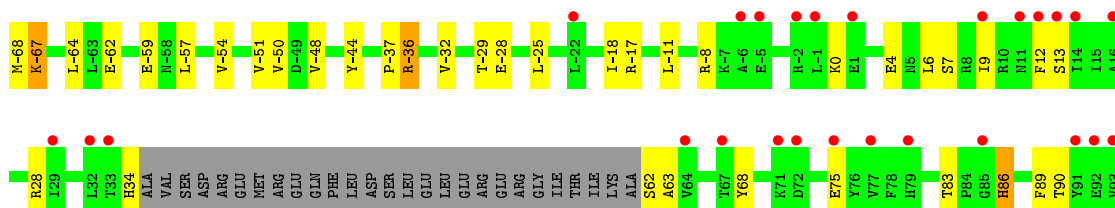
- Molecule 55: P-site tRNA



- Molecule 56: mRNA



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







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.29Å 272.85Å 431.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.90 49.76 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.76-2.90) 93.1 (49.76-2.89)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.238 , 0.304 0.239 , 0.303	Depositor DCC
$R_{free}$ test set	29295 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 66.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	152111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GDP, ZN, MIA, SF4, MG, F3O, 4SU, 7MG, PSU

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

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

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

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

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

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	1	G	OP3-P	-10.81	1.48	1.61
34	a	1125	U	P-O5'	7.89	1.67	1.59
1	A	945	A	N9-C4	-7.33	1.33	1.37
1	A	945	A	N3-C4	-7.19	1.30	1.34
1	A	2790	A	N9-C4	7.08	1.42	1.37
34	a	1125	U	O3'-P	6.66	1.69	1.61
34	a	1323	G	N7-C5	-6.48	1.35	1.39
1	A	2765	A	N9-C4	-6.40	1.34	1.37
1	A	2287	A	N9-C4	-6.38	1.34	1.37
55	w	45	U	N1-C2	6.25	1.44	1.38
3	D	237	GLU	CG-CD	6.19	1.61	1.51
34	a	975	A	N9-C4	-6.08	1.34	1.37
1	A	2058	A	N9-C4	-6.02	1.34	1.37
1	A	2566	A	N3-C4	-5.96	1.31	1.34
34	a	563	A	N9-C4	-5.68	1.34	1.37
34	a	767	A	N9-C4	5.67	1.41	1.37
1	A	265	A	N9-C4	-5.65	1.34	1.37
1	A	1021	A	C5-C6	-5.62	1.35	1.41
1	A	1571	A	N9-C4	-5.61	1.34	1.37
1	A	1021	A	N9-C4	-5.59	1.34	1.37
1	A	1667	G	N9-C8	-5.59	1.33	1.37
1	A	2765	A	N7-C5	-5.57	1.35	1.39
34	a	563	A	N3-C4	-5.57	1.31	1.34
34	a	1227	A	N9-C4	-5.56	1.34	1.37
34	a	1281	U	N1-C2	5.52	1.43	1.38
1	A	197	A	N9-C4	-5.50	1.34	1.37
57	y	141	PRO	N-CD	5.47	1.55	1.47
1	A	526	A	N9-C4	-5.46	1.34	1.37
1	A	1021	A	N7-C5	-5.45	1.35	1.39
1	A	1190	G	C6-N1	5.45	1.43	1.39
57	y	299	PRO	N-CD	5.45	1.55	1.47
34	a	1530	G	N9-C4	-5.42	1.33	1.38
34	a	983	A	N7-C5	-5.38	1.36	1.39
57	y	188	PRO	N-CD	5.38	1.55	1.47
1	A	973	A	N9-C4	-5.30	1.34	1.37
1	A	959	A	N9-C4	-5.29	1.34	1.37
57	y	195	PRO	N-CD	5.26	1.55	1.47
57	y	374	PRO	N-CD	5.24	1.55	1.47
57	y	397	PRO	N-CD	5.22	1.55	1.47
1	A	1674	G	N7-C5	-5.21	1.36	1.39
34	a	397	A	N7-C5	-5.20	1.36	1.39
1	A	820	A	N3-C4	-5.18	1.31	1.34
57	y	529	PRO	N-CD	5.18	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1142(A)	A	N9-C4	-5.17	1.34	1.37
57	y	288	PRO	N-CD	5.17	1.55	1.47
1	A	1322	A	N9-C4	-5.15	1.34	1.37
1	A	958	U	N1-C2	5.15	1.43	1.38
57	y	189	LYS	C-N	5.14	1.42	1.33
34	a	975	A	C5-C6	-5.14	1.36	1.41
57	y	334	PRO	N-CD	5.13	1.55	1.47
1	A	1919	A	C6-N1	-5.10	1.31	1.35
57	y	408	PRO	N-CD	5.09	1.54	1.47
34	a	1125	U	C4'-C3'	5.09	1.58	1.53
1	A	2506	U	C2-N3	5.08	1.41	1.37
57	y	292	PRO	N-CD	5.08	1.54	1.47
57	y	460	LEU	C-O	5.08	1.32	1.23
1	A	1828	G	N1-C2	-5.05	1.33	1.37
1	A	528	A	C5-C6	-5.04	1.36	1.41
1	A	2242	G	N9-C4	-5.03	1.33	1.38

All (1866) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2096	U	O5'-P-OP1	-18.05	89.04	110.70
34	a	1281	U	N3-C2-O2	-14.81	111.83	122.20
1	A	1021	A	C2-N3-C4	-13.57	103.82	110.60
1	A	945	A	N1-C6-N6	13.26	126.56	118.60
1	A	1190	G	N1-C6-O6	13.08	127.75	119.90
1	A	945	A	C6-C5-N7	-12.08	123.84	132.30
1	A	1190	G	C5-C6-O6	-12.00	121.40	128.60
34	a	1281	U	N1-C2-N3	11.79	121.97	114.90
1	A	2200	C	C6-N1-C2	-11.61	115.66	120.30
34	a	1126	U	C5-C6-N1	11.60	128.50	122.70
1	A	1791	A	O5'-P-OP1	-11.36	95.48	105.70
1	A	945	A	C2-N3-C4	-11.33	104.94	110.60
1	A	814	C	O5'-P-OP2	-11.04	95.77	105.70
34	a	1127	G	N3-C4-N9	-10.99	119.40	126.00
1	A	1798	U	O5'-P-OP2	-10.83	95.95	105.70
34	a	1281	U	C6-N1-C2	-10.79	114.52	121.00
1	A	2059	A	N1-C6-N6	10.64	124.99	118.60
34	a	1129	C	C6-N1-C2	-10.45	116.12	120.30
34	a	1125	U	N3-C2-O2	10.12	129.29	122.20
34	a	1126	U	C2-N1-C1'	10.03	129.73	117.70
1	A	1021	A	N1-C6-N6	9.91	124.55	118.60
34	a	365	U	C5-C6-N1	-9.91	117.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	518	C	C5-C4-N4	9.90	127.13	120.20
34	a	975	A	N1-C6-N6	9.90	124.54	118.60
1	A	1776	G	O5'-P-OP2	-9.88	96.81	105.70
1	A	945	A	C5-N7-C8	-9.86	98.97	103.90
1	A	1021	A	C5-N7-C8	-9.82	98.99	103.90
1	A	2791	C	C6-N1-C2	-9.72	116.41	120.30
34	a	975	A	C5-N7-C8	-9.68	99.06	103.90
34	a	518	C	N3-C4-N4	-9.63	111.26	118.00
34	a	365	U	C2-N1-C1'	-9.61	106.17	117.70
1	A	2539	C	O5'-P-OP2	-9.56	97.09	105.70
1	A	2096	U	C5-C6-N1	9.52	127.46	122.70
34	a	518	C	C6-N1-C1'	9.49	132.18	120.80
34	a	1281	U	C5-C4-O4	9.45	131.57	125.90
34	a	1279	A	N7-C8-N9	9.43	118.51	113.80
1	A	945	A	C5-C6-N1	-9.42	112.99	117.70
1	A	1142(A)	A	C2-N3-C4	-9.39	105.91	110.60
1	A	2202	C	C6-N1-C2	-9.38	116.55	120.30
34	a	560	U	O5'-P-OP2	-9.31	97.32	105.70
34	a	792	A	O4'-C1'-N9	9.29	115.64	108.20
1	A	2610	C	C6-N1-C2	-9.19	116.62	120.30
1	A	632	A	C8-N9-C4	9.15	109.46	105.80
1	A	1977	A	C2-N3-C4	-9.14	106.03	110.60
34	a	518	C	C2-N1-C1'	-9.11	108.78	118.80
1	A	945	A	C4-C5-C6	9.09	121.55	117.00
34	a	1127	G	C8-N9-C1'	9.09	138.81	127.00
1	A	2059	A	C5-C6-N6	-9.07	116.44	123.70
34	a	527	G	C8-N9-C4	-9.04	102.78	106.40
1	A	774	A	O5'-P-OP2	-9.03	97.58	105.70
34	a	527	G	N9-C4-C5	9.03	109.01	105.40
34	a	253	U	O5'-P-OP1	-8.99	97.61	105.70
1	A	2501	C	O5'-P-OP2	-8.99	97.61	105.70
34	a	1129	C	O4'-C1'-N1	8.98	115.39	108.20
1	A	1021	A	N7-C8-N9	8.97	118.28	113.80
1	A	528	A	N7-C8-N9	8.96	118.28	113.80
1	A	528	A	C5-N7-C8	-8.96	99.42	103.90
1	A	1109	C	C2-N1-C1'	8.93	128.62	118.80
1	A	197	A	O5'-P-OP2	-8.91	97.68	105.70
34	a	975	A	C4-C5-N7	8.88	115.14	110.70
1	A	253	C	C6-N1-C2	8.88	123.85	120.30
1	A	383	U	O4'-C1'-N1	8.87	115.30	108.20
1	A	1109	C	C5-C6-N1	8.85	125.42	121.00
1	A	1967	C	O5'-P-OP2	-8.80	97.78	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	x	50	U	C5-C4-O4	8.77	131.16	125.90
34	a	1279	A	C8-N9-C4	-8.77	102.29	105.80
1	A	2506	U	C5-C6-N1	8.75	127.08	122.70
1	A	2496	C	N3-C2-O2	-8.74	115.78	121.90
1	A	1190	G	C4-C5-N7	8.68	114.27	110.80
1	A	1647	G	O5'-P-OP1	-8.67	97.89	105.70
1	A	1558	A	N1-C6-N6	8.65	123.79	118.60
1	A	2096	U	C2-N1-C1'	8.64	128.07	117.70
57	y	463	PHE	N-CA-C	8.64	134.32	111.00
1	A	1792	G	O5'-P-OP2	-8.63	97.93	105.70
34	a	1127	G	N9-C4-C5	8.62	108.85	105.40
34	a	1524	C	N3-C4-C5	8.58	125.33	121.90
34	a	1530	G	N3-C4-C5	8.58	132.89	128.60
1	A	1021	A	N1-C2-N3	8.56	133.58	129.30
34	a	1150	U	C5-C4-O4	8.56	131.04	125.90
1	A	2503	A	C2-N3-C4	8.55	114.88	110.60
1	A	1558	A	C2-N3-C4	-8.54	106.33	110.60
33	x	50	U	C2-N3-C4	8.54	132.12	127.00
34	a	266	G	C5-N7-C8	-8.53	100.03	104.30
55	w	73	A	O4'-C1'-N9	8.51	115.01	108.20
1	A	1983	C	N1-C2-O2	-8.50	113.80	118.90
1	A	1781	C	N1-C2-O2	8.46	123.98	118.90
1	A	2073	C	O5'-P-OP2	-8.46	98.09	105.70
1	A	973	A	C2-N3-C4	-8.45	106.37	110.60
1	A	2448	A	N1-C6-N6	8.45	123.67	118.60
34	a	1257	U	N1-C2-O2	8.45	128.71	122.80
1	A	330	A	C2-N3-C4	-8.44	106.38	110.60
1	A	1109	C	C6-N1-C2	-8.43	116.93	120.30
34	a	1116	C	C6-N1-C2	8.42	123.67	120.30
1	A	1153	C	C6-N1-C2	-8.41	116.93	120.30
34	a	1127	G	C4-N9-C1'	-8.38	115.61	126.50
1	A	1021	A	C6-C5-N7	-8.37	126.44	132.30
1	A	1350	C	O5'-P-OP1	-8.35	98.19	105.70
1	A	2554	U	C5-C4-O4	-8.31	120.91	125.90
1	A	1599	C	C6-N1-C2	-8.29	116.99	120.30
1	A	528	A	C2-N3-C4	-8.28	106.46	110.60
1	A	945	A	N1-C2-N3	8.27	133.43	129.30
55	w	45	U	N3-C2-O2	-8.26	116.42	122.20
34	a	575	G	C5-C6-O6	-8.26	123.65	128.60
34	a	1123	A	C5-C6-N6	8.26	130.30	123.70
1	A	1131	G	O5'-P-OP2	-8.24	98.28	105.70
1	A	1300	U	N3-C2-O2	-8.21	116.45	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1380	G	O5'-P-OP2	-8.20	98.32	105.70
1	A	746	A	O4'-C1'-N9	8.19	114.75	108.20
1	A	2242	G	N3-C4-C5	8.19	132.69	128.60
34	a	1530	G	N3-C4-N9	-8.19	121.09	126.00
33	x	68	C	N1-C2-O2	8.18	123.81	118.90
1	A	693	C	N3-C2-O2	-8.17	116.18	121.90
34	a	365	U	N1-C2-N3	8.17	119.80	114.90
34	a	436	C	C5-C6-N1	8.17	125.08	121.00
34	a	776	G	O5'-P-OP1	-8.16	98.36	105.70
1	A	782	A	C8-N9-C4	8.15	109.06	105.80
1	A	2275	C	O5'-P-OP2	-8.15	98.37	105.70
1	A	1021	A	C5-C6-N1	-8.13	113.63	117.70
34	a	333	G	C5-C6-O6	-8.13	123.72	128.60
1	A	2424	C	C6-N1-C2	-8.12	117.05	120.30
1	A	530	G	N1-C6-O6	-8.11	115.04	119.90
34	a	1322	C	O5'-P-OP2	-8.10	98.41	105.70
34	a	117	G	N9-C4-C5	-8.10	102.16	105.40
1	A	1981	A	N1-C6-N6	8.08	123.45	118.60
33	x	64	A	C6-N1-C2	8.08	123.45	118.60
1	A	2202	C	C5-C6-N1	8.07	125.03	121.00
1	A	528	A	C6-C5-N7	-8.05	126.67	132.30
1	A	240	G	C4-C5-N7	-8.05	107.58	110.80
34	a	91	C	N1-C2-O2	8.03	123.72	118.90
1	A	1952	A	N1-C6-N6	8.03	123.42	118.60
1	A	263	C	N1-C2-O2	7.99	123.69	118.90
34	a	266	G	P-O3'-C3'	7.96	129.26	119.70
34	a	10	A	N1-C6-N6	7.94	123.36	118.60
1	A	528	A	N1-C6-N6	7.93	123.36	118.60
34	a	1074	G	C5-C6-O6	-7.92	123.85	128.60
34	a	70	G	C5-C6-O6	-7.89	123.87	128.60
1	A	2239	G	O5'-P-OP2	-7.89	98.60	105.70
1	A	2774	C	C6-N1-C2	7.89	123.45	120.30
34	a	1126	U	C6-N1-C2	-7.87	116.28	121.00
34	a	365	U	C6-N1-C1'	7.87	132.21	121.20
1	A	512	G	O4'-C1'-N9	7.86	114.49	108.20
1	A	645	C	N1-C2-O2	7.84	123.61	118.90
1	A	2506	U	N3-C4-O4	7.84	124.89	119.40
1	A	1774	C	N3-C4-C5	-7.83	118.77	121.90
34	a	975	A	C6-C5-N7	-7.83	126.82	132.30
1	A	2766	G	C6-C5-N7	-7.83	125.70	130.40
1	A	945	A	C4-C5-N7	7.82	114.61	110.70
1	A	745	G	N1-C6-O6	-7.80	115.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1002	G	O5'-P-OP2	-7.79	98.69	105.70
1	A	2024	G	C8-N9-C4	-7.78	103.29	106.40
55	w	73	A	N7-C8-N9	7.77	117.69	113.80
34	a	976	G	N1-C6-O6	7.77	124.56	119.90
1	A	1021	A	C8-N9-C4	-7.76	102.69	105.80
34	a	1107	C	N1-C2-O2	-7.75	114.25	118.90
1	A	1108	U	C2-N1-C1'	7.74	126.99	117.70
1	A	528	A	C8-N9-C4	-7.74	102.70	105.80
34	a	820	U	N3-C2-O2	-7.73	116.79	122.20
1	A	1667	G	C8-N9-C4	7.73	109.49	106.40
34	a	1065	U	O5'-P-OP2	-7.73	98.74	105.70
1	A	12	U	N1-C2-O2	7.73	128.21	122.80
34	a	1392	G	C5-C6-O6	7.72	133.23	128.60
34	a	266	G	N7-C8-N9	7.72	116.96	113.10
1	A	2227	A	O5'-P-OP2	-7.71	98.76	105.70
1	A	2271	G	N3-C4-N9	7.69	130.62	126.00
1	A	2638	G	N3-C4-C5	-7.69	124.76	128.60
1	A	2394	C	C2-N1-C1'	7.68	127.25	118.80
1	A	364	C	C6-N1-C2	-7.68	117.23	120.30
1	A	530	G	C5-C6-O6	7.67	133.20	128.60
1	A	80	G	N1-C6-O6	7.65	124.49	119.90
1	A	678	C	N3-C4-C5	-7.65	118.84	121.90
1	A	581	C	C6-N1-C2	-7.63	117.25	120.30
1	A	1645	G	O5'-P-OP2	-7.63	98.84	105.70
1	A	1653	G	C4-N9-C1'	7.62	136.41	126.50
1	A	1189	A	O5'-P-OP2	-7.62	98.84	105.70
1	A	2499	C	N1-C2-O2	-7.62	114.33	118.90
1	A	2605	U	C6-N1-C2	-7.61	116.43	121.00
34	a	1524	C	C6-N1-C2	7.61	123.34	120.30
34	a	1257	U	N3-C2-O2	-7.60	116.88	122.20
34	a	241	C	C6-N1-C2	7.59	123.34	120.30
1	A	1272	A	O4'-C1'-N9	7.59	114.27	108.20
34	a	1511	G	C5-C6-O6	-7.58	124.05	128.60
34	a	333	G	N1-C6-O6	7.58	124.45	119.90
34	a	1076	C	C6-N1-C2	-7.58	117.27	120.30
1	A	1108	U	N1-C2-O2	7.58	128.10	122.80
33	x	56	C	N1-C2-O2	7.58	123.45	118.90
34	a	266	G	C4-C5-N7	7.57	113.83	110.80
34	a	1127	G	C6-C5-N7	7.57	134.94	130.40
1	A	566	U	C6-N1-C2	-7.56	116.46	121.00
1	A	392	C	N1-C2-O2	7.56	123.44	118.90
1	A	2391	G	O4'-C1'-N9	7.56	114.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2271	G	N9-C4-C5	-7.54	102.38	105.40
34	a	976	G	C5-C6-N1	-7.54	107.73	111.50
34	a	1123	A	N3-C4-N9	-7.54	121.37	127.40
34	a	1125	U	C6-N1-C2	7.51	125.51	121.00
1	A	2503	A	O5'-P-OP1	-7.51	98.94	105.70
1	A	13	A	C8-N9-C4	-7.50	102.80	105.80
1	A	1005	C	N1-C2-O2	7.50	123.40	118.90
34	a	797	C	N1-C2-O2	-7.50	114.40	118.90
1	A	591	C	C6-N1-C2	-7.50	117.30	120.30
1	A	1653	G	C6-C5-N7	-7.50	125.90	130.40
1	A	933	A	O4'-C1'-N9	7.50	114.20	108.20
1	A	2573	C	N3-C2-O2	7.49	127.14	121.90
1	A	2496	C	N1-C2-O2	7.49	123.39	118.90
1	A	1918	A	N1-C6-N6	-7.47	114.12	118.60
34	a	971	G	O4'-C1'-N9	7.47	114.18	108.20
1	A	746	A	C8-N9-C4	-7.47	102.81	105.80
1	A	1030	G	C5-C6-O6	-7.47	124.12	128.60
1	A	584	C	N3-C2-O2	-7.46	116.68	121.90
1	A	129	C	C6-N1-C2	7.46	123.28	120.30
1	A	531	C	N3-C2-O2	-7.46	116.68	121.90
1	A	1030	G	N9-C4-C5	-7.45	102.42	105.40
1	A	226	G	N1-C6-O6	-7.44	115.43	119.90
34	a	91	C	C2-N3-C4	7.44	123.62	119.90
34	a	1027	C	N1-C2-O2	7.42	123.35	118.90
1	A	141	A	N1-C6-N6	7.41	123.05	118.60
55	w	20	U	C2-N1-C1'	7.41	126.59	117.70
34	a	819	A	N1-C6-N6	7.40	123.04	118.60
1	A	1980	G	C8-N9-C4	7.40	109.36	106.40
1	A	2200	C	N3-C2-O2	-7.40	116.72	121.90
34	a	317	G	C6-C5-N7	-7.38	125.97	130.40
34	a	509	A	C8-N9-C4	-7.38	102.85	105.80
1	A	2605	U	N3-C2-O2	-7.38	117.03	122.20
1	A	486	C	C6-N1-C2	7.37	123.25	120.30
1	A	2200	C	C5-C6-N1	7.37	124.69	121.00
1	A	2820	A	N1-C6-N6	7.37	123.02	118.60
1	A	2620	C	O5'-P-OP2	-7.36	99.08	105.70
1	A	240	G	C5-C6-O6	7.36	133.01	128.60
1	A	819	A	N1-C6-N6	7.36	123.01	118.60
1	A	1681	G	N3-C4-C5	7.36	132.28	128.60
1	A	2428	G	P-O3'-C3'	7.35	128.52	119.70
34	a	1202	G	O5'-P-OP2	-7.35	99.08	105.70
33	x	64	A	C5-C6-N6	7.33	129.56	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1061	U	O4'-C1'-N1	7.32	114.06	108.20
34	a	1502	A	C6-C5-N7	-7.32	127.18	132.30
34	a	510	A	C5-C6-N6	7.32	129.55	123.70
1	A	1021	A	C4-C5-N7	7.31	114.36	110.70
1	A	985	C	C6-N1-C2	7.31	123.22	120.30
34	a	976	G	C4-C5-C6	7.31	123.18	118.80
34	a	1219	U	C2-N3-C4	-7.30	122.62	127.00
34	a	1486	G	C5-C6-O6	-7.29	124.22	128.60
1	A	1212	G	C8-N9-C4	7.29	109.32	106.40
1	A	1665	A	C8-N9-C4	7.29	108.72	105.80
1	A	438	G	N1-C6-O6	7.28	124.27	119.90
1	A	1002	G	O5'-P-OP1	7.28	119.44	110.70
1	A	531	C	N3-C4-C5	-7.28	118.99	121.90
34	a	1125	U	N1-C2-O2	-7.27	117.71	122.80
34	a	834	C	C6-N1-C2	7.27	123.21	120.30
1	A	2059	A	N9-C4-C5	-7.26	102.89	105.80
1	A	2443	C	C5-C6-N1	-7.26	117.37	121.00
1	A	2494	G	C5-C6-O6	-7.26	124.25	128.60
34	a	813	U	O5'-P-OP1	7.23	119.37	110.70
34	a	1123	A	C6-N1-C2	7.22	122.93	118.60
1	A	1406	U	O5'-P-OP1	-7.21	99.21	105.70
1	A	2088	G	N3-C4-N9	-7.19	121.68	126.00
34	a	1304	G	N1-C6-O6	7.19	124.21	119.90
34	a	1520	G	O5'-P-OP2	-7.19	99.23	105.70
1	A	1634	A	C8-N9-C4	7.18	108.67	105.80
34	a	955	U	C5-C4-O4	7.18	130.21	125.90
1	A	226	G	O4'-C1'-N9	7.18	113.94	108.20
1	A	1300	U	N1-C2-O2	7.17	127.82	122.80
34	a	366	C	N3-C2-O2	-7.17	116.88	121.90
34	a	1198	G	O5'-P-OP2	7.17	119.31	110.70
1	A	2572	A	N1-C6-N6	-7.17	114.30	118.60
34	a	916	G	C8-N9-C4	-7.17	103.53	106.40
34	a	385	C	C6-N1-C2	-7.17	117.43	120.30
34	a	515	G	N1-C6-O6	7.17	124.20	119.90
1	A	528	A	N1-C2-N3	7.17	132.88	129.30
1	A	2202	C	C2-N1-C1'	7.16	126.68	118.80
1	A	2275	C	C6-N1-C2	7.16	123.17	120.30
1	A	859	G	N3-C4-N9	-7.16	121.70	126.00
55	w	9	A	C8-N9-C4	7.16	108.67	105.80
34	a	266	G	C8-N9-C4	-7.15	103.54	106.40
34	a	1502	A	C2-N3-C4	-7.15	107.03	110.60
34	a	972	C	C6-N1-C2	-7.14	117.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1036	G	C4-N9-C1'	7.14	135.79	126.50
1	A	570	G	C4-C5-N7	-7.14	107.94	110.80
34	a	1511	G	N1-C6-O6	7.14	124.18	119.90
1	A	2439	A	O4'-C1'-N9	-7.13	102.50	108.20
55	w	73	A	C5-N7-C8	-7.12	100.34	103.90
1	A	1691	C	N1-C2-O2	-7.12	114.63	118.90
34	a	1331	G	O4'-C1'-N9	7.12	113.90	108.20
1	A	2834	G	N1-C6-O6	-7.12	115.63	119.90
1	A	1698	A	C6-C5-N7	-7.11	127.32	132.30
1	A	2766	G	N1-C6-O6	7.11	124.17	119.90
1	A	528	A	C4-C5-N7	7.11	114.25	110.70
1	A	1613	G	C4-C5-N7	-7.10	107.96	110.80
34	a	873	A	C2-N3-C4	7.09	114.15	110.60
34	a	510	A	N1-C6-N6	-7.09	114.34	118.60
1	A	915	C	N3-C2-O2	-7.09	116.94	121.90
1	A	2022	U	N1-C2-O2	-7.08	117.84	122.80
1	A	1800	C	N1-C2-O2	-7.08	114.65	118.90
1	A	399	G	N3-C4-C5	7.08	132.14	128.60
1	A	2582	G	C2-N3-C4	7.07	115.44	111.90
1	A	2617	C	C6-N1-C2	-7.07	117.47	120.30
1	A	2790	A	C2-N3-C4	7.06	114.13	110.60
1	A	2500	U	O5'-P-OP1	-7.06	99.34	105.70
34	a	529	G	N1-C6-O6	7.06	124.14	119.90
1	A	1300	U	C2-N1-C1'	7.06	126.17	117.70
1	A	340	A	O5'-P-OP1	-7.05	99.35	105.70
1	A	2516	G	N1-C6-O6	7.05	124.13	119.90
1	A	645	C	C2-N1-C1'	7.05	126.55	118.80
1	A	2197	U	N3-C2-O2	-7.04	117.27	122.20
34	a	374	A	N1-C6-N6	7.04	122.83	118.60
55	w	45	U	C6-N1-C2	-7.04	116.78	121.00
34	a	1324	A	C8-N9-C4	-7.03	102.99	105.80
1	A	1633	G	N1-C6-O6	7.03	124.12	119.90
1	A	933	A	C5-N7-C8	-7.03	100.39	103.90
1	A	1950	G	C5-C6-O6	7.02	132.81	128.60
1	A	2011	U	OP1-P-O3'	7.02	120.64	105.20
1	A	2287	A	C2-N3-C4	-7.02	107.09	110.60
1	A	2325	G	C8-N9-C4	-7.02	103.59	106.40
1	A	859	G	C4-N9-C1'	-7.01	117.38	126.50
1	A	30	G	N3-C4-N9	7.00	130.20	126.00
1	A	1501	C	C5-C6-N1	7.00	124.50	121.00
1	A	1614	A	O5'-P-OP1	-7.00	99.40	105.70
1	A	446	G	C8-N9-C4	-6.99	103.60	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	436	C	C2-N1-C1'	6.99	126.49	118.80
1	A	818	G	N1-C6-O6	6.99	124.09	119.90
1	A	2394	C	N1-C2-O2	6.99	123.09	118.90
1	A	2509	G	C5-C6-O6	-6.99	124.41	128.60
1	A	1796	U	C5-C4-O4	6.98	130.09	125.90
1	A	2605	U	C5-C6-N1	6.98	126.19	122.70
1	A	2765	A	C2-N3-C4	-6.98	107.11	110.60
1	A	2056	G	C4-C5-N7	6.97	113.59	110.80
1	A	1782	C	C6-N1-C2	-6.97	117.51	120.30
1	A	958	U	N3-C2-O2	-6.97	117.32	122.20
34	a	757	U	O5'-P-OP2	-6.96	99.43	105.70
1	A	2096	U	N1-C2-O2	6.96	127.67	122.80
1	A	945	A	O5'-P-OP2	-6.96	99.44	105.70
34	a	1124	G	N3-C4-C5	-6.96	125.12	128.60
34	a	1322	C	C6-N1-C2	6.96	123.08	120.30
34	a	366	C	N1-C2-O2	6.95	123.07	118.90
45	l	84	LEU	CA-CB-CG	6.94	131.27	115.30
1	A	693	C	C6-N1-C2	-6.94	117.52	120.30
1	A	2789	C	O4'-C1'-N1	6.94	113.75	108.20
34	a	888	G	O5'-P-OP2	-6.94	99.45	105.70
1	A	2229	C	N3-C2-O2	-6.94	117.04	121.90
1	A	584	C	C2-N1-C1'	6.93	126.42	118.80
34	a	728	A	N1-C6-N6	6.93	122.76	118.60
1	A	2624	G	N3-C4-N9	6.93	130.16	126.00
1	A	2766	G	C4-C5-N7	6.92	113.57	110.80
1	A	1204	A	C2-N3-C4	-6.91	107.14	110.60
1	A	2056	G	C6-C5-N7	-6.91	126.25	130.40
34	a	852	G	N1-C2-N2	-6.91	109.98	116.20
34	a	38	G	N1-C6-O6	6.90	124.04	119.90
1	A	945	A	C4-N9-C1'	6.90	138.71	126.30
34	a	959	A	C8-N9-C4	6.89	108.56	105.80
1	A	734	A	C8-N9-C4	6.88	108.55	105.80
1	A	2609	U	C5-C6-N1	-6.88	119.26	122.70
1	A	1776	G	C8-N9-C4	6.88	109.15	106.40
34	a	1502	A	C5-N7-C8	-6.88	100.46	103.90
1	A	1827	C	C6-N1-C2	-6.87	117.55	120.30
1	A	1966	A	O5'-P-OP1	-6.87	99.52	105.70
34	a	1494	G	N3-C4-C5	-6.86	125.17	128.60
1	A	1647	G	O5'-P-OP2	6.86	118.93	110.70
34	a	576	G	C6-C5-N7	-6.86	126.29	130.40
1	A	2767	C	N1-C2-O2	6.86	123.01	118.90
57	y	215	LEU	N-CA-C	-6.86	92.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	679	C	C5-C6-N1	-6.85	117.57	121.00
34	a	894	G	N1-C6-O6	6.85	124.01	119.90
55	w	62	C	N3-C4-C5	-6.84	119.16	121.90
34	a	573	A	O5'-P-OP2	-6.84	99.54	105.70
1	A	1698	A	N1-C6-N6	6.83	122.70	118.60
34	a	1331	G	N1-C6-O6	-6.83	115.80	119.90
1	A	945	A	C8-N9-C1'	-6.83	115.41	127.70
2	B	70	C	C6-N1-C2	-6.82	117.57	120.30
34	a	1290	G	N1-C6-O6	6.82	123.99	119.90
34	a	1503	A	O4'-C1'-N9	6.81	113.65	108.20
1	A	2229	C	O5'-P-OP2	-6.81	99.57	105.70
1	A	740	U	OP1-P-OP2	-6.81	109.39	119.60
1	A	933	A	N7-C8-N9	6.80	117.20	113.80
57	y	215	LEU	CB-CG-CD1	6.80	122.56	111.00
1	A	90	U	C5-C6-N1	6.80	126.10	122.70
1	A	1745	C	C5-C6-N1	6.79	124.40	121.00
1	A	561	G	C8-N9-C4	6.79	109.12	106.40
55	w	29	G	N1-C6-O6	6.79	123.97	119.90
1	A	1991	U	C5-C6-N1	-6.78	119.31	122.70
1	A	451	C	N3-C4-N4	6.78	122.75	118.00
1	A	1796	U	C2-N1-C1'	-6.78	109.56	117.70
1	A	2791	C	C2-N1-C1'	6.77	126.25	118.80
1	A	1191	G	N3-C4-C5	6.77	131.98	128.60
1	A	265	A	C2-N3-C4	-6.76	107.22	110.60
1	A	801	G	N1-C6-O6	-6.76	115.84	119.90
34	a	510	A	N9-C4-C5	6.76	108.50	105.80
1	A	1823	G	O5'-P-OP2	6.75	118.80	110.70
1	A	12	U	N3-C2-O2	-6.75	117.48	122.20
1	A	1253	A	OP1-P-OP2	6.75	129.72	119.60
34	a	929	G	N1-C6-O6	-6.74	115.85	119.90
1	A	2200	C	C2-N1-C1'	6.74	126.22	118.80
1	A	798	G	OP1-P-OP2	-6.74	109.49	119.60
1	A	945	A	N7-C8-N9	6.74	117.17	113.80
34	a	1126	U	C5-C4-O4	-6.74	121.86	125.90
1	A	1799	G	N1-C6-O6	-6.73	115.86	119.90
1	A	1927	A	C8-N9-C4	6.73	108.49	105.80
34	a	105	G	O5'-P-OP2	-6.73	99.64	105.70
8	J	77	PRO	N-CA-CB	6.73	111.37	103.30
1	A	1030	G	C8-N9-C4	6.72	109.09	106.40
1	A	1622	G	C5-C6-O6	-6.72	124.57	128.60
1	A	2566	A	N9-C4-C5	6.72	108.49	105.80
34	a	687	A	P-O3'-C3'	6.72	127.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	45	U	O4'-C1'-N1	6.72	113.58	108.20
1	A	1677	A	N1-C6-N6	-6.72	114.57	118.60
1	A	584	C	C6-N1-C2	-6.71	117.61	120.30
1	A	573	G	C5-C6-O6	-6.71	124.57	128.60
1	A	2582	G	C5-C6-N1	6.71	114.86	111.50
1	A	2073	C	N1-C2-O2	6.70	122.92	118.90
1	A	2712(A)	A	N9-C4-C5	6.70	108.48	105.80
34	a	365	U	C5-C4-O4	6.70	129.92	125.90
1	A	234	C	N1-C2-O2	6.70	122.92	118.90
1	A	1958	C	O5'-P-OP1	6.70	118.73	110.70
1	A	2199	A	OP2-P-O3'	6.69	119.92	105.20
34	a	963	G	C2-N3-C4	-6.68	108.56	111.90
34	a	975	A	C2-N3-C4	-6.68	107.26	110.60
34	a	1234	C	C6-N1-C2	-6.68	117.63	120.30
1	A	2040	C	N3-C2-O2	-6.68	117.22	121.90
1	A	1778	U	N3-C4-C5	6.67	118.60	114.60
34	a	1511	G	C6-C5-N7	-6.65	126.41	130.40
1	A	206	U	N3-C2-O2	-6.65	117.55	122.20
1	A	1300	U	P-O3'-C3'	6.65	127.68	119.70
1	A	773	U	C6-N1-C2	6.64	124.99	121.00
1	A	1694	C	N1-C2-O2	-6.64	114.92	118.90
1	A	1190	G	C5-N7-C8	-6.64	100.98	104.30
1	A	2034	U	C2-N1-C1'	6.64	125.67	117.70
55	w	1	G	C8-N9-C4	-6.63	103.75	106.40
1	A	986	C	C6-N1-C2	6.63	122.95	120.30
1	A	1790	C	N3-C2-O2	6.63	126.54	121.90
1	A	1698	A	N7-C8-N9	6.62	117.11	113.80
34	a	320	C	C6-N1-C2	6.62	122.95	120.30
34	a	91	C	N3-C4-C5	-6.62	119.25	121.90
34	a	839	U	C2-N1-C1'	6.61	125.64	117.70
34	a	812	C	N1-C2-O2	6.61	122.86	118.90
1	A	859	G	N3-C4-C5	6.60	131.90	128.60
34	a	822	C	N1-C2-O2	-6.60	114.94	118.90
1	A	1129	A	N1-C6-N6	-6.59	114.64	118.60
1	A	2646	C	C6-N1-C2	-6.59	117.66	120.30
1	A	1095	A	O4'-C1'-N9	6.59	113.47	108.20
55	w	20	U	N1-C2-O2	6.59	127.41	122.80
1	A	844	C	C6-N1-C2	6.59	122.93	120.30
1	A	2080	G	C5-C6-O6	-6.59	124.65	128.60
1	A	531	C	C4-C5-C6	6.58	120.69	117.40
34	a	515	G	C5-C6-O6	-6.57	124.66	128.60
1	A	1227	G	N1-C6-O6	6.57	123.84	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	A	N1-C2-N3	6.57	132.58	129.30
1	A	582	G	C8-N9-C4	-6.57	103.77	106.40
34	a	980	C	C5-C6-N1	6.57	124.28	121.00
34	a	1530	G	C4-N9-C1'	-6.56	117.97	126.50
34	a	1127	G	C4-C5-N7	-6.56	108.17	110.80
1	A	1634	A	N7-C8-N9	-6.55	110.52	113.80
34	a	1027	C	N3-C2-O2	-6.55	117.32	121.90
1	A	1313	U	C2-N1-C1'	6.55	125.56	117.70
1	A	673	C	N3-C4-N4	6.55	122.58	118.00
1	A	2506	U	O5'-P-OP2	6.55	118.56	110.70
1	A	1837	C	N1-C2-O2	-6.54	114.97	118.90
1	A	1721	G	C4-C5-N7	6.54	113.42	110.80
34	a	1129	C	P-O3'-C3'	6.54	127.55	119.70
34	a	813	U	OP1-P-OP2	-6.53	109.80	119.60
1	A	990	A	N1-C6-N6	6.53	122.52	118.60
1	A	392	C	N3-C2-O2	-6.53	117.33	121.90
34	a	1432	G	C8-N9-C4	-6.53	103.79	106.40
1	A	1038	C	C6-N1-C2	-6.53	117.69	120.30
1	A	116	C	O5'-P-OP2	-6.52	99.83	105.70
1	A	830	G	O5'-P-OP1	-6.52	99.83	105.70
1	A	1981	A	C5-C6-N6	-6.52	118.48	123.70
1	A	2499	C	C2-N3-C4	-6.52	116.64	119.90
33	x	4	C	C6-N1-C2	-6.52	117.69	120.30
34	a	1331	G	C8-N9-C4	-6.52	103.79	106.40
1	A	1791	A	OP2-P-O3'	6.52	119.54	105.20
34	a	916	G	C4-N9-C1'	6.52	134.97	126.50
1	A	733	G	C4-C5-N7	6.51	113.41	110.80
1	A	561	G	N7-C8-N9	-6.51	109.84	113.10
1	A	210	C	C5-C6-N1	-6.51	117.75	121.00
34	a	839	U	N1-C2-O2	6.51	127.35	122.80
34	a	1117	G	C8-N9-C4	6.50	109.00	106.40
1	A	1899	G	N1-C2-N2	-6.50	110.35	116.20
1	A	2463	C	C5-C6-N1	6.50	124.25	121.00
34	a	861	G	N3-C4-N9	6.50	129.90	126.00
34	a	975	A	C5-C6-N6	-6.49	118.50	123.70
1	A	1667	G	N7-C8-N9	-6.49	109.86	113.10
1	A	2200	C	N1-C2-O2	6.49	122.79	118.90
34	a	778	G	O5'-P-OP2	-6.49	99.86	105.70
34	a	1502	A	N1-C6-N6	6.48	122.49	118.60
1	A	679	C	C2-N3-C4	-6.48	116.66	119.90
1	A	1897	G	N9-C4-C5	-6.47	102.81	105.40
1	A	573	G	O5'-P-OP2	-6.47	99.87	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1653	G	C4-C5-C6	6.47	122.68	118.80
1	A	2766	G	C5-C6-O6	-6.47	124.72	128.60
34	a	769	G	N3-C4-N9	6.47	129.88	126.00
34	a	514	C	C6-N1-C2	6.47	122.89	120.30
34	a	1526	G	C6-C5-N7	-6.46	126.52	130.40
55	w	74	C	C6-N1-C2	-6.46	117.72	120.30
1	A	1030	G	N3-C4-N9	6.46	129.88	126.00
1	A	1775	U	C5-C6-N1	-6.46	119.47	122.70
1	A	452	G	N1-C6-O6	6.46	123.77	119.90
33	x	4	C	N3-C2-O2	-6.46	117.38	121.90
1	A	1190	G	C6-C5-N7	-6.45	126.53	130.40
1	A	1629	U	N1-C2-N3	6.45	118.77	114.90
1	A	866	A	C8-N9-C4	-6.45	103.22	105.80
1	A	1108	U	C6-N1-C1'	-6.45	112.17	121.20
1	A	2073	C	N3-C2-O2	-6.45	117.39	121.90
1	A	945	A	O4'-C1'-N9	6.45	113.36	108.20
1	A	1061	U	C2-N1-C1'	6.44	125.43	117.70
1	A	2286	A	N7-C8-N9	6.44	117.02	113.80
1	A	2448	A	N9-C4-C5	-6.44	103.22	105.80
34	a	1255	G	C8-N9-C4	6.44	108.98	106.40
1	A	2785	C	C6-N1-C2	-6.43	117.73	120.30
34	a	1248	A	C2-N3-C4	6.43	113.81	110.60
1	A	2286	A	C8-N9-C4	-6.43	103.23	105.80
1	A	2064	C	N3-C2-O2	6.42	126.39	121.90
1	A	798	G	C8-N9-C4	-6.42	103.83	106.40
1	A	2825	C	C5-C6-N1	-6.42	117.79	121.00
34	a	518	C	O4'-C1'-N1	6.42	113.33	108.20
1	A	561	G	N1-C6-O6	-6.42	116.05	119.90
1	A	182	A	C8-N9-C4	-6.42	103.23	105.80
34	a	1198	G	N3-C2-N2	-6.41	115.41	119.90
34	a	28	G	N1-C6-O6	6.41	123.75	119.90
1	A	364	C	C5-C6-N1	6.41	124.21	121.00
5	F	62	ARG	NE-CZ-NH1	-6.41	117.09	120.30
34	a	254	G	O5'-P-OP1	-6.41	99.93	105.70
57	y	416	THR	C-N-CD	6.41	141.86	128.40
1	A	958	U	C6-N1-C2	-6.40	117.16	121.00
1	A	265	A	N1-C6-N6	6.40	122.44	118.60
1	A	819	A	C4-C5-N7	6.40	113.90	110.70
1	A	2615	U	N3-C4-O4	-6.39	114.92	119.40
1	A	1758	G	C4-C5-C6	6.39	122.64	118.80
1	A	2197	U	N1-C2-O2	6.39	127.27	122.80
1	A	2052	G	C4-C5-N7	-6.39	108.25	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2789	C	C2-N1-C1'	-6.39	111.77	118.80
34	a	275	G	N3-C4-C5	-6.39	125.41	128.60
1	A	1109	C	N1-C2-O2	6.38	122.73	118.90
1	A	1962	C	C5-C6-N1	6.38	124.19	121.00
1	A	573	G	N1-C6-O6	6.38	123.73	119.90
1	A	275	G	C8-N9-C4	-6.37	103.85	106.40
1	A	1962	C	C6-N1-C2	-6.37	117.75	120.30
1	A	2751	G	C4-N9-C1'	6.37	134.78	126.50
34	a	1488	G	N1-C6-O6	6.37	123.72	119.90
1	A	1672	C	C6-N1-C2	-6.37	117.75	120.30
1	A	1629	U	C4-C5-C6	6.37	123.52	119.70
34	a	317	G	N3-C4-N9	6.36	129.82	126.00
34	a	337	C	C6-N1-C2	-6.36	117.76	120.30
34	a	981	U	N3-C2-O2	6.35	126.65	122.20
1	A	2250	G	C5-C6-N1	6.35	114.67	111.50
1	A	680	G	O5'-P-OP2	-6.35	99.99	105.70
55	w	26	A	N1-C6-N6	6.35	122.41	118.60
1	A	2049	G	C8-N9-C4	-6.34	103.86	106.40
34	a	619	U	C5-C4-O4	6.34	129.71	125.90
1	A	788	A	N9-C4-C5	-6.34	103.26	105.80
34	a	241	C	N3-C4-C5	6.34	124.44	121.90
34	a	1506	U	N1-C2-O2	-6.34	118.36	122.80
1	A	208	C	N1-C2-O2	-6.34	115.10	118.90
1	A	580	C	N1-C2-O2	-6.34	115.10	118.90
1	A	1300	U	C6-N1-C2	-6.34	117.20	121.00
1	A	2050	C	O5'-P-OP1	-6.34	100.00	105.70
1	A	577	G	C8-N9-C4	-6.34	103.87	106.40
8	J	86	PRO	N-CA-CB	6.33	110.89	103.30
1	A	1698	A	C2-N3-C4	-6.32	107.44	110.60
1	A	2048	G	N1-C6-O6	6.32	123.69	119.90
1	A	531	C	C6-N1-C2	-6.32	117.77	120.30
1	A	139(A)	G	N3-C4-C5	-6.32	125.44	128.60
1	A	2549	G	O5'-P-OP2	-6.31	100.02	105.70
1	A	1328	G	N1-C6-O6	6.31	123.69	119.90
34	a	78	G	N1-C6-O6	-6.31	116.12	119.90
1	A	1204	A	N1-C6-N6	6.30	122.38	118.60
1	A	1558	A	C4-C5-N7	6.30	113.85	110.70
1	A	1212	G	N7-C8-N9	-6.30	109.95	113.10
1	A	1153	C	N3-C4-C5	-6.30	119.38	121.90
1	A	2516	G	C5-C6-O6	-6.30	124.82	128.60
1	A	1322	A	C2-N3-C4	-6.30	107.45	110.60
1	A	2820	A	O5'-P-OP2	-6.29	100.03	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2723	C	C6-N1-C2	-6.29	117.78	120.30
34	a	1123	A	C5-C6-N1	-6.29	114.55	117.70
1	A	915	C	N1-C2-O2	6.29	122.67	118.90
34	a	1127	G	N3-C4-C5	6.29	131.74	128.60
1	A	1460	A	O4'-C1'-N9	6.28	113.23	108.20
1	A	803	U	N1-C2-N3	6.28	118.67	114.90
34	a	864	A	N1-C6-N6	6.28	122.37	118.60
1	A	961	C	N3-C4-N4	6.28	122.40	118.00
1	A	2559	C	C4-C5-C6	6.28	120.54	117.40
34	a	527	G	C4-C5-N7	-6.27	108.29	110.80
34	a	1132	C	C6-N1-C2	-6.27	117.79	120.30
1	A	2022	U	N3-C2-O2	6.27	126.59	122.20
1	A	2271	G	C8-N9-C1'	-6.27	118.85	127.00
34	a	1461	G	C4-N9-C1'	6.27	134.65	126.50
1	A	1621	U	O5'-P-OP2	-6.27	100.06	105.70
34	a	1063	C	C2-N1-C1'	-6.27	111.91	118.80
55	w	41	C	N3-C4-C5	6.27	124.41	121.90
1	A	239	U	C6-N1-C2	6.26	124.76	121.00
1	A	265	A	C5-C6-N1	-6.26	114.57	117.70
1	A	275	G	C4-N9-C1'	6.26	134.64	126.50
1	A	1998	G	O5'-P-OP1	-6.26	100.06	105.70
1	A	2820	A	C5-N7-C8	-6.26	100.77	103.90
1	A	246	C	N1-C2-O2	-6.25	115.15	118.90
1	A	275	G	N7-C8-N9	6.25	116.23	113.10
1	A	1957	C	OP2-P-O3'	6.25	118.96	105.20
1	A	2065	C	O5'-P-OP1	-6.25	100.07	105.70
1	A	2522	U	N3-C4-O4	6.25	123.78	119.40
34	a	115	G	C5-C6-O6	-6.25	124.85	128.60
1	A	2576	G	C4-N9-C1'	6.25	134.63	126.50
34	a	1505	G	C4-C5-N7	-6.25	108.30	110.80
34	a	880	C	C6-N1-C2	6.24	122.80	120.30
1	A	1619	G	N3-C2-N2	-6.24	115.53	119.90
34	a	365	U	C4-C5-C6	6.24	123.44	119.70
1	A	561	G	C6-C5-N7	6.24	134.14	130.40
34	a	119	A	N1-C6-N6	-6.23	114.86	118.60
33	x	64	A	C5-C6-N1	-6.23	114.58	117.70
34	a	314	C	N3-C2-O2	-6.23	117.54	121.90
1	A	459	U	C5-C4-O4	-6.23	122.16	125.90
34	a	1125	U	O5'-P-OP2	6.23	118.17	110.70
1	A	491	G	N3-C4-N9	-6.22	122.27	126.00
1	A	1645	G	N3-C4-N9	6.22	129.73	126.00
1	A	364	C	C2-N1-C1'	6.22	125.64	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	748	C	C6-N1-C2	-6.22	117.81	120.30
34	a	841	U	C5-C6-N1	6.21	125.81	122.70
1	A	1430	C	C6-N1-C2	-6.21	117.82	120.30
34	a	1279	A	C5-N7-C8	-6.21	100.80	103.90
1	A	272	G	N1-C6-O6	6.21	123.63	119.90
1	A	1813	G	C8-N9-C4	6.21	108.88	106.40
1	A	1256	G	C8-N9-C4	-6.21	103.92	106.40
1	A	1772	G	C2-N3-C4	-6.21	108.80	111.90
1	A	2056	G	N1-C6-O6	6.20	123.62	119.90
34	a	940	C	N1-C2-O2	-6.20	115.18	118.90
1	A	129	C	C5-C6-N1	-6.20	117.90	121.00
34	a	860	A	C2-N3-C4	-6.20	107.50	110.60
1	A	467	G	C2-N3-C4	-6.20	108.80	111.90
1	A	2638	G	C8-N9-C4	-6.20	103.92	106.40
1	A	774	A	N1-C2-N3	6.20	132.40	129.30
1	A	1214	A	N1-C6-N6	-6.20	114.88	118.60
34	a	957	U	N1-C2-O2	-6.20	118.46	122.80
34	a	117	G	C6-C5-N7	-6.19	126.68	130.40
34	a	117	G	N3-C4-N9	6.19	129.72	126.00
35	b	213	LEU	CA-CB-CG	6.19	129.54	115.30
1	A	2059	A	C6-C5-N7	-6.19	127.97	132.30
34	a	1206	G	N3-C2-N2	-6.19	115.57	119.90
34	a	1036	G	C8-N9-C1'	-6.19	118.95	127.00
34	a	1187	G	C8-N9-C4	-6.19	103.92	106.40
1	A	2774	C	N3-C4-C5	6.19	124.37	121.90
1	A	592	G	N1-C6-O6	6.18	123.61	119.90
34	a	1053	G	N7-C8-N9	-6.18	110.01	113.10
1	A	190	A	OP2-P-O3'	6.18	118.79	105.20
1	A	2742	C	N1-C2-O2	-6.18	115.19	118.90
34	a	1151	A	N1-C6-N6	-6.18	114.89	118.60
34	a	319	G	N1-C6-O6	-6.17	116.20	119.90
1	A	13	A	N9-C4-C5	6.17	108.27	105.80
1	A	2717	G	N1-C6-O6	6.17	123.60	119.90
8	J	69	PRO	N-CA-CB	6.17	110.70	103.30
34	a	117	G	C4-C5-N7	6.17	113.27	110.80
34	a	805	C	C5-C6-N1	6.17	124.08	121.00
8	J	101	PRO	N-CA-CB	6.16	110.69	103.30
1	A	1034	G	C5-C6-O6	-6.16	124.91	128.60
1	A	788	A	C8-N9-C4	6.15	108.26	105.80
34	a	1363	C	C6-N1-C1'	6.15	128.18	120.80
1	A	584	C	N1-C2-O2	6.15	122.59	118.90
1	A	1190	G	N9-C4-C5	-6.15	102.94	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1944	U	C4-C5-C6	6.15	123.39	119.70
1	A	2474	C	N1-C2-O2	6.14	122.58	118.90
1	A	452	G	C5-C6-O6	-6.14	124.92	128.60
1	A	963	U	N1-C2-N3	-6.14	111.22	114.90
1	A	778	G	C5-C6-O6	-6.14	124.92	128.60
1	A	1166	C	C6-N1-C2	-6.14	117.84	120.30
34	a	115	G	P-O3'-C3'	6.14	127.06	119.70
1	A	450	G	C5-C6-N1	-6.13	108.43	111.50
1	A	2394	C	C6-N1-C2	-6.13	117.85	120.30
34	a	819	A	C6-C5-N7	-6.13	128.01	132.30
1	A	685	A	O5'-P-OP2	-6.13	100.18	105.70
1	A	961	C	C6-N1-C2	-6.13	117.85	120.30
1	A	2466	C	C6-N1-C2	6.13	122.75	120.30
34	a	123	C	C6-N1-C2	6.13	122.75	120.30
1	A	1271	G	C5-C6-N1	-6.13	108.44	111.50
1	A	1698	A	O4'-C1'-N9	6.13	113.10	108.20
1	A	2434	A	O5'-P-OP2	-6.13	100.19	105.70
33	x	23	A	N1-C6-N6	-6.13	114.92	118.60
1	A	795	C	C6-N1-C2	-6.12	117.85	120.30
1	A	2509	G	N1-C6-O6	6.12	123.57	119.90
1	A	687	C	C6-N1-C2	-6.12	117.85	120.30
34	a	852	G	N3-C2-N2	6.12	124.18	119.90
1	A	1939	U	O5'-P-OP1	-6.12	100.19	105.70
1	A	2095	C	O3'-P-O5'	6.12	115.62	104.00
1	A	2779	U	O5'-P-OP2	-6.12	100.19	105.70
1	A	565	C	OP1-P-OP2	-6.12	110.43	119.60
34	a	1363	C	O4'-C1'-N1	6.12	113.09	108.20
34	a	959	A	N1-C6-N6	6.11	122.27	118.60
34	a	1351	U	N1-C2-O2	-6.11	118.52	122.80
34	a	1432	G	N3-C4-C5	-6.11	125.54	128.60
1	A	570	G	C5-C6-O6	6.11	132.27	128.60
1	A	1245	G	N1-C6-O6	-6.11	116.23	119.90
34	a	1123	A	N9-C4-C5	6.11	108.24	105.80
34	a	1237	C	N3-C4-C5	6.11	124.34	121.90
1	A	866	A	N7-C8-N9	6.10	116.85	113.80
1	A	1320	C	C5-C4-N4	-6.10	115.93	120.20
34	a	605	U	C5-C4-O4	6.09	129.56	125.90
34	a	1491	G	C8-N9-C4	-6.09	103.96	106.40
1	A	985	C	C5-C6-N1	-6.09	117.95	121.00
1	A	2394	C	N3-C2-O2	-6.09	117.64	121.90
1	A	2610	C	N3-C2-O2	-6.09	117.64	121.90
34	a	1126	U	N3-C4-O4	6.09	123.66	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1620	G	C5-C6-N1	-6.08	108.46	111.50
2	B	96	U	N3-C2-O2	-6.08	117.94	122.20
1	A	1970	A	N1-C6-N6	6.08	122.25	118.60
1	A	1999	C	C6-N1-C2	6.08	122.73	120.30
1	A	2570	G	C8-N9-C4	6.07	108.83	106.40
8	J	105	PRO	N-CA-CB	6.07	110.58	103.30
1	A	2712(A)	A	C8-N9-C4	-6.06	103.38	105.80
34	a	117	G	C5-C6-O6	-6.06	124.96	128.60
34	a	1054	C	N1-C2-O2	6.06	122.54	118.90
1	A	1191	G	N3-C4-N9	-6.06	122.36	126.00
34	a	855	G	N1-C6-O6	6.06	123.53	119.90
1	A	1667	G	C5-N7-C8	6.05	107.33	104.30
34	a	748	C	N1-C2-O2	6.05	122.53	118.90
1	A	1214	A	N9-C4-C5	6.05	108.22	105.80
1	A	2592	G	C6-C5-N7	-6.05	126.77	130.40
1	A	1046	A	O4'-C1'-N9	6.05	113.04	108.20
1	A	1424	G	N3-C4-N9	6.05	129.63	126.00
1	A	2820	A	N9-C4-C5	-6.05	103.38	105.80
34	a	515	G	C6-C5-N7	-6.05	126.77	130.40
1	A	1617	C	C2-N1-C1'	-6.05	112.15	118.80
1	A	1992	G	P-O3'-C3'	6.05	126.96	119.70
55	w	57	G	C8-N9-C4	-6.04	103.98	106.40
1	A	1424	G	C6-C5-N7	-6.04	126.78	130.40
1	A	2324	C	C6-N1-C2	6.04	122.71	120.30
1	A	391	G	N1-C6-O6	6.03	123.52	119.90
1	A	806	C	N3-C4-C5	6.03	124.31	121.90
1	A	2417	C	C6-N1-C2	6.03	122.71	120.30
57	y	282	LEU	N-CA-C	-6.03	94.71	111.00
1	A	2019	A	C8-N9-C4	-6.03	103.39	105.80
1	A	298	G	N1-C6-O6	6.03	123.52	119.90
1	A	1653	G	N3-C4-C5	-6.03	125.58	128.60
34	a	1124	G	C8-N9-C4	-6.03	103.99	106.40
1	A	2780	G	N3-C4-N9	6.03	129.62	126.00
1	A	941	A	C8-N9-C4	6.03	108.21	105.80
34	a	527	G	C5-C6-O6	6.03	132.22	128.60
1	A	240	G	N9-C4-C5	6.02	107.81	105.40
1	A	1958	C	N3-C4-N4	6.02	122.22	118.00
1	A	1306	C	N1-C2-O2	6.02	122.51	118.90
1	A	2460	U	C5-C6-N1	-6.02	119.69	122.70
34	a	575	G	N1-C6-O6	6.02	123.51	119.90
1	A	328	U	C6-N1-C2	-6.02	117.39	121.00
1	A	2810	A	C8-N9-C4	6.02	108.21	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1221	G	C4-C5-N7	-6.02	108.39	110.80
1	A	733	G	C5-N7-C8	-6.01	101.29	104.30
1	A	2093	G	N9-C4-C5	6.01	107.81	105.40
34	a	394	G	O5'-P-OP2	-6.01	100.29	105.70
11	O	8	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	2078	C	O5'-P-OP1	-6.01	100.29	105.70
1	A	2856	C	N3-C2-O2	-6.00	117.70	121.90
1	A	1343	G	C8-N9-C4	-6.00	104.00	106.40
34	a	562	C	N3-C4-C5	6.00	124.30	121.90
55	w	57	G	N3-C4-C5	-6.00	125.60	128.60
1	A	2071	A	N1-C6-N6	6.00	122.20	118.60
1	A	781	A	C5-C6-N1	6.00	120.70	117.70
1	A	991	C	C6-N1-C2	-6.00	117.90	120.30
34	a	314	C	N1-C2-O2	5.99	122.50	118.90
1	A	818	G	O5'-P-OP1	5.99	117.89	110.70
1	A	446	G	O5'-P-OP2	-5.99	100.31	105.70
57	y	291	TYR	C-N-CD	5.99	140.98	128.40
1	A	2064	C	N1-C2-O2	-5.99	115.31	118.90
34	a	1258	G	C5-C6-N1	5.99	114.49	111.50
34	a	1502	A	C4-C5-N7	5.99	113.69	110.70
1	A	1555	G	N1-C6-O6	5.99	123.49	119.90
1	A	961	C	C4-C5-C6	5.98	120.39	117.40
1	A	964	C	N3-C4-C5	5.98	124.29	121.90
1	A	2610	C	N3-C4-C5	-5.98	119.51	121.90
1	A	2820	A	C4-C5-N7	5.98	113.69	110.70
2	B	71	C	N1-C2-O2	5.98	122.49	118.90
1	A	1698	A	C5-N7-C8	-5.98	100.91	103.90
1	A	379	G	C8-N9-C4	-5.98	104.01	106.40
1	A	1936	A	O4'-C1'-N9	5.98	112.98	108.20
1	A	1202	C	N1-C2-O2	-5.97	115.31	118.90
1	A	2586	C	N1-C2-O2	-5.97	115.32	118.90
1	A	2576	G	C8-N9-C1'	-5.97	119.23	127.00
57	y	159	PRO	C-N-CA	-5.97	106.77	121.70
34	a	855	G	C6-C5-N7	-5.97	126.82	130.40
39	f	75	LEU	CA-CB-CG	5.97	129.02	115.30
1	A	1899	G	C4-N9-C1'	5.96	134.25	126.50
8	J	33	PRO	N-CA-CB	5.96	110.46	103.30
34	a	1036	G	N3-C4-N9	5.96	129.58	126.00
34	a	748	C	P-O3'-C3'	5.96	126.86	119.70
1	A	1021	A	O5'-P-OP1	-5.96	100.34	105.70
1	A	1919	A	C8-N9-C4	-5.96	103.42	105.80
34	a	1124	G	C4-C5-N7	-5.96	108.42	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1628	G	C6-C5-N7	-5.96	126.83	130.40
34	a	1068	G	C4-N9-C1'	5.96	134.24	126.50
55	w	29	G	C6-C5-N7	-5.96	126.83	130.40
57	y	191	ASP	C-N-CD	5.95	140.90	128.40
1	A	512	G	N1-C6-O6	-5.95	116.33	119.90
34	a	401	C	C6-N1-C2	-5.95	117.92	120.30
34	a	575	G	O5'-P-OP2	-5.95	100.35	105.70
1	A	570	G	N9-C4-C5	5.95	107.78	105.40
1	A	1285	G	OP2-P-O3'	5.95	118.28	105.20
1	A	1897	G	C8-N9-C4	5.95	108.78	106.40
1	A	1227	G	C2-N3-C4	-5.94	108.93	111.90
1	A	1758	G	C6-C5-N7	-5.94	126.84	130.40
1	A	1653	G	P-O3'-C3'	5.94	126.82	119.70
1	A	714	U	C5-C6-N1	-5.93	119.74	122.70
1	A	2789	C	C6-N1-C2	5.93	122.67	120.30
34	a	573	A	C8-N9-C4	-5.93	103.43	105.80
34	a	23	C	C6-N1-C2	-5.92	117.93	120.30
34	a	1076	C	N3-C2-O2	-5.92	117.75	121.90
34	a	855	G	C5-C6-O6	-5.92	125.05	128.60
1	A	1958	C	OP1-P-OP2	-5.91	110.73	119.60
34	a	1219	U	N1-C2-O2	-5.91	118.66	122.80
34	a	1227	A	C2-N3-C4	-5.91	107.64	110.60
1	A	252	G	C6-C5-N7	-5.91	126.85	130.40
1	A	1698	A	N1-C2-N3	5.91	132.25	129.30
34	a	1254	C	C6-N1-C2	5.91	122.66	120.30
1	A	692	C	N3-C2-O2	-5.91	117.76	121.90
1	A	2889	C	C2-N1-C1'	5.91	125.30	118.80
34	a	515	G	C4-C5-N7	5.91	113.16	110.80
1	A	2395	C	C6-N1-C2	-5.90	117.94	120.30
34	a	258	G	C8-N9-C1'	-5.90	119.33	127.00
34	a	805	C	C5-C4-N4	-5.90	116.07	120.20
34	a	91	C	N3-C2-O2	-5.90	117.77	121.90
1	A	526	A	N1-C6-N6	-5.90	115.06	118.60
34	a	301	G	N1-C6-O6	5.90	123.44	119.90
1	A	451	C	N3-C2-O2	5.89	126.03	121.90
1	A	1034	G	N1-C6-O6	5.89	123.44	119.90
33	x	15	G	N3-C2-N2	5.89	124.03	119.90
1	A	742	G	C8-N9-C4	5.89	108.76	106.40
34	a	1525	G	C5-N7-C8	-5.89	101.36	104.30
1	A	1772	G	N1-C6-O6	5.89	123.43	119.90
1	A	1896	G	N1-C6-O6	5.89	123.43	119.90
57	y	441	LEU	C-N-CD	5.89	140.76	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	A	N7-C8-N9	5.88	116.74	113.80
1	A	661	C	C6-N1-C2	5.88	122.65	120.30
1	A	701	G	C8-N9-C4	5.88	108.75	106.40
1	A	1653	G	C8-N9-C4	-5.88	104.05	106.40
34	a	258	G	C6-C5-N7	-5.88	126.87	130.40
34	a	717	C	N3-C2-O2	5.88	126.02	121.90
1	A	859	G	C8-N9-C1'	5.88	134.64	127.00
1	A	944	G	C6-C5-N7	-5.88	126.87	130.40
1	A	1992	G	O4'-C1'-N9	-5.88	103.50	108.20
34	a	1150	U	C2-N3-C4	5.88	130.53	127.00
1	A	1950	G	N1-C6-O6	-5.88	116.37	119.90
34	a	394	G	C5-C6-O6	5.88	132.12	128.60
34	a	1187	G	N9-C4-C5	5.88	107.75	105.40
1	A	1992	G	N3-C4-N9	5.87	129.52	126.00
1	A	139(A)	G	C8-N9-C4	-5.87	104.05	106.40
34	a	117	G	N1-C6-O6	5.87	123.42	119.90
34	a	1527	C	C4-C5-C6	-5.87	114.47	117.40
1	A	558	G	N1-C6-O6	5.86	123.42	119.90
1	A	1061	U	C5-C6-N1	5.86	125.63	122.70
1	A	2624	G	N3-C4-C5	-5.86	125.67	128.60
1	A	190	A	N1-C6-N6	-5.86	115.08	118.60
1	A	2242	G	N3-C4-N9	-5.86	122.48	126.00
34	a	954	G	C8-N9-C4	5.86	108.74	106.40
34	a	1356	G	C5-C6-O6	5.86	132.11	128.60
37	d	139	ARG	NE-CZ-NH1	5.86	123.23	120.30
34	a	1254	C	N3-C4-C5	5.85	124.24	121.90
1	A	645	C	C6-N1-C2	-5.85	117.96	120.30
1	A	1796	U	C5-C6-N1	-5.85	119.78	122.70
34	a	79	G	N1-C6-O6	-5.85	116.39	119.90
1	A	1404	C	C2-N1-C1'	5.85	125.23	118.80
2	B	7	G	C8-N9-C4	-5.85	104.06	106.40
1	A	2443	C	C2-N3-C4	-5.85	116.98	119.90
55	w	73	A	C8-N9-C4	-5.84	103.46	105.80
1	A	1328	G	C5-C6-O6	-5.84	125.10	128.60
1	A	1299	G	O5'-P-OP2	-5.84	100.44	105.70
57	y	303	ALA	N-CA-C	-5.84	95.23	111.00
1	A	1973	G	N9-C4-C5	5.84	107.73	105.40
1	A	2096	U	OP1-P-OP2	5.84	128.35	119.60
57	y	557	ASP	C-N-CA	5.84	136.29	121.70
1	A	2038	G	OP2-P-O3'	5.83	118.03	105.20
1	A	335	C	C5-C6-N1	5.83	123.92	121.00
1	A	2286	A	C2-N3-C4	-5.83	107.69	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2450	A	O5'-P-OP1	-5.83	100.45	105.70
34	a	333	G	C4-C5-N7	5.83	113.13	110.80
1	A	961	C	N3-C4-C5	-5.83	119.57	121.90
34	a	1280	A	N3-C4-C5	-5.83	122.72	126.80
1	A	2084	C	N3-C4-C5	5.82	124.23	121.90
1	A	2324	C	C5-C6-N1	-5.82	118.09	121.00
1	A	800	A	O5'-P-OP2	-5.82	100.46	105.70
1	A	1654	A	O5'-P-OP1	-5.82	100.46	105.70
1	A	797	C	O5'-P-OP2	-5.82	100.47	105.70
1	A	2566	A	N1-C6-N6	-5.82	115.11	118.60
57	y	407	GLU	C-N-CD	5.82	140.62	128.40
1	A	1239	G	C8-N9-C4	-5.81	104.08	106.40
34	a	509	A	N7-C8-N9	5.81	116.70	113.80
34	a	851	G	N1-C6-O6	5.81	123.39	119.90
1	A	2439	A	OP1-P-O3'	5.81	117.98	105.20
1	A	2559	C	C5-C6-N1	-5.81	118.10	121.00
1	A	2791	C	N3-C4-N4	5.81	122.06	118.00
1	A	195	A	C4-C5-N7	5.81	113.60	110.70
34	a	78	G	C5-C6-O6	5.80	132.08	128.60
34	a	1266	G	N3-C4-N9	-5.80	122.52	126.00
1	A	1921	G	N1-C6-O6	5.80	123.38	119.90
1	A	2789	C	C5-C6-N1	-5.80	118.10	121.00
1	A	1955	U	C5-C4-O4	5.80	129.38	125.90
34	a	1206	G	C5-C6-O6	-5.80	125.12	128.60
1	A	307	G	C8-N9-C4	-5.79	104.08	106.40
1	A	797	C	O5'-P-OP1	5.79	117.65	110.70
1	A	2179	C	N1-C2-O2	5.79	122.38	118.90
17	U	92	ARG	NE-CZ-NH1	-5.79	117.40	120.30
34	a	327	A	N1-C6-N6	5.79	122.08	118.60
34	a	330	C	OP1-P-O3'	5.79	117.95	105.20
34	a	1442	G	N1-C6-O6	5.79	123.38	119.90
1	A	1980	G	N9-C4-C5	-5.79	103.08	105.40
34	a	1124	G	N9-C4-C5	5.79	107.72	105.40
1	A	1343	G	C4-N9-C1'	5.79	134.03	126.50
1	A	531	C	N1-C2-O2	5.79	122.37	118.90
1	A	818	G	O5'-P-OP2	-5.78	100.49	105.70
1	A	1325	G	O4'-C1'-N9	5.78	112.83	108.20
33	x	56	C	N3-C2-O2	-5.78	117.85	121.90
34	a	258	G	C4-N9-C1'	5.78	134.02	126.50
34	a	406	G	N3-C4-N9	5.78	129.47	126.00
34	a	1123	A	N1-C6-N6	-5.78	115.13	118.60
1	A	808	G	C4-N9-C1'	5.78	134.01	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2448	A	C5-C6-N6	-5.78	119.08	123.70
1	A	2030	A	O4'-C1'-N9	5.78	112.82	108.20
34	a	976	G	C4-N9-C1'	5.77	134.00	126.50
1	A	1919	A	N1-C6-N6	-5.77	115.14	118.60
1	A	1979	C	C6-N1-C2	5.77	122.61	120.30
1	A	2174	C	C2-N3-C4	5.77	122.78	119.90
1	A	2335	A	O4'-C1'-N9	5.77	112.82	108.20
34	a	569	C	C6-N1-C2	5.77	122.61	120.30
1	A	945	A	N9-C4-C5	-5.77	103.49	105.80
1	A	2501	C	C5-C6-N1	-5.77	118.12	121.00
7	H	3	ARG	NE-CZ-NH1	5.76	123.18	120.30
34	a	1461	G	C6-C5-N7	-5.76	126.94	130.40
37	d	194	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	329	G	N3-C4-N9	5.76	129.46	126.00
34	a	362	G	N1-C6-O6	5.76	123.36	119.90
34	a	1237	C	C6-N1-C2	5.76	122.60	120.30
34	a	1343	G	N1-C2-N3	5.76	127.36	123.90
34	a	1420	C	N1-C2-O2	-5.76	115.44	118.90
57	y	553	ALA	N-CA-C	5.76	126.55	111.00
1	A	1653	G	C8-N9-C1'	-5.76	119.52	127.00
34	a	1036	G	N3-C4-C5	-5.76	125.72	128.60
33	x	68	C	C5-C6-N1	5.76	123.88	121.00
34	a	1402	C	C6-N1-C2	-5.75	118.00	120.30
1	A	868	U	C5-C6-N1	-5.75	119.82	122.70
1	A	1272	A	N1-C2-N3	5.75	132.18	129.30
1	A	1519	G	N3-C4-C5	-5.75	125.72	128.60
1	A	565	C	O5'-P-OP1	-5.75	100.53	105.70
1	A	572	A	N1-C6-N6	5.75	122.05	118.60
34	a	841	U	C6-N1-C2	-5.75	117.55	121.00
1	A	586	A	C2-N3-C4	-5.75	107.73	110.60
1	A	2458	G	N3-C2-N2	-5.74	115.88	119.90
1	A	2095	C	OP1-P-O3'	-5.74	92.57	105.20
4	E	47	VAL	CB-CA-C	-5.74	100.50	111.40
34	a	1392	G	C5-C6-N1	-5.74	108.63	111.50
55	w	40	C	N1-C2-O2	5.74	122.34	118.90
34	a	962	C	N1-C2-O2	-5.73	115.46	118.90
34	a	1359	C	N1-C2-O2	5.73	122.34	118.90
34	a	1290	G	C5-C6-O6	-5.73	125.16	128.60
34	a	1486	G	C4-N9-C1'	5.73	133.95	126.50
34	a	79	G	C5-C6-O6	5.73	132.03	128.60
34	a	1386	G	N3-C2-N2	-5.72	115.89	119.90
34	a	1530	G	C8-N9-C1'	5.72	134.44	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1758	G	C4-N9-C1'	5.72	133.94	126.50
1	A	1138	G	C5-C6-N1	5.72	114.36	111.50
1	A	973	A	N1-C2-N3	5.72	132.16	129.30
34	a	263	A	C5-C6-N1	5.72	120.56	117.70
1	A	2230	G	C5-C6-O6	5.72	132.03	128.60
34	a	1053	G	C8-N9-C4	5.72	108.69	106.40
1	A	1558	A	C5-N7-C8	-5.71	101.04	103.90
1	A	2243	U	O5'-P-OP1	5.71	117.55	110.70
34	a	37	U	N3-C4-O4	5.71	123.39	119.40
34	a	15	G	C4-C5-N7	5.71	113.08	110.80
34	a	936	C	C6-N1-C2	-5.71	118.02	120.30
34	a	717	C	N1-C2-O2	-5.71	115.48	118.90
34	a	1330	U	N3-C2-O2	-5.70	118.21	122.20
56	v	13	A	C8-N9-C4	-5.70	103.52	105.80
57	y	333	GLU	C-N-CD	5.70	140.37	128.40
1	A	1767	C	C6-N1-C2	-5.70	118.02	120.30
34	a	1227	A	C5-N7-C8	-5.70	101.05	103.90
1	A	330	A	C5-N7-C8	-5.69	101.05	103.90
1	A	781	A	C2-N3-C4	5.69	113.45	110.60
34	a	752	G	N1-C6-O6	-5.69	116.48	119.90
34	a	1456	G	N3-C4-C5	5.69	131.45	128.60
57	y	287	THR	C-N-CD	5.69	140.35	128.40
1	A	2556	C	N3-C4-N4	5.69	121.98	118.00
1	A	2611	U	C5-C4-O4	-5.69	122.48	125.90
34	a	1516	G	N3-C4-C5	5.69	131.44	128.60
34	a	1230	C	C5-C6-N1	5.69	123.84	121.00
1	A	1189	A	N1-C6-N6	5.69	122.01	118.60
1	A	1218	C	C6-N1-C2	-5.68	118.03	120.30
34	a	897	C	O5'-P-OP2	-5.68	100.58	105.70
1	A	2140	C	C5-C4-N4	5.68	124.18	120.20
34	a	232	G	N1-C6-O6	5.68	123.31	119.90
1	A	1902	C	N3-C2-O2	-5.68	117.92	121.90
1	A	2283	C	C6-N1-C2	-5.67	118.03	120.30
34	a	288	A	C4-C5-C6	5.67	119.84	117.00
1	A	80	G	C5-C6-O6	-5.67	125.20	128.60
1	A	581	C	C2-N1-C1'	5.67	125.04	118.80
1	A	1491	G	N1-C6-O6	-5.67	116.50	119.90
1	A	1369	G	C8-N9-C4	-5.67	104.13	106.40
1	A	1697	G	C5-C6-O6	-5.67	125.20	128.60
34	a	233	C	C6-N1-C2	-5.67	118.03	120.30
34	a	863	U	C2-N1-C1'	-5.67	110.89	117.70
1	A	979	G	N7-C8-N9	5.67	115.94	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1899	G	N3-C4-C5	-5.67	125.77	128.60
34	a	300	A	C8-N9-C4	-5.67	103.53	105.80
1	A	830	G	C5-C6-O6	5.67	132.00	128.60
34	a	91	C	C6-N1-C2	-5.67	118.03	120.30
1	A	1936	A	C8-N9-C4	-5.66	103.53	105.80
34	a	959	A	N9-C4-C5	-5.66	103.53	105.80
34	a	1229	A	OP1-P-O3'	5.66	117.66	105.20
1	A	1899	G	C8-N9-C1'	-5.66	119.64	127.00
1	A	1772	G	C6-C5-N7	-5.66	127.00	130.40
34	a	619	U	C6-N1-C1'	5.66	129.13	121.20
1	A	1972	A	O5'-P-OP1	-5.66	100.61	105.70
33	x	60	U	C2-N1-C1'	5.66	124.49	117.70
34	a	913	A	C4-C5-C6	5.66	119.83	117.00
34	a	406	G	C5-C6-O6	-5.66	125.21	128.60
34	a	1067	A	N1-C6-N6	-5.66	115.21	118.60
1	A	139(A)	G	N1-C6-O6	-5.66	116.51	119.90
1	A	399	G	C2-N3-C4	-5.65	109.07	111.90
1	A	1416	G	O4'-C1'-N9	5.65	112.72	108.20
1	A	2070	G	C5-C6-N1	5.65	114.33	111.50
1	A	1657	C	N3-C4-N4	-5.65	114.04	118.00
1	A	2612	C	C6-N1-C2	5.65	122.56	120.30
34	a	302	G	N1-C6-O6	-5.65	116.51	119.90
34	a	572	A	N1-C2-N3	-5.65	126.47	129.30
1	A	645	C	C5-C6-N1	5.65	123.83	121.00
1	A	141	A	C5-N7-C8	-5.65	101.08	103.90
34	a	1514	C	C4-C5-C6	5.65	120.22	117.40
1	A	1493	C	C6-N1-C2	-5.65	118.04	120.30
1	A	2503	A	N1-C2-N3	-5.65	126.48	129.30
1	A	263	C	C2-N1-C1'	5.64	125.01	118.80
1	A	2276	G	N3-C4-N9	5.64	129.38	126.00
1	A	803	U	C4-C5-C6	5.64	123.08	119.70
34	a	10	A	C5-C6-N6	-5.64	119.19	123.70
34	a	369	C	C6-N1-C2	-5.64	118.04	120.30
34	a	549	C	N1-C2-O2	-5.64	115.52	118.90
1	A	1214	A	C5-C6-N6	5.64	128.21	123.70
1	A	1572	A	N1-C6-N6	5.64	121.98	118.60
34	a	1324	A	N9-C4-C5	5.64	108.05	105.80
34	a	1326	C	N1-C2-O2	-5.64	115.52	118.90
1	A	272(A)	U	C5-C6-N1	5.63	125.52	122.70
1	A	2828	C	C5-C6-N1	-5.63	118.19	121.00
34	a	325	A	C8-N9-C4	5.63	108.05	105.80
1	A	576	U	C5-C6-N1	5.63	125.51	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	331	G	OP1-P-O3'	5.63	117.58	105.20
34	a	880	C	C5-C6-N1	-5.63	118.19	121.00
34	a	1029	C	P-O3'-C3'	5.63	126.45	119.70
12	P	44	GLY	N-CA-C	-5.63	99.04	113.10
1	A	570	G	C8-N9-C4	-5.62	104.15	106.40
1	A	2508	G	O5'-P-OP2	-5.62	100.64	105.70
34	a	117	G	C8-N9-C1'	-5.62	119.69	127.00
1	A	983	A	N1-C6-N6	5.62	121.97	118.60
1	A	1797	C	C6-N1-C2	5.62	122.55	120.30
1	A	961	C	OP1-P-OP2	5.62	128.03	119.60
1	A	2693	A	C8-N9-C4	-5.62	103.55	105.80
34	a	1402	C	N3-C4-C5	-5.62	119.65	121.90
1	A	737	C	C6-N1-C2	5.62	122.55	120.30
1	A	1052	C	C5-C6-N1	5.62	123.81	121.00
47	n	44	LEU	CA-CB-CG	5.62	128.22	115.30
8	J	129	PRO	N-CA-CB	5.62	110.04	103.30
34	a	1125	U	C2-N1-C1'	-5.62	110.96	117.70
1	A	2638	G	N3-C4-N9	5.62	129.37	126.00
34	a	975	A	N7-C8-N9	5.62	116.61	113.80
1	A	945	A	N9-C1'-C2'	5.62	121.30	114.00
1	A	1787	A	C4-N9-C1'	5.62	136.41	126.30
1	A	2519	U	C2-N3-C4	-5.62	123.63	127.00
34	a	1399	C	O5'-P-OP1	-5.61	100.65	105.70
1	A	527	C	N3-C2-O2	-5.61	117.97	121.90
34	a	803	G	C5-C6-O6	5.61	131.96	128.60
34	a	976	G	N3-C2-N2	-5.61	115.97	119.90
55	w	29	G	C5-C6-O6	-5.61	125.23	128.60
34	a	569	C	C5-C6-N1	-5.61	118.20	121.00
57	y	140	LEU	C-N-CD	5.61	140.17	128.40
1	A	695	G	N1-C6-O6	5.60	123.26	119.90
1	A	137	C	C6-N1-C2	-5.60	118.06	120.30
1	A	569	U	N3-C2-O2	-5.60	118.28	122.20
1	A	1913	A	N1-C6-N6	5.60	121.96	118.60
1	A	571	A	O5'-P-OP1	-5.60	100.66	105.70
34	a	406	G	C4-N9-C1'	5.60	133.78	126.50
1	A	963	U	C6-N1-C2	5.60	124.36	121.00
1	A	1955	U	N1-C2-N3	5.60	118.26	114.90
1	A	2432	A	C8-N9-C4	5.59	108.04	105.80
34	a	1526	G	N1-C6-O6	5.59	123.26	119.90
1	A	830	G	N1-C6-O6	-5.59	116.55	119.90
1	A	2638	G	C4-N9-C1'	5.59	133.77	126.50
1	A	2503	A	N3-C4-N9	5.59	131.87	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	C	O5'-P-OP2	-5.59	100.67	105.70
34	a	796	C	C6-N1-C2	5.59	122.53	120.30
1	A	335	C	C6-N1-C2	-5.58	118.07	120.30
34	a	44	G	N1-C6-O6	-5.58	116.55	119.90
34	a	353	A	OP2-P-O3'	5.58	117.49	105.20
1	A	2554	U	N3-C4-O4	5.58	123.31	119.40
1	A	742	G	N1-C6-O6	5.58	123.25	119.90
34	a	345	C	N3-C2-O2	-5.58	117.99	121.90
34	a	750	G	N3-C4-C5	-5.58	125.81	128.60
1	A	581	C	N3-C2-O2	-5.58	118.00	121.90
1	A	1006	C	C5-C6-N1	5.58	123.79	121.00
1	A	1571	A	N1-C6-N6	-5.58	115.25	118.60
1	A	1721	G	C5-C6-O6	-5.58	125.25	128.60
1	A	1973	G	N3-C2-N2	-5.58	116.00	119.90
55	w	73	A	C4-C5-N7	5.58	113.49	110.70
34	a	937	A	N1-C6-N6	-5.58	115.25	118.60
1	A	1617	C	N1-C2-O2	-5.58	115.56	118.90
1	A	1562	A	N1-C6-N6	5.57	121.94	118.60
1	A	1314	C	C2-N1-C1'	5.57	124.93	118.80
1	A	1617	C	C6-N1-C1'	5.57	127.49	120.80
34	a	1363	C	N1-C2-O2	-5.57	115.56	118.90
1	A	1191	G	C4-N9-C1'	-5.57	119.27	126.50
1	A	141	A	C6-C5-N7	-5.56	128.41	132.30
1	A	263	C	C6-N1-C1'	-5.56	114.12	120.80
34	a	258	G	N3-C4-N9	5.56	129.34	126.00
34	a	899	C	C6-N1-C2	5.56	122.53	120.30
1	A	574	C	C6-N1-C2	5.56	122.53	120.30
1	A	973	A	C5-C6-N1	-5.56	114.92	117.70
1	A	2027	G	O5'-P-OP2	-5.56	100.69	105.70
1	A	2496	C	C5-C6-N1	-5.56	118.22	121.00
1	A	2546	U	N3-C2-O2	-5.56	118.31	122.20
55	w	45	U	N3-C4-O4	-5.56	115.51	119.40
1	A	1992	G	C5-C6-N1	5.56	114.28	111.50
26	3	31	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	841	A	O5'-P-OP2	-5.56	100.70	105.70
1	A	2638	G	C6-C5-N7	-5.56	127.07	130.40
34	a	1396	A	N1-C2-N3	5.56	132.08	129.30
1	A	815	C	C2-N1-C1'	5.55	124.91	118.80
34	a	365	U	N1-C2-O2	-5.55	118.91	122.80
34	a	1344	C	C6-N1-C2	5.55	122.52	120.30
1	A	399	G	C8-N9-C4	5.55	108.62	106.40
34	a	973	G	C4-C5-N7	-5.55	108.58	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1320	C	C6-N1-C1'	-5.55	114.14	120.80
1	A	2419	U	O5'-P-OP2	-5.55	100.71	105.70
1	A	2820	A	C6-C5-N7	-5.55	128.42	132.30
1	A	805	G	C8-N9-C4	5.54	108.62	106.40
34	a	1129	C	N3-C2-O2	-5.54	118.02	121.90
34	a	559	A	O5'-P-OP2	-5.54	100.71	105.70
34	a	1206	G	N1-C6-O6	5.54	123.22	119.90
1	A	381	G	N1-C6-O6	5.54	123.22	119.90
1	A	501	A	N1-C6-N6	-5.54	115.28	118.60
34	a	111	G	C5-C6-O6	-5.54	125.28	128.60
34	a	816	A	C8-N9-C4	5.54	108.02	105.80
1	A	803	U	C5-C6-N1	-5.54	119.93	122.70
1	A	1628	G	N1-C6-O6	5.54	123.22	119.90
1	A	1992	G	N3-C4-C5	-5.54	125.83	128.60
1	A	1208	C	C5-C6-N1	5.54	123.77	121.00
1	A	2308	G	O4'-C1'-N9	-5.53	103.77	108.20
1	A	307	G	N7-C8-N9	5.53	115.87	113.10
1	A	2766	G	C4-N9-C1'	5.53	133.69	126.50
34	a	651	C	C6-N1-C2	-5.53	118.09	120.30
1	A	195	A	C5-N7-C8	-5.53	101.14	103.90
1	A	1681	G	N3-C4-N9	-5.53	122.68	126.00
1	A	2198	A	OP1-P-O3'	5.53	117.36	105.20
1	A	2550	G	C6-C5-N7	-5.53	127.08	130.40
1	A	2579	C	N1-C2-O2	-5.53	115.58	118.90
1	A	751	A	N1-C2-N3	-5.52	126.54	129.30
1	A	1277	G	C8-N9-C4	5.52	108.61	106.40
34	a	913	A	P-O3'-C3'	5.52	126.33	119.70
1	A	1252	G	C6-C5-N7	-5.52	127.09	130.40
1	A	2503	A	C5-C6-N6	-5.52	119.28	123.70
34	a	1366	C	N1-C2-O2	-5.52	115.59	118.90
1	A	1199	U	C5-C6-N1	-5.52	119.94	122.70
1	A	1620	G	N1-C6-O6	5.52	123.21	119.90
34	a	881	G	O5'-P-OP2	5.52	117.32	110.70
1	A	614	U	O4'-C1'-N1	5.51	112.61	108.20
34	a	1524	C	C2-N3-C4	-5.51	117.14	119.90
1	A	561	G	C5-C6-N1	5.51	114.25	111.50
1	A	2742	C	C6-N1-C2	5.51	122.50	120.30
57	y	155	VAL	CB-CA-C	-5.51	100.93	111.40
34	a	981	U	C5-C4-O4	-5.51	122.59	125.90
34	a	878	G	N1-C6-O6	5.51	123.20	119.90
34	a	1346	A	C8-N9-C4	5.51	108.00	105.80
1	A	857	C	N1-C2-O2	-5.51	115.60	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2040	C	N1-C2-O2	5.51	122.20	118.90
1	A	2235	G	C6-C5-N7	-5.50	127.10	130.40
55	w	12	U	C5-C6-N1	-5.50	119.95	122.70
1	A	2001	A	N1-C2-N3	5.50	132.05	129.30
1	A	2638	G	C4-C5-C6	5.50	122.10	118.80
34	a	1346	A	OP1-P-O3'	5.50	117.31	105.20
34	a	976	G	C8-N9-C1'	-5.50	119.85	127.00
57	y	187	PRO	C-N-CD	5.50	139.95	128.40
1	A	1598	C	C5-C4-N4	-5.50	116.35	120.20
34	a	271	C	C6-N1-C2	-5.50	118.10	120.30
1	A	2546	U	C5-C6-N1	-5.50	119.95	122.70
47	n	53	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	997	G	O5'-P-OP1	-5.49	100.76	105.70
34	a	25	C	C6-N1-C2	-5.49	118.10	120.30
1	A	1761	C	C6-N1-C2	5.49	122.50	120.30
55	w	24	G	C5-N7-C8	-5.49	101.55	104.30
1	A	364	C	N1-C2-O2	5.49	122.19	118.90
34	a	1486	G	N3-C4-C5	-5.49	125.86	128.60
34	a	481	G	C5-C6-O6	-5.49	125.31	128.60
1	A	1778	U	N3-C4-O4	-5.48	115.56	119.40
34	a	1230	C	C6-N1-C2	-5.48	118.11	120.30
1	A	979	G	N1-C6-O6	5.48	123.19	119.90
1	A	1202	C	N3-C2-O2	5.48	125.74	121.90
34	a	1502	A	N7-C8-N9	5.48	116.54	113.80
34	a	1248	A	C5-C6-N1	5.48	120.44	117.70
57	y	103	VAL	CB-CA-C	-5.48	101.00	111.40
1	A	948	G	N1-C6-O6	5.47	123.18	119.90
1	A	1702	G	N9-C4-C5	5.47	107.59	105.40
34	a	559	A	C2-N3-C4	5.47	113.34	110.60
34	a	1494	G	N3-C4-N9	5.47	129.28	126.00
1	A	693	C	N1-C2-O2	5.47	122.18	118.90
1	A	2239	G	N1-C6-O6	5.47	123.18	119.90
1	A	2612	C	N3-C4-C5	5.47	124.09	121.90
1	A	1950	G	N9-C4-C5	5.47	107.59	105.40
1	A	2262	U	O5'-P-OP1	-5.47	100.78	105.70
34	a	1221	G	C5-C6-O6	5.47	131.88	128.60
1	A	941	A	O5'-P-OP1	-5.47	100.78	105.70
1	A	1395	A	O4'-C1'-N9	5.47	112.58	108.20
33	x	50	U	N3-C4-C5	-5.46	111.32	114.60
34	a	400	C	N3-C4-C5	-5.46	119.71	121.90
34	a	1083	U	C2-N3-C4	5.46	130.28	127.00
1	A	266	G	C6-C5-N7	-5.46	127.12	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	374	PRO	CA-N-CD	-5.46	103.85	111.50
1	A	22	C	N1-C2-O2	5.46	122.17	118.90
34	a	1195	C	N1-C2-O2	-5.46	115.62	118.90
1	A	2047	U	N1-C2-N3	5.46	118.17	114.90
1	A	2767	C	C2-N1-C1'	5.46	124.80	118.80
34	a	369	C	C5-C6-N1	5.46	123.73	121.00
1	A	298	G	C4-C5-N7	5.46	112.98	110.80
1	A	2581	G	O4'-C1'-N9	5.46	112.56	108.20
1	A	2088	G	N9-C4-C5	5.45	107.58	105.40
34	a	70	G	N1-C6-O6	5.45	123.17	119.90
34	a	976	G	C6-C5-N7	-5.45	127.13	130.40
34	a	1461	G	C8-N9-C1'	-5.45	119.91	127.00
1	A	1938	A	C8-N9-C4	5.45	107.98	105.80
55	w	70	G	N1-C6-O6	5.45	123.17	119.90
55	w	73	A	C6-C5-N7	-5.45	128.49	132.30
1	A	796	C	OP1-P-OP2	5.45	127.77	119.60
34	a	225	C	C5-C6-N1	-5.45	118.28	121.00
34	a	1502	A	C5-C6-N1	-5.45	114.98	117.70
1	A	1142(A)	A	N3-C4-C5	5.44	130.61	126.80
34	a	295	C	C6-N1-C2	5.44	122.48	120.30
1	A	1950	G	C4-C5-N7	-5.44	108.62	110.80
34	a	508	C	N1-C2-O2	-5.44	115.64	118.90
34	a	529	G	C5-C6-O6	-5.44	125.34	128.60
34	a	975	A	N9-C4-C5	-5.44	103.62	105.80
1	A	1799	G	C4-C5-N7	-5.44	108.62	110.80
34	a	397	A	C4-C5-C6	5.44	119.72	117.00
34	a	61	G	N1-C6-O6	5.43	123.16	119.90
1	A	2584	U	C5-C4-O4	5.43	129.16	125.90
34	a	317	G	C5-C6-O6	-5.43	125.34	128.60
34	a	1496	C	N1-C2-O2	-5.43	115.64	118.90
34	a	1525	G	C4-C5-N7	5.43	112.97	110.80
1	A	2252	G	OP2-P-O3'	5.43	117.14	105.20
1	A	1108	U	P-O3'-C3'	5.43	126.21	119.70
1	A	90	U	N1-C2-O2	5.43	126.60	122.80
34	a	940	C	N3-C2-O2	5.43	125.70	121.90
1	A	1599	C	C5-C6-N1	5.42	123.71	121.00
34	a	929	G	C6-C5-N7	5.42	133.65	130.40
1	A	933	A	C6-C5-N7	-5.42	128.51	132.30
1	A	24	G	N1-C6-O6	5.42	123.15	119.90
1	A	1109	C	C6-N1-C1'	-5.42	114.30	120.80
1	A	1700	A	N1-C6-N6	5.42	121.85	118.60
33	x	23	A	C4-C5-C6	-5.42	114.29	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	x	68	C	N3-C2-O2	-5.42	118.11	121.90
34	a	986	A	C5-C6-N6	-5.42	119.37	123.70
1	A	48	G	N9-C4-C5	5.41	107.56	105.40
1	A	997	G	C8-N9-C4	5.41	108.56	106.40
1	A	1493	C	C2-N1-C1'	5.41	124.75	118.80
1	A	47	C	O5'-P-OP1	-5.41	100.83	105.70
1	A	436	C	N1-C2-O2	5.41	122.14	118.90
1	A	810	U	C5-C6-N1	-5.41	120.00	122.70
1	A	1138	G	N1-C6-O6	-5.41	116.65	119.90
34	a	819	A	C5-N7-C8	-5.41	101.20	103.90
1	A	1019	U	N3-C2-O2	-5.41	118.42	122.20
1	A	2059	A	C4-C5-N7	5.41	113.40	110.70
34	a	667	G	C8-N9-C4	-5.41	104.24	106.40
1	A	2502	G	O5'-P-OP2	-5.40	100.84	105.70
1	A	1842	G	C6-C5-N7	-5.40	127.16	130.40
34	a	1225	A	N1-C2-N3	-5.40	126.60	129.30
1	A	673	C	C5-C4-N4	-5.40	116.42	120.20
1	A	2178	C	C5-C4-N4	5.40	123.98	120.20
1	A	562	U	OP1-P-OP2	5.40	127.70	119.60
34	a	576	G	C4-N9-C1'	5.40	133.52	126.50
57	y	213	PRO	CA-N-CD	-5.40	103.94	111.50
34	a	194	C	C5-C4-N4	-5.40	116.42	120.20
1	A	661	C	N3-C2-O2	5.39	125.68	121.90
1	A	959	A	C6-N1-C2	5.39	121.84	118.60
1	A	1314	C	N1-C2-O2	5.39	122.14	118.90
34	a	436	C	C5-C4-N4	-5.39	116.42	120.20
1	A	1136	G	N1-C6-O6	5.39	123.14	119.90
34	a	1074	G	C8-N9-C4	5.39	108.56	106.40
34	a	365	U	O4'-C1'-N1	5.39	112.51	108.20
34	a	436	C	C6-N1-C2	-5.39	118.14	120.30
1	A	979	G	N1-C2-N3	5.39	127.13	123.90
1	A	2257	U	N3-C2-O2	5.39	125.97	122.20
1	A	1990	C	N3-C4-C5	-5.39	119.75	121.90
1	A	1702	G	C8-N9-C4	-5.38	104.25	106.40
1	A	1955	U	C5-C6-N1	-5.38	120.01	122.70
1	A	2573	C	N3-C4-N4	5.38	121.77	118.00
34	a	515	G	C5-N7-C8	-5.38	101.61	104.30
34	a	1221	G	C5-N7-C8	5.38	106.99	104.30
34	a	1266	G	C8-N9-C1'	5.38	134.00	127.00
55	w	10	G	C5-N7-C8	-5.38	101.61	104.30
57	y	246	THR	C-N-CD	5.38	139.70	128.40
1	A	2325	G	N1-C6-O6	-5.38	116.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2501	C	C6-N1-C2	5.38	122.45	120.30
1	A	818	G	C6-C5-N7	-5.38	127.17	130.40
1	A	2096	U	C6-N1-C2	-5.38	117.77	121.00
34	a	20	U	N3-C2-O2	5.38	125.97	122.20
34	a	924	C	C2-N3-C4	5.38	122.59	119.90
1	A	298	G	C5-N7-C8	-5.38	101.61	104.30
1	A	1794	U	O5'-P-OP1	-5.38	100.86	105.70
34	a	769	G	N3-C4-C5	-5.38	125.91	128.60
34	a	728	A	C6-C5-N7	-5.38	128.54	132.30
1	A	1204	A	O4'-C1'-N9	5.37	112.50	108.20
1	A	2096	U	N3-C2-O2	-5.37	118.44	122.20
34	a	1461	G	N3-C4-N9	5.37	129.22	126.00
1	A	1069	A	P-O3'-C3'	5.37	126.15	119.70
1	A	2587	A	OP2-P-O3'	5.37	117.02	105.20
1	A	2820	A	C2-N3-C4	-5.37	107.92	110.60
1	A	1210	A	C5-C6-N1	5.37	120.38	117.70
34	a	548	G	C5-C6-O6	-5.37	125.38	128.60
34	a	1281	U	N3-C4-O4	-5.37	115.64	119.40
1	A	2271	G	N1-C2-N2	-5.37	111.37	116.20
2	B	75	G	C8-N9-C4	-5.37	104.25	106.40
34	a	20	U	N1-C2-O2	-5.37	119.04	122.80
34	a	1491	G	N3-C4-C5	-5.37	125.92	128.60
1	A	489	G	C6-C5-N7	-5.37	127.18	130.40
1	A	1932	A	N1-C6-N6	5.37	121.82	118.60
1	A	2095	C	P-O3'-C3'	-5.37	113.26	119.70
34	a	894	G	C5-C6-O6	-5.37	125.38	128.60
55	w	70	G	N3-C2-N2	-5.37	116.14	119.90
2	B	96	U	C6-N1-C2	-5.36	117.78	121.00
1	A	2250	G	C8-N9-C4	5.36	108.54	106.40
1	A	22	C	N3-C2-O2	-5.36	118.15	121.90
1	A	255	A	C2-N3-C4	-5.36	107.92	110.60
1	A	1343	G	N7-C8-N9	5.36	115.78	113.10
1	A	1655	A	N1-C6-N6	5.36	121.81	118.60
1	A	206	U	N1-C2-N3	5.36	118.11	114.90
1	A	462	C	C6-N1-C2	5.36	122.44	120.30
1	A	819	A	C5-N7-C8	-5.36	101.22	103.90
1	A	2024	G	N7-C8-N9	5.36	115.78	113.10
1	A	2056	G	C5-C6-O6	-5.36	125.39	128.60
1	A	2454	G	C6-N1-C2	-5.36	121.89	125.10
34	a	219	C	N3-C2-O2	-5.35	118.15	121.90
1	A	340	A	C2-N3-C4	-5.35	107.93	110.60
1	A	752	A	P-O3'-C3'	5.35	126.12	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1190	G	N3-C2-N2	-5.35	116.16	119.90
34	a	852	G	N9-C4-C5	-5.35	103.26	105.40
1	A	2080	G	C4-C5-N7	5.35	112.94	110.80
1	A	602	G	C4-N9-C1'	5.35	133.45	126.50
1	A	1123	C	C4-C5-C6	5.35	120.07	117.40
1	A	2503	A	C5-C6-N1	5.35	120.37	117.70
1	A	1822	G	C8-N9-C4	5.34	108.54	106.40
34	a	886	G	C5-C6-O6	-5.34	125.39	128.60
1	A	1667	G	C8-N9-C1'	-5.34	120.06	127.00
1	A	2088	G	C8-N9-C1'	5.34	133.94	127.00
1	A	2341	G	C5-C6-O6	-5.34	125.39	128.60
34	a	748	C	N3-C2-O2	-5.34	118.16	121.90
57	y	159	PRO	O-C-N	-5.34	114.16	122.70
1	A	786	C	C6-N1-C2	5.34	122.44	120.30
1	A	1278	A	C2-N3-C4	-5.34	107.93	110.60
1	A	311	A	N1-C6-N6	5.34	121.80	118.60
1	A	1828	G	N1-C6-O6	-5.34	116.70	119.90
34	a	1186	G	C8-N9-C1'	5.34	133.94	127.00
1	A	83	G	O5'-P-OP1	-5.33	100.90	105.70
1	A	977	G	C5-N7-C8	5.33	106.97	104.30
1	A	1628	G	C4-N9-C1'	5.33	133.43	126.50
1	A	1669	A	C6-N1-C2	-5.33	115.40	118.60
1	A	2271	G	C4-C5-N7	5.33	112.93	110.80
1	A	933	A	C8-N9-C4	-5.33	103.67	105.80
1	A	2276	G	N9-C4-C5	-5.33	103.27	105.40
1	A	48	G	C5-C6-O6	5.33	131.80	128.60
1	A	1817	G	O5'-P-OP2	-5.33	100.90	105.70
1	A	2370	G	O5'-P-OP1	-5.33	100.90	105.70
34	a	913	A	N1-C2-N3	5.33	131.96	129.30
1	A	298	G	N7-C8-N9	5.33	115.76	113.10
1	A	782	A	N7-C8-N9	-5.33	111.14	113.80
1	A	1721	G	N9-C4-C5	-5.33	103.27	105.40
34	a	993	G	C4-N9-C1'	5.33	133.43	126.50
1	A	2507	C	C2-N1-C1'	5.33	124.66	118.80
1	A	2611	U	N3-C4-O4	5.33	123.13	119.40
1	A	2751	G	C8-N9-C1'	-5.33	120.08	127.00
34	a	1126	U	C6-N1-C1'	-5.33	113.74	121.20
1	A	986	C	C2-N1-C1'	-5.32	112.94	118.80
1	A	1558	A	C6-C5-N7	-5.32	128.57	132.30
34	a	619	U	C2-N1-C1'	-5.32	111.31	117.70
34	a	1514	C	C5-C6-N1	-5.32	118.34	121.00
1	A	1823	G	N9-C4-C5	-5.32	103.27	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	362	G	C6-C5-N7	-5.32	127.21	130.40
1	A	1199	U	O5'-P-OP2	-5.32	100.92	105.70
34	a	908	A	OP2-P-O3'	5.32	116.89	105.20
1	A	958	U	N1-C2-O2	5.31	126.52	122.80
1	A	2439	A	P-O3'-C3'	5.31	126.08	119.70
1	A	459	U	N3-C4-O4	5.31	123.12	119.40
34	a	527	G	N3-C4-N9	-5.31	122.81	126.00
1	A	2506	U	C5-C4-O4	-5.31	122.71	125.90
34	a	1505	G	C5-C6-O6	5.31	131.79	128.60
1	A	1656	C	C4-C5-C6	5.31	120.05	117.40
1	A	1954	G	C5-C6-O6	-5.31	125.42	128.60
57	y	343	GLY	O-C-N	-5.31	114.20	122.70
34	a	12	U	N1-C2-N3	5.31	118.08	114.90
34	a	317	G	N1-C6-O6	5.30	123.08	119.90
34	a	1198	G	N9-C4-C5	5.30	107.52	105.40
34	a	532	A	N1-C6-N6	5.30	121.78	118.60
34	a	869	G	N3-C4-N9	-5.30	122.82	126.00
1	A	927	G	C6-C5-N7	-5.30	127.22	130.40
1	A	1005	C	N3-C4-C5	5.30	124.02	121.90
1	A	1222	C	C6-N1-C2	-5.30	118.18	120.30
34	a	839	U	N3-C2-O2	-5.30	118.49	122.20
34	a	1395	C	C5-C4-N4	5.30	123.91	120.20
34	a	1432	G	N9-C4-C5	5.30	107.52	105.40
1	A	1204	A	C4-C5-N7	5.30	113.35	110.70
1	A	1502	C	C6-N1-C2	-5.30	118.18	120.30
1	A	1781	C	N3-C2-O2	-5.30	118.19	121.90
34	a	1260	C	N1-C2-O2	5.30	122.08	118.90
1	A	195	A	C4-C5-C6	-5.29	114.35	117.00
1	A	2051	A	N1-C6-N6	5.29	121.78	118.60
1	A	1198	U	OP1-P-OP2	5.29	127.54	119.60
1	A	2384	G	C8-N9-C4	-5.29	104.28	106.40
1	A	80	G	C6-C5-N7	-5.29	127.23	130.40
1	A	600	G	C5-C6-N1	-5.29	108.86	111.50
1	A	1035	U	C5-C4-O4	5.29	129.07	125.90
1	A	2253	G	N1-C6-O6	5.29	123.07	119.90
34	a	1224	G	N1-C6-O6	-5.29	116.73	119.90
1	A	1911	U	N3-C2-O2	-5.29	118.50	122.20
1	A	2811	G	C4-C5-N7	5.29	112.91	110.80
1	A	678	C	C6-N1-C2	-5.28	118.19	120.30
1	A	775	G	O5'-P-OP1	-5.28	100.94	105.70
34	a	275	G	N3-C4-N9	5.28	129.17	126.00
34	a	314	C	C6-N1-C2	-5.28	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	643	C	N1-C2-O2	-5.28	115.73	118.90
1	A	1395	A	N1-C6-N6	5.28	121.77	118.60
1	A	1306	C	N3-C2-O2	-5.28	118.20	121.90
34	a	750	G	C8-N9-C4	-5.28	104.29	106.40
34	a	767	A	N3-C4-C5	-5.28	123.10	126.80
34	a	1131	G	C4-N9-C1'	5.28	133.37	126.50
1	A	139(A)	G	C5-C6-N1	5.28	114.14	111.50
1	A	517	C	C6-N1-C2	-5.28	118.19	120.30
34	a	738	C	C5-C6-N1	5.28	123.64	121.00
1	A	1199	U	C2-N3-C4	-5.28	123.83	127.00
2	B	11	C	C6-N1-C2	5.28	122.41	120.30
57	y	136	ASN	N-CA-C	5.28	125.25	111.00
1	A	704	G	N1-C6-O6	-5.28	116.73	119.90
1	A	2780	G	N3-C2-N2	5.28	123.59	119.90
1	A	2642	G	OP1-P-OP2	-5.27	111.69	119.60
1	A	438	G	C5-C6-O6	-5.27	125.44	128.60
34	a	514	C	C2-N1-C1'	-5.27	113.00	118.80
34	a	333	G	N9-C4-C5	-5.27	103.29	105.40
1	A	1368	G	N1-C6-O6	-5.27	116.74	119.90
1	A	1378	A	C2-N3-C4	-5.27	107.97	110.60
1	A	2261	C	N1-C2-O2	-5.27	115.74	118.90
1	A	2049	G	O5'-P-OP2	-5.27	100.96	105.70
34	a	1257	U	C2-N1-C1'	5.27	124.02	117.70
34	a	1330	U	N1-C2-O2	5.27	126.49	122.80
1	A	2080	G	N3-C4-N9	5.27	129.16	126.00
34	a	311	C	C5-C6-N1	-5.27	118.37	121.00
34	a	1068	G	C8-N9-C1'	-5.27	120.15	127.00
1	A	602	G	C6-C5-N7	-5.26	127.24	130.40
34	a	301	G	C6-C5-N7	-5.26	127.24	130.40
34	a	1052	U	N1-C2-O2	5.26	126.49	122.80
34	a	1110	A	C8-N9-C4	-5.26	103.69	105.80
2	B	79	C	OP2-P-O3'	5.26	116.78	105.20
34	a	251	G	C5-C6-O6	-5.26	125.44	128.60
1	A	1965	C	C5-C4-N4	-5.26	116.52	120.20
1	A	2229	C	N1-C2-O2	5.26	122.06	118.90
34	a	253	U	N3-C2-O2	5.26	125.88	122.20
34	a	588	G	C8-N9-C4	-5.26	104.30	106.40
1	A	526	A	N9-C4-C5	5.26	107.90	105.80
1	A	790	C	N1-C2-O2	5.26	122.06	118.90
1	A	792	G	O4'-C1'-N9	-5.26	103.99	108.20
2	B	75	G	C6-C5-N7	-5.26	127.24	130.40
57	y	194	ALA	C-N-CD	5.26	139.45	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1662	C	OP2-P-O3'	5.26	116.77	105.20
1	A	2010	G	C8-N9-C4	-5.26	104.30	106.40
1	A	2120	G	C5-C6-O6	5.26	131.75	128.60
1	A	48	G	C5-C6-N1	-5.26	108.87	111.50
1	A	1899	G	N3-C4-N9	5.26	129.15	126.00
1	A	2516	G	N9-C4-C5	-5.26	103.30	105.40
1	A	234	C	C6-N1-C1'	-5.25	114.49	120.80
1	A	432	A	C8-N9-C4	-5.25	103.70	105.80
1	A	819	A	N9-C4-C5	-5.25	103.70	105.80
34	a	1496	C	N3-C2-O2	5.25	125.58	121.90
1	A	474	G	N3-C4-N9	5.25	129.15	126.00
1	A	979	G	C8-N9-C4	-5.25	104.30	106.40
34	a	569	C	C2-N3-C4	-5.25	117.27	119.90
1	A	808	G	C8-N9-C1'	-5.25	120.17	127.00
34	a	19	C	N3-C4-C5	-5.25	119.80	121.90
1	A	1696	G	C5-N7-C8	-5.25	101.67	104.30
1	A	1952	A	C6-C5-N7	-5.25	128.62	132.30
34	a	454	C	C6-N1-C2	-5.25	118.20	120.30
34	a	728	A	C5-C6-N6	-5.25	119.50	123.70
34	a	1358	U	C5-C6-N1	-5.25	120.08	122.70
1	A	806	C	O5'-P-OP2	-5.25	100.98	105.70
1	A	1781	C	C6-N1-C1'	-5.25	114.50	120.80
34	a	585	G	N1-C6-O6	5.25	123.05	119.90
1	A	2586	C	OP2-P-O3'	5.25	116.74	105.20
1	A	2704	C	C6-N1-C2	-5.25	118.20	120.30
34	a	267	C	N3-C4-C5	5.24	124.00	121.90
34	a	664	G	C4-C5-N7	-5.24	108.70	110.80
34	a	1198	G	C4-C5-N7	-5.24	108.70	110.80
55	w	20	U	N3-C2-O2	-5.24	118.53	122.20
1	A	2230	G	N1-C6-O6	-5.24	116.75	119.90
1	A	566	U	N3-C2-O2	-5.24	118.53	122.20
1	A	1787	A	C8-N9-C1'	-5.24	118.27	127.70
1	A	2308	G	C4-C5-N7	5.24	112.90	110.80
2	B	7	G	N7-C8-N9	5.24	115.72	113.10
55	w	74	C	N3-C4-C5	-5.24	119.80	121.90
1	A	690	G	C8-N9-C4	-5.24	104.31	106.40
34	a	684	A	C8-N9-C4	-5.24	103.70	105.80
34	a	969	A	N1-C6-N6	5.24	121.74	118.60
1	A	1300	U	C5-C6-N1	5.24	125.32	122.70
1	A	632	A	N7-C8-N9	-5.24	111.18	113.80
1	A	781	A	OP1-P-OP2	5.24	127.45	119.60
1	A	1553	A	O4'-C1'-N9	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1224	G	N9-C4-C5	5.24	107.49	105.40
1	A	678	C	N1-C2-O2	-5.23	115.76	118.90
1	A	1153	C	C5-C6-N1	5.23	123.62	121.00
1	A	1247	A	C8-N9-C4	5.23	107.89	105.80
1	A	2875	C	N1-C2-O2	-5.23	115.76	118.90
34	a	1075	C	OP1-P-O3'	5.23	116.71	105.20
1	A	239	U	N3-C4-C5	5.23	117.74	114.60
1	A	1022	G	C4-N9-C1'	-5.23	119.70	126.50
34	a	634	C	C6-N1-C2	-5.23	118.21	120.30
45	l	29	GLY	N-CA-C	-5.23	100.03	113.10
34	a	1109	C	C2-N1-C1'	5.23	124.55	118.80
57	y	417	PRO	CA-N-CD	-5.23	104.18	111.50
1	A	805	G	C8-N9-C1'	-5.23	120.20	127.00
1	A	1698	A	C4-C5-C6	5.23	119.61	117.00
1	A	1988	C	N1-C2-O2	5.23	122.04	118.90
1	A	2271	G	N3-C2-N2	5.22	123.56	119.90
1	A	2612	C	C2-N1-C1'	-5.22	113.05	118.80
34	a	1323	G	C6-C5-N7	-5.22	127.27	130.40
1	A	932	G	C4-C5-N7	-5.22	108.71	110.80
1	A	961	C	N1-C2-O2	-5.22	115.77	118.90
1	A	1629	U	N3-C4-C5	-5.22	111.47	114.60
2	B	77	U	OP1-P-O3'	5.22	116.69	105.20
34	a	406	G	C6-C5-N7	-5.22	127.27	130.40
34	a	852	G	C6-C5-N7	-5.22	127.27	130.40
1	A	141	A	N7-C8-N9	5.22	116.41	113.80
34	a	984	C	N1-C2-O2	5.22	122.03	118.90
34	a	1406	U	C5-C6-N1	-5.22	120.09	122.70
34	a	1227	A	N1-C6-N6	5.22	121.73	118.60
1	A	1357	U	N1-C2-O2	-5.22	119.15	122.80
1	A	206	U	C5-C4-O4	5.21	129.03	125.90
1	A	818	G	C5-C6-O6	-5.21	125.47	128.60
1	A	1251	C	C6-N1-C2	-5.21	118.21	120.30
1	A	2573	C	C5-C4-N4	-5.21	116.55	120.20
1	A	2592	G	N1-C6-O6	5.21	123.03	119.90
1	A	1787	A	O4'-C1'-N9	-5.21	104.03	108.20
1	A	1982	C	N3-C4-N4	5.21	121.65	118.00
1	A	470	A	O5'-P-OP1	-5.21	101.01	105.70
1	A	1699	G	O5'-P-OP2	-5.21	101.01	105.70
34	a	106	C	N1-C2-O2	-5.21	115.77	118.90
34	a	394	G	N1-C6-O6	-5.21	116.77	119.90
1	A	583	G	C8-N9-C4	-5.21	104.32	106.40
1	A	782	A	N9-C4-C5	-5.21	103.72	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	855	G	C4-C5-N7	5.21	112.88	110.80
55	w	26	A	N9-C4-C5	-5.21	103.72	105.80
1	A	526	A	C5-C6-N6	5.21	127.87	123.70
1	A	915	C	C6-N1-C2	-5.21	118.22	120.30
34	a	1363	C	C2-N1-C1'	-5.21	113.07	118.80
1	A	1191	G	C8-N9-C4	5.21	108.48	106.40
1	A	340	A	C5-C6-N1	-5.20	115.10	117.70
1	A	517	C	N3-C4-N4	5.20	121.64	118.00
1	A	808	G	N1-C6-O6	5.20	123.02	119.90
1	A	1813	G	N7-C8-N9	-5.20	110.50	113.10
34	a	1127	G	N3-C2-N2	-5.20	116.26	119.90
1	A	2873	A	O4'-C1'-N9	5.20	112.36	108.20
34	a	1506	U	N3-C2-O2	5.20	125.84	122.20
1	A	1958	C	C5-C4-N4	-5.20	116.56	120.20
34	a	1290	G	C6-C5-N7	-5.20	127.28	130.40
55	w	20	U	C6-N1-C1'	-5.20	113.92	121.20
34	a	1131	G	C4-C5-C6	5.20	121.92	118.80
1	A	103	A	N1-C6-N6	5.20	121.72	118.60
1	A	234	C	C2-N1-C1'	5.20	124.51	118.80
34	a	397	A	C6-C5-N7	-5.20	128.66	132.30
1	A	514	A	C5-C6-N1	-5.19	115.10	117.70
1	A	825	C	N3-C4-C5	-5.19	119.82	121.90
34	a	1281	U	C4-C5-C6	5.19	122.82	119.70
1	A	807	U	C5-C4-O4	-5.19	122.79	125.90
34	a	1232	U	N1-C2-O2	5.19	126.43	122.80
1	A	265	A	O4'-C1'-N9	5.19	112.35	108.20
1	A	531	C	C2-N1-C1'	5.19	124.50	118.80
1	A	2054	A	OP2-P-O3'	5.19	116.61	105.20
34	a	585	G	C6-C5-N7	-5.19	127.29	130.40
34	a	916	G	C5-C6-O6	5.19	131.71	128.60
57	y	292	PRO	CA-N-CD	-5.19	104.24	111.50
1	A	1007	C	N3-C4-N4	5.18	121.63	118.00
1	A	1161	C	N1-C2-O2	5.18	122.01	118.90
1	A	2627	G	C6-C5-N7	-5.18	127.29	130.40
34	a	782	A	N1-C6-N6	-5.18	115.49	118.60
1	A	734	A	C2-N3-C4	-5.18	108.01	110.60
1	A	1227	G	C6-C5-N7	-5.18	127.29	130.40
1	A	2571	C	C6-N1-C2	5.18	122.37	120.30
1	A	445	C	OP2-P-O3'	5.18	116.59	105.20
34	a	317	G	C4-C5-N7	5.18	112.87	110.80
2	B	71	C	C5-C6-N1	5.18	123.59	121.00
34	a	396	G	C8-N9-C4	-5.18	104.33	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	662	G	O4'-C1'-N9	5.18	112.34	108.20
34	a	1524	C	C5-C6-N1	-5.18	118.41	121.00
1	A	187	G	N1-C6-O6	5.17	123.00	119.90
1	A	1637	A	C8-N9-C4	5.17	107.87	105.80
55	w	24	G	N3-C4-N9	-5.17	122.89	126.00
1	A	944	G	C4-N9-C1'	5.17	133.22	126.50
1	A	1666	G	O5'-P-OP2	5.17	116.91	110.70
1	A	1136	G	C5-C6-O6	-5.17	125.50	128.60
1	A	2765	A	C6-C5-N7	-5.17	128.68	132.30
34	a	406	G	N3-C4-C5	-5.17	126.01	128.60
34	a	1356	G	C4-C5-N7	-5.17	108.73	110.80
34	a	1513	A	N9-C4-C5	5.17	107.87	105.80
34	a	916	G	N3-C4-C5	-5.17	126.02	128.60
1	A	727	A	N1-C6-N6	5.17	121.70	118.60
1	A	949	C	C6-N1-C2	-5.17	118.23	120.30
1	A	1339	G	C8-N9-C4	-5.17	104.33	106.40
34	a	1416	G	C2-N3-C4	-5.17	109.32	111.90
34	a	1486	G	N3-C4-N9	5.17	129.10	126.00
47	n	18	VAL	CB-CA-C	-5.17	101.58	111.40
1	A	572	A	C6-C5-N7	-5.17	128.68	132.30
1	A	2730	C	OP1-P-O3'	5.17	116.56	105.20
1	A	2574	G	N3-C4-N9	-5.16	122.90	126.00
1	A	2791	C	N3-C4-C5	-5.16	119.83	121.90
34	a	1115	C	C6-N1-C2	5.16	122.37	120.30
1	A	577	G	OP1-P-O3'	5.16	116.56	105.20
57	y	528	ILE	C-N-CD	5.16	139.24	128.40
1	A	1021	A	N3-C4-C5	5.16	130.41	126.80
1	A	1424	G	C8-N9-C1'	-5.16	120.30	127.00
1	A	2605	U	N1-C2-O2	5.16	126.41	122.80
55	w	43	C	C5-C6-N1	-5.16	118.42	121.00
56	v	18	C	N3-C2-O2	-5.16	118.29	121.90
1	A	467	G	N1-C6-O6	5.16	122.99	119.90
1	A	729	G	C6-C5-N7	-5.16	127.31	130.40
1	A	2690	C	N1-C2-O2	5.16	121.99	118.90
34	a	378	G	N1-C6-O6	5.16	122.99	119.90
34	a	436	C	N3-C4-N4	5.16	121.61	118.00
34	a	1214	C	N3-C4-C5	-5.16	119.84	121.90
1	A	2525	G	N3-C2-N2	5.15	123.51	119.90
1	A	115	C	OP2-P-O3'	5.15	116.53	105.20
1	A	1667	G	N3-C4-N9	5.15	129.09	126.00
1	A	2608	G	C8-N9-C4	5.15	108.46	106.40
1	A	2617	C	C4-C5-C6	5.15	119.98	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	A	C5-C6-N6	-5.15	119.58	123.70
1	A	857	C	C5-C6-N1	-5.15	118.42	121.00
1	A	1645	G	C5-C6-O6	-5.15	125.51	128.60
1	A	1751	C	N3-C4-N4	-5.15	114.39	118.00
1	A	1698	A	C8-N9-C4	-5.15	103.74	105.80
1	A	946	G	C5-C6-O6	-5.15	125.51	128.60
1	A	2634	G	OP2-P-O3'	5.15	116.53	105.20
1	A	265	A	C5-N7-C8	-5.15	101.33	103.90
34	a	800	G	N3-C4-C5	-5.15	126.03	128.60
1	A	586	A	OP2-P-O3'	5.14	116.52	105.20
1	A	2481	G	C5-C6-O6	-5.14	125.51	128.60
1	A	249	C	C2-N1-C1'	5.14	124.46	118.80
1	A	1665	A	N9-C4-C5	-5.14	103.74	105.80
1	A	1989	G	N1-C6-O6	5.14	122.98	119.90
34	a	297	G	N3-C4-N9	-5.14	122.92	126.00
34	a	720	C	N3-C4-C5	5.14	123.96	121.90
1	A	30	G	N9-C4-C5	-5.14	103.34	105.40
1	A	577	G	N7-C8-N9	5.14	115.67	113.10
1	A	977	G	C4-C5-N7	-5.14	108.75	110.80
1	A	1209	G	O5'-P-OP1	-5.14	101.08	105.70
1	A	1338	G	N3-C4-C5	-5.14	126.03	128.60
1	A	1813	G	C5-N7-C8	5.14	106.87	104.30
56	v	13	A	N9-C4-C5	5.14	107.86	105.80
5	F	169	ASN	N-CA-C	5.14	124.87	111.00
34	a	379	C	C2-N1-C1'	-5.14	113.15	118.80
34	a	1126	U	P-O3'-C3'	5.14	125.86	119.70
34	a	115	G	N1-C6-O6	5.14	122.98	119.90
34	a	317	G	N9-C4-C5	-5.14	103.34	105.40
34	a	820	U	N1-C2-O2	5.14	126.40	122.80
34	a	1227	A	C6-C5-N7	-5.14	128.70	132.30
1	A	207	A	C8-N9-C4	5.13	107.85	105.80
55	w	12	U	O5'-P-OP2	-5.13	101.08	105.70
1	A	1653	G	N3-C4-N9	5.13	129.08	126.00
34	a	691	G	C6-C5-N7	-5.13	127.32	130.40
34	a	1366	C	N3-C4-C5	-5.13	119.85	121.90
1	A	210	C	C2-N3-C4	-5.13	117.33	119.90
1	A	491	G	C4-N9-C1'	-5.13	119.83	126.50
1	A	499	U	N1-C2-N3	5.13	117.98	114.90
1	A	2018	G	N3-C4-N9	5.13	129.08	126.00
1	A	2073	C	N3-C4-N4	-5.13	114.41	118.00
34	a	1056	U	C2-N3-C4	5.13	130.08	127.00
1	A	581	C	OP1-P-OP2	-5.13	111.91	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2542	A	O5'-P-OP1	-5.13	101.09	105.70
1	A	2609	U	C6-N1-C2	5.13	124.08	121.00
1	A	2611	U	C2-N1-C1'	5.13	123.85	117.70
1	A	1700	A	C5-C6-N6	-5.12	119.60	123.70
1	A	1973	G	C4-C5-N7	-5.12	108.75	110.80
1	A	2059	A	C8-N9-C4	5.12	107.85	105.80
1	A	203	C	N3-C2-O2	5.12	125.48	121.90
34	a	1123	A	N3-C4-C5	5.12	130.38	126.80
1	A	1501	C	N3-C4-N4	5.12	121.58	118.00
1	A	18	C	C6-N1-C2	-5.12	118.25	120.30
1	A	857	C	C2-N1-C1'	-5.12	113.17	118.80
1	A	1128	A	N3-C4-C5	5.12	130.38	126.80
1	A	2025	C	C2-N1-C1'	5.12	124.43	118.80
34	a	225	C	C6-N1-C2	5.12	122.35	120.30
1	A	1499	C	C2-N1-C1'	-5.12	113.17	118.80
1	A	2048	G	C5-C6-O6	-5.12	125.53	128.60
1	A	2519	U	N1-C2-O2	-5.12	119.22	122.80
1	A	16	G	O5'-P-OP1	-5.11	101.10	105.70
1	A	2587	A	C2-N3-C4	5.11	113.16	110.60
34	a	613	C	C6-N1-C2	-5.11	118.25	120.30
1	A	143(A)	C	C6-N1-C2	-5.11	118.26	120.30
1	A	1142(A)	A	C5-C6-N1	-5.11	115.14	117.70
34	a	966	G	C5-C6-N1	5.11	114.06	111.50
1	A	918	A	O5'-P-OP1	-5.11	101.10	105.70
1	A	2597	G	N3-C4-C5	-5.11	126.05	128.60
1	A	328	U	C5-C6-N1	5.11	125.25	122.70
1	A	1796	U	C6-N1-C1'	5.11	128.35	121.20
1	A	2494	G	N1-C6-O6	5.11	122.96	119.90
34	a	12	U	C6-N1-C2	-5.11	117.94	121.00
34	a	354	G	N3-C4-C5	-5.11	126.05	128.60
1	A	1781	C	C2-N1-C1'	5.10	124.42	118.80
1	A	1051	G	N1-C6-O6	5.10	122.96	119.90
1	A	1204	A	C5-N7-C8	-5.10	101.35	103.90
1	A	1979	C	C5-C6-N1	-5.10	118.45	121.00
34	a	424	G	N1-C6-O6	-5.10	116.84	119.90
34	a	306	G	N1-C6-O6	-5.10	116.84	119.90
1	A	391	G	C5-C6-O6	-5.09	125.54	128.60
1	A	981	A	C2-N3-C4	-5.09	108.05	110.60
1	A	1006	C	O5'-P-OP1	-5.09	101.11	105.70
1	A	1776	G	O5'-P-OP1	5.09	116.81	110.70
1	A	2766	G	N7-C8-N9	5.09	115.65	113.10
34	a	1025	U	N1-C2-O2	5.09	126.37	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1254	C	C5-C6-N1	-5.09	118.45	121.00
1	A	1362	C	C6-N1-C2	-5.09	118.26	120.30
34	a	372	C	C5-C6-N1	5.09	123.55	121.00
34	a	1524	C	N3-C4-N4	-5.09	114.44	118.00
4	E	78	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	239	U	N1-C2-O2	5.09	126.36	122.80
1	A	491	G	C8-N9-C1'	5.09	133.62	127.00
1	A	805	G	N3-C4-N9	5.09	129.05	126.00
2	B	99	G	C4-N9-C1'	5.09	133.12	126.50
1	A	1924	C	C4-C5-C6	5.09	119.94	117.40
34	a	952	U	N3-C2-O2	5.09	125.76	122.20
1	A	688	U	N3-C4-C5	5.08	117.65	114.60
1	A	1142(A)	A	N3-C4-N9	-5.08	123.33	127.40
1	A	2249	U	N3-C4-O4	5.08	122.96	119.40
1	A	2790	A	N3-C4-N9	5.08	131.47	127.40
1	A	2185	C	C2-N3-C4	5.08	122.44	119.90
1	A	2556	C	C2-N1-C1'	5.08	124.39	118.80
34	a	60	A	OP1-P-O3'	5.08	116.38	105.20
34	a	576	G	C4-C5-C6	5.08	121.85	118.80
1	A	2188	C	N1-C2-O2	5.08	121.95	118.90
1	A	2376	A	N1-C6-N6	-5.08	115.55	118.60
1	A	2522	U	OP2-P-O3'	5.08	116.38	105.20
2	B	75	G	C4-N9-C1'	5.08	133.10	126.50
1	A	455	C	C5-C4-N4	-5.08	116.65	120.20
1	A	479	A	O4'-C1'-N9	5.08	112.26	108.20
1	A	645	C	N3-C2-O2	-5.08	118.35	121.90
1	A	745	G	C6-N1-C2	-5.08	122.06	125.10
1	A	1665	A	N7-C8-N9	-5.08	111.26	113.80
34	a	661	G	C8-N9-C4	-5.08	104.37	106.40
1	A	2096	U	C6-N1-C1'	-5.07	114.10	121.20
34	a	750	G	C4-N9-C1'	5.07	133.10	126.50
1	A	1780	A	O5'-P-OP2	-5.07	101.14	105.70
1	A	1996	C	C6-N1-C2	5.07	122.33	120.30
1	A	2597	G	C4-C5-N7	-5.07	108.77	110.80
1	A	526	A	C4-C5-N7	-5.07	108.17	110.70
1	A	1289	C	C6-N1-C2	5.07	122.33	120.30
33	x	9	A	N1-C6-N6	5.07	121.64	118.60
34	a	21	G	OP2-P-O3'	5.07	116.36	105.20
34	a	812	C	N3-C2-O2	-5.07	118.35	121.90
1	A	1257	C	C2-N1-C1'	5.07	124.38	118.80
1	A	991	C	C5-C6-N1	5.07	123.53	121.00
1	A	1673	U	C5-C4-O4	5.07	128.94	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2028	U	N3-C4-C5	-5.07	111.56	114.60
2	B	99	G	C8-N9-C1'	-5.07	120.41	127.00
34	a	283	C	O5'-P-OP1	-5.07	101.14	105.70
34	a	1374	A	C5-C6-N6	5.07	127.75	123.70
34	a	189(A)	C	O5'-P-OP2	-5.07	101.14	105.70
34	a	986	A	C6-N1-C2	-5.06	115.56	118.60
1	A	214	G	O4'-C1'-N9	5.06	112.25	108.20
1	A	1982	C	C5-C4-N4	-5.06	116.66	120.20
34	a	376	G	N1-C6-O6	5.06	122.94	119.90
55	w	27	G	C8-N9-C4	5.06	108.42	106.40
1	A	738	G	C8-N9-C4	-5.06	104.38	106.40
34	a	609	A	O5'-P-OP1	-5.06	101.15	105.70
34	a	1125	U	C5-C6-N1	-5.06	120.17	122.70
1	A	615	G	N1-C6-O6	5.06	122.93	119.90
34	a	18	C	N3-C2-O2	-5.06	118.36	121.90
34	a	1484	C	C6-N1-C2	-5.06	118.28	120.30
34	a	1494	G	C4-N9-C1'	5.06	133.07	126.50
1	A	2593	U	C5-C4-O4	-5.06	122.87	125.90
1	A	2000	G	OP1-P-OP2	5.05	127.18	119.60
34	a	1486	G	C6-C5-N7	-5.05	127.37	130.40
1	A	1774	C	C6-N1-C2	-5.05	118.28	120.30
34	a	858	G	C6-C5-N7	-5.05	127.37	130.40
1	A	594	U	C5-C6-N1	-5.05	120.17	122.70
1	A	950	G	O5'-P-OP2	-5.05	101.15	105.70
1	A	1790	C	C5-C4-N4	-5.05	116.66	120.20
34	a	1127	G	C5-C6-O6	5.05	131.63	128.60
1	A	1272	A	O5'-P-OP2	-5.05	101.16	105.70
34	a	1404	C	N3-C4-C5	5.05	123.92	121.90
1	A	263	C	N3-C2-O2	-5.05	118.37	121.90
1	A	2242	G	C2-N3-C4	-5.05	109.38	111.90
34	a	1027	C	C5-C4-N4	5.05	123.73	120.20
1	A	450	G	C4-C5-C6	5.04	121.83	118.80
1	A	824	A	O5'-P-OP1	-5.04	101.16	105.70
1	A	2088	G	N3-C2-N2	-5.04	116.37	119.90
1	A	2124	G	C5-C6-O6	5.04	131.63	128.60
1	A	19	C	C5-C6-N1	-5.04	118.48	121.00
1	A	445	C	O5'-P-OP2	-5.04	101.16	105.70
1	A	1745	C	C6-N1-C2	-5.04	118.28	120.30
1	A	1756	G	C8-N9-C4	-5.04	104.38	106.40
55	w	35	A	C2-N3-C4	-5.04	108.08	110.60
1	A	778	G	N3-C4-N9	5.04	129.02	126.00
1	A	2580	U	N3-C2-O2	-5.04	118.67	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	990	A	N7-C8-N9	5.04	116.32	113.80
1	A	2253	G	OP1-P-OP2	-5.04	112.04	119.60
1	A	2504	U	C5-C6-N1	-5.04	120.18	122.70
1	A	1372	U	C2-N1-C1'	5.04	123.74	117.70
1	A	2864	G	N1-C2-N2	-5.04	111.67	116.20
34	a	189(A)	C	N3-C4-C5	5.04	123.92	121.90
1	A	1996	C	N1-C2-O2	-5.03	115.88	118.90
34	a	585	G	N9-C4-C5	-5.03	103.39	105.40
1	A	1210	A	P-O3'-C3'	5.03	125.74	119.70
34	a	424	G	N9-C4-C5	5.03	107.41	105.40
1	A	2233	U	C5-C6-N1	-5.03	120.18	122.70
34	a	200	G	C5-C6-O6	5.03	131.62	128.60
34	a	805	C	C4-C5-C6	-5.03	114.89	117.40
57	y	230	ILE	CB-CA-C	-5.03	101.54	111.60
1	A	2645	G	O5'-P-OP2	-5.03	101.17	105.70
1	A	593	G	N1-C6-O6	5.03	122.92	119.90
1	A	1829	A	OP2-P-O3'	5.03	116.26	105.20
1	A	1934	C	C6-N1-C2	5.03	122.31	120.30
1	A	2502	G	N1-C6-O6	5.03	122.92	119.90
1	A	2609	U	N1-C2-O2	-5.03	119.28	122.80
34	a	603	U	N1-C2-O2	-5.03	119.28	122.80
34	a	863	U	O4'-C1'-N1	5.03	112.22	108.20
1	A	467	G	C6-C5-N7	-5.03	127.38	130.40
1	A	1353	A	N1-C6-N6	-5.03	115.58	118.60
34	a	1190	G	C5-C6-O6	-5.03	125.58	128.60
1	A	576	U	C5-C4-O4	-5.02	122.89	125.90
1	A	782	A	C5-C6-N6	-5.02	119.68	123.70
55	w	41	C	C2-N3-C4	-5.02	117.39	119.90
1	A	2271	G	C8-N9-C4	5.02	108.41	106.40
1	A	2285	C	C6-N1-C2	5.02	122.31	120.30
1	A	2773	C	N1-C2-O2	-5.02	115.89	118.90
34	a	570	G	OP2-P-O3'	5.02	116.25	105.20
55	w	42	C	C6-N1-C2	5.02	122.31	120.30
1	A	1368	G	C5-C6-N1	5.02	114.01	111.50
1	A	574	C	N1-C2-N3	-5.02	115.69	119.20
1	A	2864	G	C6-C5-N7	-5.02	127.39	130.40
1	A	2874	C	C6-N1-C2	5.02	122.31	120.30
1	A	1972	A	N1-C6-N6	-5.02	115.59	118.60
34	a	62	U	N1-C2-N3	5.02	117.91	114.90
34	a	279	A	N1-C6-N6	5.02	121.61	118.60
34	a	779	C	C5-C4-N4	5.02	123.71	120.20
34	a	1250	A	C8-N9-C4	-5.02	103.79	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1680	U	N1-C2-N3	5.02	117.91	114.90
34	a	791	G	O5'-P-OP2	5.02	116.72	110.70
34	a	1507	A	N3-C4-C5	-5.02	123.29	126.80
1	A	981	A	N1-C6-N6	5.01	121.61	118.60
1	A	2726	U	O5'-P-OP1	-5.01	101.19	105.70
21	Y	9	LYS	N-CA-C	-5.01	97.46	111.00
34	a	797	C	N3-C2-O2	5.01	125.41	121.90
34	a	919	A	C8-N9-C4	-5.01	103.79	105.80
34	a	1074	G	N9-C4-C5	-5.01	103.39	105.40
34	a	869	G	N3-C4-C5	5.01	131.11	128.60
1	A	441	U	C5-C6-N1	5.01	125.21	122.70
1	A	1310	G	N1-C2-N2	-5.01	111.69	116.20
1	A	2201	C	C6-N1-C2	-5.01	118.30	120.30
34	a	635	G	C6-C5-N7	-5.01	127.39	130.40
34	a	834	C	C5-C6-N1	-5.01	118.50	121.00
34	a	898	G	C5-C6-O6	-5.01	125.59	128.60
1	A	86	C	OP2-P-O3'	5.01	116.22	105.20
1	A	139(A)	G	N7-C8-N9	5.01	115.61	113.10
1	A	665	C	O5'-P-OP2	5.01	116.71	110.70
1	A	1137	G	N1-C6-O6	-5.01	116.89	119.90
1	A	1305	C	N3-C4-C5	5.01	123.90	121.90
34	a	724	G	C5-C6-O6	-5.01	125.59	128.60
1	A	1821	A	C8-N9-C4	5.01	107.80	105.80
1	A	1246	A	C8-N9-C4	5.01	107.80	105.80
1	A	1310	G	N3-C2-N2	5.01	123.40	119.90
1	A	2050	C	C5-C6-N1	-5.01	118.50	121.00
1	A	2040	C	C2-N1-C1'	5.00	124.31	118.80
1	A	918	A	N1-C6-N6	5.00	121.60	118.60
1	A	1653	G	N7-C8-N9	5.00	115.60	113.10
1	A	2606	C	C2-N3-C4	-5.00	117.40	119.90
34	a	111	G	N1-C2-N2	5.00	120.70	116.20
34	a	853	G	N3-C4-N9	5.00	129.00	126.00
34	a	924	C	C5-C4-N4	5.00	123.70	120.20
34	a	1320	C	C5-C6-N1	-5.00	118.50	121.00
1	A	330	A	N1-C6-N6	5.00	121.60	118.60
1	A	1052	C	N1-C2-O2	5.00	121.90	118.90
34	a	767	A	C4-C5-C6	5.00	119.50	117.00
34	a	1320	C	C6-N1-C2	5.00	122.30	120.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	223	GLY	Peptide
8	J	6	ASN	Peptide
42	i	45	ALA	Peptide
46	m	7	VAL	Peptide
46	m	8	GLU	Peptide
52	s	28	LYS	Peptide
53	t	10	LEU	Peptide
57	y	127	HIS	Peptide
57	y	137	LYS	Peptide
57	y	152	VAL	Peptide
57	y	171	GLY	Peptide
57	y	174	VAL	Peptide
57	y	226	ASP	Peptide
57	y	230	ILE	Peptide
57	y	235	LYS	Peptide
57	y	250	LEU	Peptide
57	y	268	ILE	Peptide
57	y	292	PRO	Peptide
57	y	294	PHE	Mainchain
57	y	301	VAL	Peptide
57	y	331	THR	Peptide
57	y	389	GLU	Peptide
57	y	395	ASP	Peptide
57	y	419	GLU	Peptide
57	y	480	GLU	Peptide
57	y	553	ALA	Peptide
57	y	554	LEU	Peptide
57	y	557	ASP	Peptide
57	y	6	LEU	Peptide
57	y	86	HIS	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	273/276 (99%)	233 (85%)	26 (10%)	14 (5%)	2	7
4	E	202/206 (98%)	165 (82%)	27 (13%)	10 (5%)	2	7
5	F	201/205 (98%)	152 (76%)	37 (18%)	12 (6%)	1	4
6	G	179/182 (98%)	143 (80%)	25 (14%)	11 (6%)	1	4
7	H	172/180 (96%)	128 (74%)	34 (20%)	10 (6%)	1	5
8	J	128/173 (74%)	69 (54%)	31 (24%)	28 (22%)	0	0
9	K	137/147 (93%)	94 (69%)	33 (24%)	10 (7%)	1	3
10	N	138/140 (99%)	106 (77%)	24 (17%)	8 (6%)	1	5
11	O	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	4	15
12	P	147/150 (98%)	108 (74%)	29 (20%)	10 (7%)	1	3
13	Q	139/141 (99%)	122 (88%)	12 (9%)	5 (4%)	3	14
14	R	116/118 (98%)	92 (79%)	21 (18%)	3 (3%)	5	20
15	S	108/112 (96%)	77 (71%)	20 (18%)	11 (10%)	0	1
16	T	129/146 (88%)	113 (88%)	15 (12%)	1 (1%)	19	51
17	U	114/118 (97%)	92 (81%)	16 (14%)	6 (5%)	2	6
18	V	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	1	1
19	W	110/113 (97%)	86 (78%)	14 (13%)	10 (9%)	1	1
20	X	93/96 (97%)	73 (78%)	12 (13%)	8 (9%)	1	2
21	Y	105/110 (96%)	82 (78%)	12 (11%)	11 (10%)	0	1
22	Z	183/206 (89%)	145 (79%)	24 (13%)	14 (8%)	1	2
23	0	72/85 (85%)	65 (90%)	6 (8%)	1 (1%)	11	36
24	1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	4
25	2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	10	34
26	3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	14
27	4	67/71 (94%)	42 (63%)	14 (21%)	11 (16%)	0	0
28	5	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	1	2
29	6	51/54 (94%)	43 (84%)	6 (12%)	2 (4%)	3	12
30	7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	7	26
31	8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
32	9	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	4	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	b	229/256 (90%)	167 (73%)	41 (18%)	21 (9%)	1	1
36	c	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	3	12
37	d	206/209 (99%)	163 (79%)	33 (16%)	10 (5%)	2	8
38	e	146/162 (90%)	108 (74%)	30 (20%)	8 (6%)	2	5
39	f	98/101 (97%)	70 (71%)	20 (20%)	8 (8%)	1	2
40	g	153/156 (98%)	123 (80%)	26 (17%)	4 (3%)	5	20
41	h	135/138 (98%)	115 (85%)	18 (13%)	2 (2%)	10	34
42	i	125/128 (98%)	98 (78%)	17 (14%)	10 (8%)	1	2
43	j	94/105 (90%)	73 (78%)	12 (13%)	9 (10%)	0	1
44	k	112/129 (87%)	88 (79%)	20 (18%)	4 (4%)	3	14
45	l	120/132 (91%)	106 (88%)	9 (8%)	5 (4%)	3	10
46	m	117/126 (93%)	91 (78%)	16 (14%)	10 (8%)	1	2
47	n	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	6
48	o	86/89 (97%)	69 (80%)	15 (17%)	2 (2%)	6	23
49	p	80/88 (91%)	61 (76%)	17 (21%)	2 (2%)	5	21
50	q	97/105 (92%)	78 (80%)	13 (13%)	6 (6%)	1	4
51	r	66/88 (75%)	57 (86%)	6 (9%)	3 (4%)	2	9
52	s	81/93 (87%)	64 (79%)	9 (11%)	8 (10%)	0	1
53	t	94/106 (89%)	74 (79%)	10 (11%)	10 (11%)	0	1
54	u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
57	y	640/679 (94%)	534 (83%)	67 (10%)	39 (6%)	1	4
All	All	6466/6910 (94%)	5145 (80%)	924 (14%)	397 (6%)	1	4

All (397) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	14	ARG
3	D	224	ALA
4	E	195	LEU
5	F	89	VAL
5	F	130	ALA
5	F	136	THR
5	F	168	ARG
5	F	169	ASN
6	G	28	VAL

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Mol	Chain	Res	Type
6	G	47	LYS
6	G	115	ARG
6	G	150	ASP
7	H	80	SER
8	J	7	VAL
8	J	53	VAL
8	J	56	ASN
8	J	74	LEU
8	J	77	PRO
8	J	80	VAL
8	J	93	LEU
8	J	99	SER
8	J	100	ASN
8	J	107	VAL
8	J	128	LEU
9	K	7	VAL
9	K	115	LEU
10	N	23	LEU
10	N	37	LYS
10	N	69	GLN
11	O	72	PRO
12	P	45	LEU
13	Q	59	ARG
13	Q	134	ARG
13	Q	135	ASP
16	T	55	ASN
17	U	86	ALA
19	W	25	ARG
19	W	36	LEU
19	W	57	ASN
20	X	18	TYR
20	X	19	ALA
20	X	77	LYS
21	Y	5	MET
21	Y	6	HIS
22	Z	161	VAL
22	Z	177	PRO
22	Z	179	ASP
22	Z	182	LYS
22	Z	184	ALA
24	1	76	ARG
24	1	77	ALA

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Mol	Chain	Res	Type
26	3	13	ILE
27	4	51	ASP
30	7	46	VAL
35	b	9	GLU
35	b	12	GLU
35	b	17	PHE
35	b	23	ARG
35	b	77	ALA
35	b	165	VAL
37	d	150	GLU
37	d	179	GLU
37	d	200	GLU
38	e	72	GLN
39	f	36	ARG
41	h	51	VAL
42	i	95	LYS
42	i	105	ASP
42	i	118	LYS
43	j	34	VAL
43	j	87	THR
44	k	122	LYS
46	m	7	VAL
46	m	8	GLU
47	n	3	ARG
47	n	41	ARG
48	o	19	PRO
49	p	67	THR
50	q	17	LYS
50	q	34	LYS
50	q	49	GLU
50	q	53	LEU
52	s	27	GLU
53	t	9	ASN
53	t	10	LEU
53	t	11	SER
53	t	46	GLU
53	t	47	GLY
53	t	100	ILE
57	y	-67	LYS
57	y	-59	GLU
57	y	9	ILE
57	y	63	ALA

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Mol	Chain	Res	Type
57	y	89	PHE
57	y	138	ILE
57	y	153	GLU
57	y	213	PRO
57	y	244	VAL
57	y	280	ILE
57	y	281	THR
57	y	373	ALA
57	y	402	ILE
57	y	437	ASN
57	y	438	MET
57	y	487	GLY
57	y	555	ARG
57	y	600	VAL
3	D	3	VAL
3	D	90	ALA
3	D	110	GLY
3	D	127	VAL
3	D	241	PRO
4	E	2	LYS
4	E	151	TYR
5	F	119	ARG
5	F	160	ASN
6	G	116	ASP
7	H	76	VAL
7	H	77	LYS
7	H	92	ILE
7	H	126	PRO
8	J	21	GLN
8	J	73	GLY
8	J	101	PRO
8	J	104	ILE
8	J	120	LYS
9	K	33	ASN
10	N	19	GLU
11	O	5	GLN
12	P	23	PRO
12	P	42	SER
12	P	132	LYS
13	Q	136	ALA
15	S	13	ARG
15	S	14	VAL

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Mol	Chain	Res	Type
15	S	57	LYS
15	S	88	ASP
15	S	102	ALA
15	S	103	GLU
17	U	79	PHE
18	V	24	LYS
18	V	54	GLY
18	V	55	ALA
19	W	67	ASP
20	X	66	LEU
20	X	68	ARG
20	X	93	GLU
21	Y	70	SER
21	Y	105	ALA
22	Z	154	ASP
22	Z	183	LEU
24	1	10	LYS
27	4	18	CYS
27	4	45	GLY
27	4	60	GLN
27	4	62	ARG
27	4	68	ARG
28	5	21	SER
28	5	35	GLU
29	6	33	LYS
35	b	8	LYS
35	b	24	TRP
35	b	131	PRO
35	b	204	ASN
35	b	227	GLY
35	b	232	PRO
36	c	22	TRP
36	c	130	VAL
37	d	5	ILE
37	d	10	ARG
37	d	151	LYS
38	e	68	GLU
38	e	85	GLY
38	e	148	VAL
38	e	149	GLU
39	f	70	ASP
40	g	7	ALA

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Mol	Chain	Res	Type
41	h	54	ASP
42	i	42	ARG
42	i	54	ASP
42	i	88	TYR
42	i	126	SER
42	i	127	LYS
43	j	27	ALA
43	j	36	GLY
43	j	77	PRO
43	j	82	ILE
44	k	103	LEU
45	l	14	GLY
46	m	68	GLY
46	m	85	GLY
49	p	46	PRO
50	q	3	LYS
50	q	54	GLY
51	r	36	ASN
52	s	14	HIS
52	s	30	LEU
52	s	71	LEU
53	t	65	LYS
53	t	99	LEU
57	y	13	SER
57	y	167	SER
57	y	215	LEU
57	y	286	PRO
57	y	301	VAL
57	y	446	LYS
57	y	486	PRO
3	D	219	PRO
4	E	52	LEU
4	E	162	ALA
5	F	165	ARG
5	F	206	ILE
6	G	43	LEU
6	G	46	ALA
6	G	55	LYS
7	H	34	GLU
7	H	65	HIS
7	H	174	GLY
8	J	23	SER

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Mol	Chain	Res	Type
8	J	30	GLN
8	J	61	LEU
8	J	69	PRO
8	J	91	LYS
9	K	11	GLN
9	K	73	PRO
9	K	87	GLY
10	N	22	THR
13	Q	60	ARG
14	R	45	ARG
14	R	93	GLY
15	S	59	LYS
15	S	79	ALA
17	U	54	LYS
17	U	98	LEU
18	V	45	THR
18	V	97	LYS
19	W	27	LYS
19	W	56	ALA
19	W	66	GLU
22	Z	93	ASP
22	Z	155	LEU
22	Z	158	PRO
27	4	55	ARG
29	6	34	LEU
35	b	20	GLU
35	b	36	ARG
35	b	76	GLN
36	c	79	ARG
37	d	26	CYS
37	d	172	PRO
37	d	191	ARG
39	f	5	GLU
39	f	62	TRP
39	f	64	GLN
39	f	71	ARG
42	i	70	LYS
42	i	99	LEU
45	l	121	GLY
45	l	125	PRO
46	m	3	ARG
46	m	49	THR

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Mol	Chain	Res	Type
47	n	32	SER
51	r	32	ARG
57	y	86	HIS
57	y	90	THR
57	y	267	ALA
4	E	72	VAL
5	F	67	GLN
5	F	194	MET
8	J	84	GLU
9	K	16	LYS
11	O	29	ASN
12	P	97	PRO
12	P	122	PRO
15	S	84	GLN
15	S	94	TYR
17	U	87	GLY
18	V	43	GLU
20	X	2	LYS
21	Y	2	ARG
21	Y	54	LYS
22	Z	160	GLY
26	3	22	ALA
27	4	43	TYR
27	4	46	GLN
28	5	24	ALA
28	5	37	LYS
35	b	30	ARG
35	b	35	GLU
35	b	122	PHE
35	b	153	ARG
36	c	99	VAL
36	c	100	ALA
38	e	9	LYS
38	e	73	ASN
39	f	51	PRO
40	g	80	VAL
43	j	78	ASN
45	l	19	ARG
46	m	40	ASN
52	s	29	ARG
53	t	66	ALA
57	y	-17	ARG

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Mol	Chain	Res	Type
57	y	417	PRO
57	y	560	ALA
3	D	223	GLY
4	E	57	LYS
4	E	73	GLU
4	E	128	SER
5	F	22	ALA
6	G	109	VAL
6	G	177	GLY
8	J	85	ASP
8	J	90	ALA
8	J	124	ALA
10	N	2	LYS
10	N	40	PRO
10	N	65	LYS
12	P	10	PRO
12	P	78	PRO
14	R	28	LEU
15	S	15	ARG
18	V	100	ARG
19	W	28	SER
19	W	51	LEU
19	W	59	VAL
21	Y	58	GLY
21	Y	69	ALA
22	Z	157	LEU
23	0	48	GLY
24	1	9	GLY
24	1	83	GLU
25	2	67	LYS
27	4	47	GLN
28	5	59	GLU
32	9	36	GLN
36	c	3	ASN
36	c	66	VAL
37	d	175	SER
39	f	96	PRO
40	g	50	ILE
43	j	83	GLU
44	k	100	ALA
46	m	67	GLU
46	m	101	GLN

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Mol	Chain	Res	Type
48	o	79	ARG
52	s	12	ASP
57	y	-36	ARG
57	y	137	LYS
57	y	303	ALA
57	y	500	VAL
57	y	594	GLN
3	D	144	ALA
4	E	178	GLU
8	J	86	PRO
9	K	24	GLY
11	O	35	VAL
24	l	51	VAL
27	4	41	PRO
38	e	39	GLY
43	j	37	PRO
51	r	60	ALA
52	s	76	PRO
57	y	448	VAL
6	G	149	VAL
9	K	23	VAL
12	P	47	ASP
21	Y	15	VAL
21	Y	27	VAL
36	c	108	ASN
57	y	-37	PRO
3	D	106	ILE
3	D	137	PRO
3	D	178	PRO
7	H	17	VAL
17	U	8	VAL
18	V	9	GLY
22	Z	27	VAL
44	k	105	VAL
46	m	38	GLY
20	X	94	GLY
21	Y	72	VAL
53	t	102	GLY
57	y	-48	VAL
7	H	4	ILE
8	J	68	LEU
8	J	129	PRO

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Mol	Chain	Res	Type
9	K	21	PRO
18	V	79	VAL
35	b	159	PRO
45	l	24	VAL
52	s	42	PRO
3	D	74	GLY
22	Z	68	PRO
40	g	130	GLY
12	P	72	PRO
35	b	125	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	215/218 (99%)	163 (76%)	52 (24%)	0	2
4	E	164/166 (99%)	134 (82%)	30 (18%)	1	5
5	F	160/162 (99%)	133 (83%)	27 (17%)	2	6
6	G	143/156 (92%)	103 (72%)	40 (28%)	0	1
7	H	144/148 (97%)	115 (80%)	29 (20%)	1	4
9	K	104/111 (94%)	84 (81%)	20 (19%)	1	4
10	N	118/119 (99%)	93 (79%)	25 (21%)	1	3
11	O	100/100 (100%)	89 (89%)	11 (11%)	6	19
12	P	115/116 (99%)	93 (81%)	22 (19%)	1	4
13	Q	111/111 (100%)	93 (84%)	18 (16%)	2	7
14	R	101/101 (100%)	83 (82%)	18 (18%)	2	5
15	S	87/88 (99%)	74 (85%)	13 (15%)	3	9
16	T	115/127 (91%)	95 (83%)	20 (17%)	2	6
17	U	93/94 (99%)	72 (77%)	21 (23%)	1	2
18	V	80/82 (98%)	63 (79%)	17 (21%)	1	3
19	W	90/92 (98%)	74 (82%)	16 (18%)	2	5

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	t	69/82 (84%)	58 (84%)	11 (16%)	2	7
54	u	18/22 (82%)	15 (83%)	3 (17%)	2	6
57	y	289/560 (52%)	193 (67%)	96 (33%)	0	0
All	All	4952/5576 (89%)	3927 (79%)	1025 (21%)	1	3

All (1025) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	3	VAL
3	D	5	LYS
3	D	13	ARG
3	D	20	ASP
3	D	22	SER
3	D	25	THR
3	D	27	THR
3	D	32	SER
3	D	34	VAL
3	D	37	LEU
3	D	38	LYS
3	D	39	LYS
3	D	50	THR
3	D	61	LEU
3	D	85	ASP
3	D	87	ASN
3	D	94	LEU
3	D	98	VAL
3	D	99	ASP
3	D	102	LYS
3	D	103	ARG
3	D	105	ILE
3	D	106	ILE
3	D	109	ASP
3	D	111	LEU
3	D	117	VAL
3	D	118	VAL
3	D	122	ASP
3	D	138	VAL
3	D	148	GLU
3	D	150	LYS
3	D	157	ARG
3	D	161	THR

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Mol	Chain	Res	Type
3	D	164	GLN
3	D	165	ILE
3	D	169	GLU
3	D	171	ASP
3	D	173	VAL
3	D	183	ARG
3	D	200	ASP
3	D	205	VAL
3	D	212	SER
3	D	215	LEU
3	D	217	ARG
3	D	221	VAL
3	D	222	ARG
3	D	229	VAL
3	D	239	ARG
3	D	257	LEU
3	D	260	ARG
3	D	267	SER
3	D	274	ARG
4	E	2	LYS
4	E	4	ILE
4	E	9	VAL
4	E	13	ARG
4	E	23	VAL
4	E	33	VAL
4	E	48	GLN
4	E	72	VAL
4	E	73	GLU
4	E	77	ILE
4	E	82	ARG
4	E	85	ASN
4	E	87	GLU
4	E	93	VAL
4	E	113	PHE
4	E	118	LYS
4	E	119	ARG
4	E	144	ARG
4	E	146	THR
4	E	149	ARG
4	E	152	LYS
4	E	165	VAL
4	E	173	VAL

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Mol	Chain	Res	Type
4	E	174	ASP
4	E	179	GLU
4	E	181	LEU
4	E	182	LEU
4	E	184	VAL
4	E	195	LEU
4	E	196	VAL
5	F	18	ARG
5	F	20	LEU
5	F	24	LEU
5	F	33	LEU
5	F	44	ARG
5	F	51	THR
5	F	53	THR
5	F	62	ARG
5	F	64	ILE
5	F	84	VAL
5	F	104	LYS
5	F	106	ARG
5	F	112	MET
5	F	148	LEU
5	F	152	GLU
5	F	162	LEU
5	F	164	ARG
5	F	169	ASN
5	F	170	LEU
5	F	175	THR
5	F	183	VAL
5	F	192	LEU
5	F	195	ASP
5	F	196	LEU
5	F	197	ASP
5	F	200	GLU
5	F	206	ILE
6	G	4	ASP
6	G	5	VAL
6	G	7	LEU
6	G	9	ARG
6	G	19	LEU
6	G	28	VAL
6	G	30	GLU
6	G	31	VAL

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Mol	Chain	Res	Type
6	G	33	ARG
6	G	34	LEU
6	G	43	LEU
6	G	51	ARG
6	G	58	GLN
6	G	62	LEU
6	G	80	PHE
6	G	81	LYS
6	G	82	LEU
6	G	90	LEU
6	G	91	ARG
6	G	99	MET
6	G	101	ILE
6	G	109	VAL
6	G	120	LEU
6	G	123	ASN
6	G	124	SER
6	G	135	LEU
6	G	136	ARG
6	G	138	GLN
6	G	139	LEU
6	G	143	GLU
6	G	146	TYR
6	G	148	MET
6	G	150	ASP
6	G	153	ARG
6	G	161	THR
6	G	164	GLU
6	G	165	THR
6	G	166	ASP
6	G	170	ARG
6	G	173	LEU
7	H	3	ARG
7	H	6	ARG
7	H	13	LYS
7	H	15	VAL
7	H	16	SER
7	H	17	VAL
7	H	23	ARG
7	H	27	LYS
7	H	32	GLU
7	H	40	GLU

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Mol	Chain	Res	Type
7	H	41	MET
7	H	43	VAL
7	H	45	VAL
7	H	47	GLU
7	H	54	ARG
7	H	57	ASP
7	H	62	LYS
7	H	69	ARG
7	H	79	VAL
7	H	88	LEU
7	H	95	ARG
7	H	98	LEU
7	H	106	THR
7	H	107	VAL
7	H	127	GLU
7	H	149	ARG
7	H	163	TYR
7	H	164	TYR
7	H	175	LYS
9	K	2	LYS
9	K	4	VAL
9	K	11	GLN
9	K	30	HIS
9	K	34	ILE
9	K	38	VAL
9	K	57	ILE
9	K	59	ILE
9	K	62	ASP
9	K	63	ARG
9	K	65	PHE
9	K	75	SER
9	K	86	LYS
9	K	95	LYS
9	K	115	LEU
9	K	116	ASN
9	K	117	THR
9	K	119	ASP
9	K	136	VAL
9	K	138	VAL
10	N	1	MET
10	N	2	LYS
10	N	17	ASP

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Mol	Chain	Res	Type
10	N	34	LEU
10	N	38	HIS
10	N	39	ARG
10	N	48	MET
10	N	51	PHE
10	N	68	GLU
10	N	70	LYS
10	N	74	ARG
10	N	87	LEU
10	N	90	MET
10	N	99	LEU
10	N	106	MET
10	N	109	LYS
10	N	115	ARG
10	N	120	LEU
10	N	122	VAL
10	N	127	ASP
10	N	131	GLN
10	N	133	GLN
10	N	137	LYS
10	N	138	LEU
10	N	140	VAL
11	O	3	GLN
11	O	8	LEU
11	O	10	VAL
11	O	14	THR
11	O	23	ARG
11	O	24	VAL
11	O	31	LYS
11	O	63	VAL
11	O	66	LYS
11	O	69	ILE
11	O	91	LEU
12	P	2	LYS
12	P	16	ARG
12	P	19	VAL
12	P	27	HIS
12	P	30	THR
12	P	40	SER
12	P	50	ARG
12	P	51	PHE
12	P	57	THR

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Mol	Chain	Res	Type
12	P	58	THR
12	P	59	LEU
12	P	65	ARG
12	P	70	GLN
12	P	71	VAL
12	P	74	GLU
12	P	96	THR
12	P	98	GLU
12	P	105	LEU
12	P	106	LEU
12	P	115	LEU
12	P	135	LEU
12	P	148	LEU
13	Q	7	MET
13	Q	21	THR
13	Q	31	ASP
13	Q	42	ILE
13	Q	45	GLN
13	Q	52	VAL
13	Q	56	ARG
13	Q	66	ILE
13	Q	72	LYS
13	Q	75	THR
13	Q	76	LYS
13	Q	82	ARG
13	Q	89	ASN
13	Q	112	GLU
13	Q	129	THR
13	Q	131	ILE
13	Q	135	ASP
13	Q	138	ASP
14	R	15	SER
14	R	18	LEU
14	R	28	LEU
14	R	30	THR
14	R	36	THR
14	R	38	VAL
14	R	44	LEU
14	R	60	LEU
14	R	65	LEU
14	R	67	LEU
14	R	71	GLN

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Mol	Chain	Res	Type
14	R	77	ARG
14	R	79	LEU
14	R	91	GLN
14	R	100	LEU
14	R	113	LEU
14	R	114	VAL
14	R	118	GLU
15	S	8	GLU
15	S	14	VAL
15	S	15	ARG
15	S	20	ARG
15	S	28	VAL
15	S	36	TYR
15	S	41	ASP
15	S	43	GLU
15	S	48	LEU
15	S	49	VAL
15	S	52	SER
15	S	53	SER
15	S	85	VAL
16	T	9	LEU
16	T	17	THR
16	T	18	ASP
16	T	23	ARG
16	T	31	SER
16	T	34	VAL
16	T	40	THR
16	T	44	ASP
16	T	49	VAL
16	T	53	ARG
16	T	54	ARG
16	T	57	PHE
16	T	59	THR
16	T	75	ILE
16	T	78	LEU
16	T	93	ARG
16	T	96	ARG
16	T	118	ARG
16	T	123	GLN
16	T	124	ASP
17	U	8	VAL
17	U	11	ARG

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Mol	Chain	Res	Type
17	U	18	LEU
17	U	19	LYS
17	U	20	LEU
17	U	33	ARG
17	U	34	LYS
17	U	36	ARG
17	U	55	ARG
17	U	56	ASP
17	U	63	VAL
17	U	64	ARG
17	U	71	GLN
17	U	74	LEU
17	U	78	THR
17	U	85	LYS
17	U	92	ARG
17	U	95	LEU
17	U	101	ARG
17	U	104	GLN
17	U	112	ARG
18	V	6	LYS
18	V	7	THR
18	V	13	ARG
18	V	14	VAL
18	V	18	LEU
18	V	25	LEU
18	V	33	VAL
18	V	38	LEU
18	V	46	VAL
18	V	51	VAL
18	V	53	GLU
18	V	70	ILE
18	V	71	LEU
18	V	72	VAL
18	V	73	SER
18	V	82	ARG
18	V	95	LEU
19	W	8	ARG
19	W	10	VAL
19	W	11	ARG
19	W	19	LEU
19	W	20	VAL
19	W	33	ARG

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Mol	Chain	Res	Type
19	W	39	THR
19	W	51	LEU
19	W	52	GLU
19	W	57	ASN
19	W	65	LEU
19	W	86	LEU
19	W	92	ARG
19	W	100	THR
19	W	107	LEU
19	W	111	HIS
20	X	2	LYS
20	X	9	LEU
20	X	23	GLU
20	X	27	THR
20	X	49	VAL
20	X	51	VAL
20	X	56	THR
20	X	57	LEU
20	X	68	ARG
20	X	75	ASP
20	X	80	ILE
20	X	92	LEU
21	Y	6	HIS
21	Y	9	LYS
21	Y	21	LYS
21	Y	23	ARG
21	Y	28	LYS
21	Y	30	VAL
21	Y	31	LEU
21	Y	38	ILE
21	Y	43	ASN
21	Y	55	TYR
21	Y	61	ILE
21	Y	62	GLU
21	Y	79	CYS
21	Y	84	ARG
21	Y	85	VAL
21	Y	90	LEU
21	Y	91	GLU
21	Y	98	VAL
21	Y	107	ASP
22	Z	24	LEU

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Mol	Chain	Res	Type
22	Z	27	VAL
22	Z	33	LEU
22	Z	41	LEU
22	Z	58	VAL
22	Z	61	LEU
22	Z	70	LEU
22	Z	72	ARG
22	Z	76	LEU
22	Z	80	ARG
22	Z	81	ARG
22	Z	85	HIS
22	Z	86	VAL
22	Z	96	VAL
22	Z	107	THR
22	Z	111	VAL
22	Z	119	GLU
22	Z	122	ARG
22	Z	132	ASN
22	Z	136	PHE
22	Z	139	VAL
22	Z	140	ASP
22	Z	141	VAL
22	Z	149	SER
22	Z	156	LYS
22	Z	161	VAL
22	Z	163	LEU
22	Z	170	THR
22	Z	179	ASP
23	0	11	ARG
23	0	19	LYS
23	0	20	ARG
23	0	25	ARG
23	0	32	ARG
23	0	41	ARG
23	0	44	ARG
23	0	46	LYS
23	0	66	VAL
24	1	2	SER
24	1	4	VAL
24	1	10	LYS
24	1	14	VAL
24	1	19	GLN

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Mol	Chain	Res	Type
24	1	20	ARG
24	1	21	ARG
24	1	40	ARG
24	1	57	GLU
24	1	59	THR
24	1	62	VAL
24	1	66	HIS
24	1	75	GLU
24	1	80	LEU
24	1	85	LEU
24	1	89	GLU
24	1	94	LEU
24	1	98	LEU
25	2	3	LEU
25	2	4	SER
25	2	16	LEU
25	2	25	VAL
25	2	30	ARG
25	2	32	LEU
25	2	34	GLU
25	2	45	SER
25	2	47	ASN
25	2	49	LYS
25	2	51	ARG
25	2	52	ASP
25	2	62	THR
25	2	65	ASN
25	2	70	GLN
26	3	4	LEU
26	3	9	VAL
26	3	32	GLN
26	3	33	GLN
26	3	37	LEU
26	3	40	THR
26	3	54	VAL
26	3	56	VAL
26	3	57	GLU
27	4	8	LYS
27	4	20	ASN
27	4	22	ILE
27	4	25	TYR
27	4	26	SER

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Mol	Chain	Res	Type
27	4	43	TYR
27	4	49	PHE
27	4	50	VAL
27	4	58	ARG
27	4	59	PHE
27	4	63	TYR
27	4	65	ASP
27	4	68	ARG
27	4	69	LYS
28	5	6	VAL
28	5	8	LYS
28	5	11	THR
28	5	25	LEU
28	5	26	THR
28	5	29	THR
28	5	35	GLU
28	5	37	LYS
28	5	40	LYS
28	5	48	GLU
28	5	49	CYS
28	5	57	VAL
29	6	3	SER
29	6	4	GLU
29	6	6	ARG
29	6	13	CYS
29	6	19	ARG
29	6	23	THR
29	6	27	LYS
29	6	28	ARG
29	6	34	LEU
29	6	36	LEU
29	6	38	LYS
29	6	46	HIS
29	6	52	VAL
30	7	1	MET
30	7	10	ARG
30	7	14	LYS
30	7	23	ARG
30	7	24	THR
30	7	41	ARG
30	7	42	LEU
30	7	46	VAL

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Mol	Chain	Res	Type
30	7	49	ARG
31	8	14	VAL
31	8	23	VAL
31	8	31	HIS
31	8	32	LEU
31	8	34	TRP
31	8	41	ILE
31	8	42	ARG
31	8	52	LYS
31	8	56	GLU
32	9	4	ARG
32	9	9	ARG
32	9	22	ARG
32	9	26	ILE
35	b	8	LYS
35	b	9	GLU
35	b	10	LEU
35	b	12	GLU
35	b	15	VAL
35	b	16	HIS
35	b	17	PHE
35	b	20	GLU
35	b	21	ARG
35	b	24	TRP
35	b	35	GLU
35	b	51	LEU
35	b	52	GLU
35	b	53	ARG
35	b	61	LEU
35	b	73	THR
35	b	79	ASP
35	b	80	ILE
35	b	87	ARG
35	b	94	ASN
35	b	96	ARG
35	b	97	TRP
35	b	107	THR
35	b	109	SER
35	b	119	GLU
35	b	122	PHE
35	b	135	GLN
35	b	136	VAL

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Mol	Chain	Res	Type
35	b	154	LEU
35	b	155	LEU
35	b	156	LYS
35	b	168	THR
35	b	169	LYS
35	b	172	ILE
35	b	175	ARG
35	b	185	ILE
35	b	187	LEU
35	b	189	ASP
35	b	190	THR
35	b	195	ASP
35	b	196	LEU
35	b	200	ILE
35	b	206	ASP
35	b	208	ILE
35	b	213	LEU
35	b	217	ARG
35	b	221	LEU
35	b	223	ILE
35	b	229	VAL
36	c	12	LEU
36	c	15	THR
36	c	37	GLN
36	c	45	LYS
36	c	49	SER
36	c	52	LEU
36	c	91	LEU
36	c	97	LYS
36	c	104	GLN
36	c	132	ARG
36	c	134	ILE
36	c	138	VAL
36	c	150	LYS
36	c	152	ILE
36	c	165	THR
36	c	179	ARG
36	c	188	LEU
36	c	190	ARG
36	c	191	THR
36	c	192	THR
36	c	195	VAL

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Mol	Chain	Res	Type
37	d	3	ARG
37	d	5	ILE
37	d	8	VAL
37	d	13	ARG
37	d	19	LEU
37	d	21	LEU
37	d	22	LYS
37	d	25	ARG
37	d	31	CYS
37	d	33	MET
37	d	52	SER
37	d	53	ASP
37	d	57	ARG
37	d	58	LEU
37	d	59	ARG
37	d	66	ARG
37	d	70	ILE
37	d	76	ARG
37	d	85	LYS
37	d	86	LYS
37	d	91	SER
37	d	97	LEU
37	d	107	ARG
37	d	108	LEU
37	d	113	SER
37	d	114	ARG
37	d	135	LEU
37	d	139	ARG
37	d	141	ARG
37	d	150	GLU
37	d	158	ILE
37	d	162	LEU
37	d	168	ARG
37	d	170	VAL
37	d	178	VAL
37	d	186	LEU
37	d	188	LEU
37	d	190	ASP
37	d	196	LEU
37	d	201	GLN
38	e	8	GLU
38	e	14	ARG

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Mol	Chain	Res	Type
38	e	19	MET
38	e	20	GLN
38	e	31	LEU
38	e	38	GLN
38	e	41	VAL
38	e	47	LYS
38	e	53	LEU
38	e	67	VAL
38	e	71	LEU
38	e	73	ASN
38	e	75	THR
38	e	79	GLU
38	e	80	ILE
38	e	81	GLU
38	e	82	VAL
38	e	87	SER
38	e	91	LEU
38	e	92	LYS
38	e	107	ARG
38	e	116	THR
38	e	123	LEU
38	e	126	ARG
38	e	135	THR
38	e	143	ARG
38	e	144	THR
38	e	147	ASP
38	e	151	LEU
38	e	152	ARG
39	f	9	VAL
39	f	10	LEU
39	f	15	ASP
39	f	16	GLN
39	f	25	ILE
39	f	31	GLU
39	f	36	ARG
39	f	43	LEU
39	f	54	LYS
39	f	64	GLN
39	f	65	VAL
39	f	69	GLU
39	f	72	VAL
39	f	73	ASN

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Mol	Chain	Res	Type
39	f	74	ASP
39	f	75	LEU
39	f	79	LEU
39	f	82	ARG
39	f	86	ARG
39	f	98	LEU
39	f	100	ASN
40	g	4	ARG
40	g	8	GLU
40	g	12	LEU
40	g	16	LEU
40	g	22	LEU
40	g	24	THR
40	g	41	ARG
40	g	42	ILE
40	g	45	ASP
40	g	56	GLN
40	g	57	GLU
40	g	75	VAL
40	g	90	GLU
40	g	92	SER
40	g	94	ARG
40	g	97	GLN
40	g	101	LEU
40	g	104	LEU
40	g	113	GLU
40	g	114	ARG
40	g	115	ARG
40	g	126	ASP
40	g	131	LYS
40	g	138	LYS
40	g	144	MET
41	h	2	LEU
41	h	3	THR
41	h	6	ILE
41	h	10	LEU
41	h	19	VAL
41	h	54	ASP
41	h	56	LYS
41	h	60	ARG
41	h	63	LEU
41	h	68	ARG

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Mol	Chain	Res	Type
41	h	75	ARG
41	h	78	GLN
41	h	84	ARG
41	h	87	SER
41	h	88	LYS
41	h	91	ARG
41	h	100	ILE
41	h	104	ARG
41	h	111	ILE
41	h	112	LEU
41	h	120	THR
41	h	122	ARG
41	h	137	VAL
42	i	23	ASN
42	i	25	LYS
42	i	27	THR
42	i	41	VAL
42	i	54	ASP
42	i	56	LEU
42	i	59	PHE
42	i	66	ARG
42	i	83	ARG
42	i	89	ASN
42	i	97	LYS
42	i	99	LEU
42	i	120	ARG
42	i	128	ARG
43	j	8	LEU
43	j	13	HIS
43	j	16	LEU
43	j	19	SER
43	j	21	GLN
43	j	35	SER
43	j	44	VAL
43	j	46	ARG
43	j	67	THR
43	j	70	ARG
43	j	71	LEU
43	j	89	ASP
43	j	92	THR
43	j	96	ILE
43	j	98	ILE

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Mol	Chain	Res	Type
43	j	100	THR
44	k	16	SER
44	k	51	LYS
44	k	62	GLN
44	k	82	VAL
44	k	109	VAL
44	k	110	ASP
44	k	114	VAL
44	k	116	HIS
44	k	119	CYS
44	k	125	PHE
44	k	126	ARG
45	l	27	LEU
45	l	33	ARG
45	l	41	ARG
45	l	44	THR
45	l	52	LEU
45	l	54	LYS
45	l	55	VAL
45	l	57	LYS
45	l	66	VAL
45	l	67	THR
45	l	84	LEU
45	l	86	ARG
45	l	89	ARG
45	l	97	ARG
45	l	100	ILE
46	m	3	ARG
46	m	11	ARG
46	m	15	VAL
46	m	19	LEU
46	m	48	LEU
46	m	49	THR
46	m	54	VAL
46	m	56	LEU
46	m	59	TYR
46	m	73	GLU
46	m	78	ILE
46	m	80	ARG
46	m	86	CYS
46	m	114	ARG
46	m	115	LYS

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Mol	Chain	Res	Type
46	m	120	LYS
47	n	3	ARG
47	n	6	LEU
47	n	7	ILE
47	n	9	LYS
47	n	13	THR
47	n	16	PHE
47	n	18	VAL
47	n	19	ARG
47	n	29	ARG
47	n	31	ARG
47	n	32	SER
47	n	41	ARG
47	n	44	LEU
48	o	17	ARG
48	o	26	GLU
48	o	38	ARG
48	o	39	LEU
48	o	66	LEU
48	o	71	GLN
48	o	77	ARG
48	o	82	ILE
48	o	83	GLU
48	o	87	ILE
49	p	2	VAL
49	p	8	ARG
49	p	19	ILE
49	p	20	VAL
49	p	27	LYS
49	p	28	ARG
49	p	31	LYS
49	p	40	ASP
49	p	45	THR
49	p	50	LYS
49	p	60	LEU
49	p	61	SER
49	p	67	THR
50	q	9	VAL
50	q	15	MET
50	q	16	GLN
50	q	25	ARG
50	q	35	VAL

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Mol	Chain	Res	Type
50	q	36	ILE
50	q	49	GLU
50	q	57	VAL
50	q	59	ILE
50	q	60	ILE
50	q	63	ARG
50	q	68	ARG
50	q	74	LEU
50	q	78	GLU
50	q	86	GLU
50	q	96	GLU
51	r	26	LEU
51	r	31	LEU
51	r	32	ARG
51	r	33	ASP
51	r	35	ARG
51	r	49	LYS
51	r	55	ARG
51	r	58	LEU
51	r	68	LYS
51	r	70	ILE
51	r	75	ILE
51	r	76	LEU
51	r	84	LYS
52	s	4	SER
52	s	6	LYS
52	s	12	ASP
52	s	14	HIS
52	s	22	LEU
52	s	27	GLU
52	s	28	LYS
52	s	31	ILE
52	s	32	LYS
52	s	37	ARG
52	s	38	SER
52	s	39	THR
52	s	41	VAL
52	s	48	THR
52	s	63	THR
52	s	65	ASN
52	s	76	PRO
52	s	78	ARG

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Mol	Chain	Res	Type
53	t	8	ARG
53	t	19	SER
53	t	22	ARG
53	t	50	GLU
53	t	56	MET
53	t	62	LEU
53	t	80	ARG
53	t	83	ARG
53	t	84	LEU
53	t	92	LEU
53	t	93	GLU
54	u	9	ARG
54	u	18	TYR
54	u	24	ARG
57	y	-68	MET
57	y	-67	LYS
57	y	-64	LEU
57	y	-62	GLU
57	y	-57	LEU
57	y	-54	VAL
57	y	-51	VAL
57	y	-50	VAL
57	y	-44	TYR
57	y	-36	ARG
57	y	-32	VAL
57	y	-29	THR
57	y	-28	GLU
57	y	-25	LEU
57	y	-18	ILE
57	y	-11	LEU
57	y	-8	ARG
57	y	0	LYS
57	y	4	GLU
57	y	7	SER
57	y	12	PHE
57	y	28	ARG
57	y	34	HIS
57	y	62	SER
57	y	68	TYR
57	y	75	GLU
57	y	83	THR
57	y	103	VAL

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Mol	Chain	Res	Type
57	y	105	LEU
57	y	108	ASP
57	y	114	GLU
57	y	117	THR
57	y	127	HIS
57	y	129	HIS
57	y	142	ASN
57	y	154	GLU
57	y	167	SER
57	y	170	THR
57	y	183	GLN
57	y	211	VAL
57	y	215	LEU
57	y	219	GLU
57	y	221	ARG
57	y	223	ARG
57	y	228	ILE
57	y	250	LEU
57	y	265	VAL
57	y	292	PRO
57	y	312	ASP
57	y	335	GLU
57	y	338	THR
57	y	340	LEU
57	y	351	LEU
57	y	358	GLN
57	y	359	GLU
57	y	360	ARG
57	y	361	LEU
57	y	363	ARG
57	y	369	LEU
57	y	375	SER
57	y	377	VAL
57	y	392	ASN
57	y	412	LEU
57	y	413	THR
57	y	423	SER
57	y	424	LEU
57	y	429	GLN
57	y	434	ARG
57	y	436	VAL
57	y	440	TYR

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Mol	Chain	Res	Type
57	y	461	TYR
57	y	462	ASP
57	y	469	SER
57	y	479	TYR
57	y	484	TYR
57	y	493	ASN
57	y	505	THR
57	y	506	PHE
57	y	507	ILE
57	y	509	HIS
57	y	512	LYS
57	y	531	GLN
57	y	532	LEU
57	y	533	PHE
57	y	534	GLU
57	y	544	LYS
57	y	548	ARG
57	y	551	VAL
57	y	554	LEU
57	y	556	LYS
57	y	557	ASP
57	y	568	THR
57	y	570	LYS
57	y	584	LEU
57	y	587	ILE
57	y	602	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	164	GLN
3	D	166	GLN
3	D	220	HIS
3	D	253	GLN
4	E	85	ASN
5	F	69	HIS
5	F	169	ASN
6	G	41	GLN
6	G	58	GLN
6	G	123	ASN
9	K	29	GLN
9	K	42	ASN

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Mol	Chain	Res	Type
9	K	89	HIS
10	N	8	GLN
11	O	29	ASN
12	P	128	HIS
13	Q	13	GLN
13	Q	57	HIS
14	R	50	HIS
14	R	91	GLN
15	S	34	HIS
16	T	58	ASN
17	U	72	HIS
18	V	80	GLN
20	X	31	HIS
20	X	82	GLN
21	Y	6	HIS
22	Z	34	ASN
22	Z	50	GLN
22	Z	65	GLN
22	Z	73	GLN
22	Z	132	ASN
23	0	17	GLN
24	1	56	GLN
25	2	9	GLN
25	2	46	GLN
25	2	47	ASN
25	2	65	ASN
26	3	32	GLN
27	4	20	ASN
29	6	29	ASN
31	8	35	GLN
32	9	36	GLN
35	b	19	HIS
35	b	45	GLN
35	b	94	ASN
36	c	37	GLN
36	c	102	ASN
36	c	104	GLN
36	c	136	GLN
36	c	162	GLN
36	c	176	HIS
36	c	181	ASN
37	d	42	GLN

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Mol	Chain	Res	Type
37	d	123	HIS
37	d	125	HIS
38	e	38	GLN
38	e	73	ASN
38	e	141	GLN
39	f	73	ASN
39	f	94	GLN
39	f	100	ASN
40	g	28	ASN
40	g	68	ASN
40	g	86	GLN
41	h	82	HIS
42	i	89	ASN
42	i	124	GLN
43	j	56	HIS
44	k	38	ASN
45	l	99	HIS
46	m	12	ASN
46	m	92	HIS
48	o	28	GLN
48	o	71	GLN
49	p	76	GLN
50	q	26	GLN
52	s	14	HIS
52	s	47	HIS
52	s	56	GLN
52	s	65	ASN
52	s	83	HIS
53	t	16	HIS
53	t	75	ASN
57	y	127	HIS
57	y	142	ASN
57	y	183	GLN
57	y	426	GLN
57	y	493	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2865/2915 (98%)	639 (22%)	38 (1%)
2	B	119/122 (97%)	18 (15%)	0

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

All (1027) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	15	G
1	A	22	C
1	A	23	G
1	A	28	A
1	A	35	G
1	A	41	C
1	A	45	C
1	A	49	A
1	A	51	G
1	A	54	G
1	A	55	G
1	A	61	G
1	A	64	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	81	G
1	A	84	A
1	A	90	U
1	A	92	A
1	A	95	G
1	A	102	G
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	123	G
1	A	125	G
1	A	131	G
1	A	135	G
1	A	141	A
1	A	148	C

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Mol	Chain	Res	Type
1	A	154(A)	C
1	A	181	A
1	A	182	A
1	A	196	A
1	A	197	A
1	A	200	U
1	A	205	G
1	A	206	U
1	A	212	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	227	A
1	A	228	A
1	A	229	A
1	A	230	U
1	A	233	A
1	A	248	G
1	A	250	G
1	A	252	G
1	A	264	C
1	A	265	A
1	A	266	G
1	A	267	C
1	A	271(F)	C
1	A	271(H)	G
1	A	271(I)	G
1	A	271(K)	U
1	A	271(L)	U
1	A	271(M)	G
1	A	271(N)	U
1	A	271(O)	C
1	A	271(R)	G
1	A	271(Y)	U
1	A	272(A)	U
1	A	272(B)	G
1	A	272(G)	C
1	A	272(H)	C
1	A	274	G
1	A	279	C
1	A	294	A

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Mol	Chain	Res	Type
1	A	296	C
1	A	299	A
1	A	310	A
1	A	311	A
1	A	324	A
1	A	329	G
1	A	330	A
1	A	345	A
1	A	352	G
1	A	353	G
1	A	362	U
1	A	363	G
1	A	363(E)	U
1	A	366	C
1	A	384	U
1	A	385	C
1	A	386	G
1	A	396	G
1	A	404	C
1	A	405	U
1	A	406	G
1	A	407	G
1	A	408	G
1	A	411	G
1	A	420	C
1	A	423	A
1	A	434	U
1	A	435	C
1	A	444	C
1	A	448	U
1	A	451	C
1	A	455	C
1	A	457	A
1	A	470	A
1	A	471	A
1	A	472	A
1	A	481	G
1	A	491	G
1	A	504	U
1	A	505	A
1	A	508	G
1	A	509	C

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Mol	Chain	Res	Type
1	A	530	G
1	A	531	C
1	A	532	A
1	A	536	A
1	A	545	G
1	A	549	G
1	A	556	G
1	A	563	G
1	A	572	A
1	A	573	G
1	A	575	A
1	A	584	C
1	A	594	U
1	A	603	A
1	A	604	G
1	A	607	U
1	A	614(A)	U
1	A	614(B)	G
1	A	615	G
1	A	627	A
1	A	628	G
1	A	631	A
1	A	637	A
1	A	645	C
1	A	646	A
1	A	652(B)	A
1	A	652(E)	G
1	A	652(T)	C
1	A	652(U)	G
1	A	652(V)	C
1	A	654	A
1	A	668	G
1	A	669	G
1	A	670	A
1	A	684	G
1	A	686	G
1	A	694	U
1	A	695	G
1	A	717	G
1	A	730	C
1	A	738	G
1	A	752	A

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Mol	Chain	Res	Type
1	A	753	C
1	A	764	A
1	A	775	G
1	A	776	G
1	A	782	A
1	A	783	A
1	A	784	A
1	A	785	G
1	A	792	G
1	A	794	G
1	A	800	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	829	A
1	A	830	G
1	A	832	G
1	A	842	G
1	A	859	G
1	A	860	U
1	A	866	A
1	A	870	A
1	A	875	G
1	A	881	G
1	A	886	C
1	A	887	A
1	A	888	C
1	A	889	C
1	A	890	A
1	A	895	U
1	A	896	A
1	A	897	C
1	A	906	G
1	A	907	U
1	A	910	A
1	A	911	A
1	A	917	A
1	A	931	G
1	A	932	G
1	A	936	C

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Mol	Chain	Res	Type
1	A	941	A
1	A	945	A
1	A	946	G
1	A	953	A
1	A	957	A
1	A	959	A
1	A	961	C
1	A	974	G
1	A	975	C
1	A	975(A)	G
1	A	976	C
1	A	982	C
1	A	983	A
1	A	996	A
1	A	1005	C
1	A	1008	C
1	A	1012	U
1	A	1013	C
1	A	1015	G
1	A	1017	G
1	A	1022	G
1	A	1025	G
1	A	1027	A
1	A	1033	U
1	A	1034	G
1	A	1036	G
1	A	1038	C
1	A	1041	C
1	A	1042	G
1	A	1045	A
1	A	1046	A
1	A	1047	G
1	A	1052	C
1	A	1053	C
1	A	1054	A
1	A	1055	G
1	A	1058	G
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1067	A

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Mol	Chain	Res	Type
1	A	1070	A
1	A	1073	A
1	A	1076	C
1	A	1079	C
1	A	1083	U
1	A	1084	A
1	A	1085	A
1	A	1088	A
1	A	1089	G
1	A	1095	A
1	A	1109	C
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1115	G
1	A	1119	C
1	A	1124	C
1	A	1127	A
1	A	1128	A
1	A	1129	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1137	G
1	A	1142(A)	A
1	A	1143	A
1	A	1149	G
1	A	1152	C
1	A	1155	A
1	A	1156	A
1	A	1157	G
1	A	1171	G
1	A	1173	G
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1177	A
1	A	1206	G
1	A	1210	A
1	A	1211	U
1	A	1219	G
1	A	1220	A

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Mol	Chain	Res	Type
1	A	1224	C
1	A	1230	C
1	A	1236	G
1	A	1244	G
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1275	A
1	A	1300	U
1	A	1301	A
1	A	1308	A
1	A	1313	U
1	A	1320	C
1	A	1321	A
1	A	1329	U
1	A	1332	G
1	A	1342	A
1	A	1347	G
1	A	1359	A
1	A	1360	A
1	A	1363	C
1	A	1365	A
1	A	1369	G
1	A	1373	A
1	A	1378	A
1	A	1380	G
1	A	1384	A
1	A	1385	G
1	A	1386	C
1	A	1398	C
1	A	1413	G
1	A	1416	G
1	A	1417	C
1	A	1420	U
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1436	G
1	A	1437	C

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Mol	Chain	Res	Type
1	A	1445	A
1	A	1450	G
1	A	1451	C
1	A	1455	G
1	A	1459	G
1	A	1460	A
1	A	1461	G
1	A	1467	C
1	A	1471	A
1	A	1481	U
1	A	1482	G
1	A	1490	A
1	A	1492	G
1	A	1493	C
1	A	1507	A
1	A	1508	A
1	A	1509	C
1	A	1509(A)	A
1	A	1511	C
1	A	1523	U
1	A	1526	G
1	A	1542	A
1	A	1543	C
1	A	1547	C
1	A	1553	A
1	A	1554	A
1	A	1558	A
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1581	G
1	A	1582	C
1	A	1584	C
1	A	1586	A
1	A	1588	C
1	A	1595	G
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1613	G
1	A	1617	C
1	A	1631(A)	A

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Mol	Chain	Res	Type
1	A	1644	C
1	A	1648	C
1	A	1649	G
1	A	1651	G
1	A	1654	A
1	A	1674	G
1	A	1695	G
1	A	1696	G
1	A	1700	A
1	A	1702	G
1	A	1705	G
1	A	1721	G
1	A	1722	A
1	A	1740	G
1	A	1745(A)	C
1	A	1746	G
1	A	1747	G
1	A	1756	G
1	A	1758	G
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1781	C
1	A	1791	A
1	A	1800	C
1	A	1802	A
1	A	1812	A
1	A	1816	G
1	A	1817	G
1	A	1820	U
1	A	1821	A
1	A	1828	G
1	A	1829	A
1	A	1838	C
1	A	1847	A
1	A	1877	A
1	A	1878	G
1	A	1889	A
1	A	1895	C
1	A	1900	A
1	A	1903	G

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Mol	Chain	Res	Type
1	A	1906	G
1	A	1913	A
1	A	1914	C
1	A	1920	C
1	A	1921	G
1	A	1929	G
1	A	1930	G
1	A	1934	C
1	A	1937	A
1	A	1938	A
1	A	1939	U
1	A	1941	C
1	A	1943	U
1	A	1955	U
1	A	1958	C
1	A	1960	A
1	A	1963	U
1	A	1964	G
1	A	1967	C
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1983	C
1	A	1992	G
1	A	1993	U
1	A	1996	C
1	A	1997	G
1	A	2020	A
1	A	2021	C
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2034	U
1	A	2035	G
1	A	2043	C
1	A	2049	G
1	A	2050	C
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G

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Mol	Chain	Res	Type
1	A	2062	A
1	A	2063	C
1	A	2069	G
1	A	2070	G
1	A	2077	A
1	A	2087	G
1	A	2091	U
1	A	2096	U
1	A	2098	U
1	A	2105	C
1	A	2110	G
1	A	2111	C
1	A	2113	U
1	A	2115	G
1	A	2116	G
1	A	2119	A
1	A	2127	G
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2135	A
1	A	2136	C
1	A	2137	C
1	A	2138	C
1	A	2141	G
1	A	2142	C
1	A	2146	C
1	A	2157	G
1	A	2158	A
1	A	2159	G
1	A	2161	C
1	A	2166	G
1	A	2167	U
1	A	2168	G
1	A	2169	A
1	A	2172	U
1	A	2178	C
1	A	2182	G
1	A	2184	G
1	A	2186	G
1	A	2187	G
1	A	2188	C

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Mol	Chain	Res	Type
1	A	2189	U
1	A	2198	A
1	A	2199	A
1	A	2200	C
1	A	2201	C
1	A	2203	U
1	A	2206	G
1	A	2207	G
1	A	2208	A
1	A	2223	G
1	A	2225	A
1	A	2226	C
1	A	2235	G
1	A	2238	G
1	A	2239	G
1	A	2243	U
1	A	2246	G
1	A	2251	G
1	A	2265	U
1	A	2268	A
1	A	2271	G
1	A	2273	A
1	A	2275	C
1	A	2279	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2305	A
1	A	2307	G
1	A	2308	G
1	A	2311	A
1	A	2319	G
1	A	2320	A
1	A	2321	G
1	A	2322	A
1	A	2325	G
1	A	2334	G
1	A	2336	A
1	A	2338	G
1	A	2343	C
1	A	2345	G
1	A	2347	C

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Mol	Chain	Res	Type
1	A	2350	C
1	A	2374	C
1	A	2383	G
1	A	2385	C
1	A	2406	U
1	A	2408	U
1	A	2410	G
1	A	2414	G
1	A	2422	A
1	A	2424	C
1	A	2425	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2434	A
1	A	2439	A
1	A	2441	C
1	A	2447	G
1	A	2448	A
1	A	2460	U
1	A	2469	A
1	A	2471	C
1	A	2474	C
1	A	2476	A
1	A	2478	A
1	A	2482	G
1	A	2491	U
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2505	G
1	A	2507	C
1	A	2511	U
1	A	2518	A
1	A	2519	U
1	A	2520	C
1	A	2528	U
1	A	2529	G
1	A	2535	G
1	A	2545	G
1	A	2554	U
1	A	2564	A

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Mol	Chain	Res	Type
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2574	G
1	A	2581	G
1	A	2582	G
1	A	2586	C
1	A	2602	A
1	A	2605	U
1	A	2609	U
1	A	2611	U
1	A	2612	C
1	A	2621	A
1	A	2629	A
1	A	2630	G
1	A	2639	A
1	A	2645	G
1	A	2654	A
1	A	2660	A
1	A	2663	G
1	A	2669	G
1	A	2679	A
1	A	2686	G
1	A	2689	U
1	A	2691	C
1	A	2702	U
1	A	2703	C
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U
1	A	2733	A
1	A	2744	G
1	A	2751	G
1	A	2755	C
1	A	2757	A
1	A	2758	A
1	A	2764	A
1	A	2765	A
1	A	2766	G
1	A	2778	A
1	A	2780	G

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Mol	Chain	Res	Type
1	A	2784	C
1	A	2790	A
1	A	2791	C
1	A	2792	G
1	A	2802	G
1	A	2811	G
1	A	2818	G
1	A	2820	A
1	A	2821	A
1	A	2831	G
1	A	2833	G
1	A	2835	A
1	A	2872	G
1	A	2880	C
1	A	2887	U
1	A	2889	C
1	A	2895	U
1	A	2897	U
2	B	7	G
2	B	9	G
2	B	10	C
2	B	13	A
2	B	24	G
2	B	25	A
2	B	35	U
2	B	40	U
2	B	42	C
2	B	44	G
2	B	45	A
2	B	56	G
2	B	73	A
2	B	77	U
2	B	78	A
2	B	110	G
2	B	119	G
2	B	120	A
33	x	2	C
33	x	4	C
33	x	5	G
33	x	7	A
33	x	9	A
33	x	10	G

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Mol	Chain	Res	Type
33	x	11	C
33	x	14	A
33	x	19	G
33	x	20	U
33	x	21	A
33	x	23	A
33	x	25	C
33	x	26	A
33	x	32	PSU
33	x	34	G
33	x	39	PSU
33	x	41	C
33	x	42	C
33	x	44	G
33	x	45	U
33	x	46	7MG
33	x	47	U
33	x	48	C
33	x	49	C
33	x	54	5MU
33	x	56	C
33	x	57	G
33	x	58	A
33	x	59	U
33	x	60	U
33	x	61	C
33	x	62	C
33	x	67	C
33	x	68	C
33	x	69	G
33	x	73	A
34	a	7	G
34	a	9	G
34	a	15	G
34	a	22	G
34	a	31	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	50	A
34	a	51	A

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Mol	Chain	Res	Type
34	a	61	G
34	a	73	G
34	a	77	G
34	a	78	G
34	a	79	G
34	a	92	C
34	a	96	U
34	a	97	G
34	a	101	A
34	a	110	C
34	a	116	A
34	a	120	A
34	a	121	C
34	a	131	C
34	a	133	U
34	a	144	G
34	a	151	A
34	a	159	G
34	a	163	C
34	a	167	G
34	a	171	A
34	a	182	U
34	a	189(G)	G
34	a	194	C
34	a	197	A
34	a	202	U
34	a	203	U
34	a	204	U
34	a	216	G
34	a	232	G
34	a	236	G
34	a	247	G
34	a	251	G
34	a	253	U
34	a	266	G
34	a	267	C
34	a	280	C
34	a	289	G
34	a	291	C
34	a	305	G
34	a	306	G
34	a	317	G

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Mol	Chain	Res	Type
34	a	321	A
34	a	325	A
34	a	328	C
34	a	331	G
34	a	332	G
34	a	346	G
34	a	347	G
34	a	348	G
34	a	351	G
34	a	352	C
34	a	353	A
34	a	354	G
34	a	355	C
34	a	366	C
34	a	367	U
34	a	369	C
34	a	372	C
34	a	374	A
34	a	378	G
34	a	382	A
34	a	384	G
34	a	398	C
34	a	406	G
34	a	412	A
34	a	413	G
34	a	422	C
34	a	423	G
34	a	429	U
34	a	430	A
34	a	437	U
34	a	439	A
34	a	441	A
34	a	444	C
34	a	452	A
34	a	453	A
34	a	461	A
34	a	470	C
34	a	472	A
34	a	485	G
34	a	496	A
34	a	498	U
34	a	505	G

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Mol	Chain	Res	Type
34	a	506	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	518	C
34	a	525	C
34	a	527	G
34	a	532	A
34	a	533	A
34	a	546	G
34	a	547	A
34	a	559	A
34	a	561	U
34	a	562	C
34	a	564	C
34	a	565	U
34	a	572	A
34	a	573	A
34	a	576	G
34	a	577	G
34	a	596	C
34	a	597	G
34	a	607	A
34	a	630	G
34	a	631	G
34	a	641	U
34	a	653	A
34	a	661	G
34	a	665	A
34	a	666	G
34	a	687	A
34	a	688	G
34	a	693	G
34	a	697	U
34	a	702	A
34	a	704	A
34	a	707	C
34	a	718	G
34	a	723	U
34	a	731	G
34	a	734	G
34	a	749	C

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Mol	Chain	Res	Type
34	a	750	G
34	a	752	G
34	a	753	A
34	a	755	G
34	a	760	G
34	a	764	C
34	a	777	A
34	a	786	G
34	a	790	A
34	a	792	A
34	a	793	U
34	a	794	A
34	a	802	A
34	a	816	A
34	a	817	C
34	a	821	G
34	a	828	A
34	a	836	G
34	a	839	U
34	a	840	C
34	a	841	U
34	a	848	C
34	a	853	G
34	a	859	A
34	a	860	A
34	a	863	U
34	a	870	U
34	a	873	A
34	a	874	G
34	a	896	C
34	a	902	G
34	a	914	A
34	a	916	G
34	a	919	A
34	a	922	G
34	a	926	G
34	a	927	G
34	a	928	G
34	a	934	C
34	a	935	A
34	a	936	C
34	a	938	A

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Mol	Chain	Res	Type
34	a	960	U
34	a	961	U
34	a	968	A
34	a	969	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	984	C
34	a	993	G
34	a	997	U
34	a	998	G
34	a	1006	C
34	a	1009	G
34	a	1016	A
34	a	1024	G
34	a	1026	G
34	a	1027	C
34	a	1028	C
34	a	1029	C
34	a	1030	C
34	a	1030(A)	G
34	a	1030(B)	C
34	a	1030(C)	G
34	a	1032	G
34	a	1033	G
34	a	1036	G
34	a	1044	A
34	a	1053	G
34	a	1054	C
34	a	1055	A
34	a	1062	U
34	a	1064	G
34	a	1070	U
34	a	1090	U
34	a	1094	G
34	a	1095	U
34	a	1101	A
34	a	1103	C
34	a	1121	U
34	a	1124	G
34	a	1125	U
34	a	1126	U

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Mol	Chain	Res	Type
34	a	1127	G
34	a	1129	C
34	a	1130	A
34	a	1131	G
34	a	1137	C
34	a	1139	G
34	a	1146	A
34	a	1151	A
34	a	1152	A
34	a	1157	A
34	a	1159	U
34	a	1170	A
34	a	1181	G
34	a	1182	G
34	a	1183	A
34	a	1184	G
34	a	1193	G
34	a	1196	U
34	a	1197	G
34	a	1212	U
34	a	1213	A
34	a	1227	A
34	a	1236	A
34	a	1238	A
34	a	1250	A
34	a	1251	A
34	a	1253	G
34	a	1256	A
34	a	1257	U
34	a	1258	G
34	a	1259	C
34	a	1260	C
34	a	1268	A
34	a	1270	C
34	a	1273	G
34	a	1278	U
34	a	1279	A
34	a	1280	A
34	a	1281	U
34	a	1282	C
34	a	1287	A
34	a	1299	A

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Mol	Chain	Res	Type
34	a	1300	G
34	a	1302	U
34	a	1304	G
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1322	C
34	a	1323	G
34	a	1338	G
34	a	1340	A
34	a	1346	A
34	a	1347	G
34	a	1364	U
34	a	1365	G
34	a	1370	G
34	a	1376	U
34	a	1379	G
34	a	1383	C
34	a	1392	G
34	a	1397	C
34	a	1398	A
34	a	1400	C
34	a	1411	C
34	a	1419	G
34	a	1442	G
34	a	1442(B)	A
34	a	1445	C
34	a	1446	U
34	a	1447	A
34	a	1452	C
34	a	1456	G
34	a	1457	G
34	a	1458	G
34	a	1486	G
34	a	1487	G
34	a	1497	G
34	a	1498	U
34	a	1502	A
34	a	1503	A
34	a	1504	G
34	a	1506	U
34	a	1507	A

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Mol	Chain	Res	Type
34	a	1517	G
34	a	1519	A
34	a	1520	G
34	a	1529	G
34	a	1530	G
34	a	1531	A
55	w	10	G
55	w	13	C
55	w	16	U
55	w	17	C
55	w	18	G
55	w	19	G
55	w	20	U
55	w	21	A
55	w	22	G
55	w	35	A
55	w	38	A
55	w	41	C
55	w	44	G
55	w	45	U
55	w	46	7MG
55	w	47	U
55	w	48	C
55	w	49	C
55	w	61	C
55	w	64	A
55	w	71	G
56	v	18	C

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	34	C
1	A	90	U
1	A	196	A
1	A	266	G
1	A	278	A
1	A	328	U
1	A	529	A
1	A	685	A
1	A	746	A
1	A	752	A

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Mol	Chain	Res	Type
1	A	774	A
1	A	895	U
1	A	1033	U
1	A	1052	C
1	A	1069	A
1	A	1078	U
1	A	1108	U
1	A	1145	C
1	A	1174	A
1	A	1176	G
1	A	1210	A
1	A	1300	U
1	A	1379	A
1	A	1529	G
1	A	1608	A
1	A	1617	C
1	A	1653	G
1	A	1992	G
1	A	2110	G
1	A	2132	U
1	A	2183	C
1	A	2187	G
1	A	2318	G
1	A	2428	G
1	A	2439	A
1	A	2611	U
1	A	2756	U
1	A	2873	A

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

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

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

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	4SU	w	8	55	-	0/5/25/26	0/2/2/2
33	MIA	x	37	33	-	3/3/25/34	0/3/3/3
33	PSU	x	55	33	-	0/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/5/25/26	0/2/2/2
33	5MU	x	54	33	-	3/5/25/26	0/2/2/2
33	PSU	x	32	33	-	2/7/25/26	0/2/2/2
55	PSU	w	32	55	-	0/7/25/26	0/2/2/2
55	PSU	w	39	55	-	0/7/25/26	0/2/2/2
55	MIA	w	37	55	-	4/11/33/34	0/3/3/3
55	PSU	w	55	55	-	0/7/25/26	0/2/2/2
55	F3O	w	76	55,58	-	6/15/37/38	0/4/4/4
33	4SU	x	8	33	-	0/5/25/26	0/2/2/2
33	PSU	x	39	33	-	2/7/25/26	0/2/2/2
33	7MG	x	46	33	-	4/7/37/38	0/3/3/3
55	7MG	w	46	55	-	1/7/37/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	37	MIA	C2-S10	-9.18	1.67	1.75
55	w	37	MIA	C13-C14	7.75	1.54	1.32
55	w	46	7MG	C6-C5	5.33	1.48	1.41
33	x	55	PSU	C5-C1'	-4.75	1.48	1.52
33	x	46	7MG	C5-C4	4.38	1.47	1.39
55	w	55	PSU	C5-C1'	-4.18	1.48	1.52
33	x	8	4SU	C4-S4	-4.09	1.60	1.67
33	x	46	7MG	C6-C5	4.07	1.47	1.41
55	w	39	PSU	C4-C5	4.01	1.50	1.41
33	x	39	PSU	C5-C1'	-3.96	1.48	1.52
55	w	32	PSU	C5-C1'	-3.89	1.48	1.52
33	x	32	PSU	C4-C5	3.85	1.49	1.41
55	w	46	7MG	C5-C4	3.80	1.46	1.39
55	w	8	4SU	C4-S4	-3.65	1.60	1.67
33	x	46	7MG	C5-N7	-3.55	1.33	1.39
33	x	54	5MU	C4-C5	3.48	1.48	1.41
33	x	39	PSU	C4-C5	3.43	1.48	1.41
55	w	76	F3O	O3'-C	3.41	1.42	1.34
33	x	55	PSU	C4-C5	3.36	1.48	1.41
55	w	32	PSU	C4-C5	3.35	1.48	1.41
55	w	55	PSU	C4-C5	3.20	1.48	1.41
33	x	32	PSU	C5-C1'	-3.20	1.49	1.52
55	w	39	PSU	C5-C1'	-3.13	1.49	1.52
55	w	54	5MU	C4-C5	3.10	1.48	1.41
33	x	37	MIA	C5-C4	2.82	1.48	1.40
33	x	37	MIA	C2-N3	2.81	1.36	1.32
55	w	46	7MG	C4-N9	-2.74	1.33	1.38
55	w	37	MIA	C5-C4	2.73	1.48	1.40
55	w	37	MIA	C2-N1	2.73	1.38	1.34
55	w	46	7MG	C5-N7	-2.72	1.35	1.39
55	w	37	MIA	C6-N1	2.58	1.36	1.32
55	w	55	PSU	C2-N3	-2.49	1.33	1.38
55	w	32	PSU	O4'-C1'	-2.12	1.41	1.44
33	x	46	7MG	C4-N3	2.10	1.36	1.34
33	x	55	PSU	O4'-C1'	-2.09	1.41	1.44
55	w	39	PSU	O4'-C1'	-2.03	1.41	1.44
55	w	54	5MU	C2-N3	-2.02	1.34	1.38

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	37	MIA	C11-S10-C2	-15.14	90.96	102.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	x	46	7MG	N3-C4-N9	11.28	141.39	126.91
55	w	32	PSU	N1-C2-N3	-9.58	120.81	128.43
33	x	39	PSU	N1-C2-N3	-8.88	121.37	128.43
33	x	32	PSU	N1-C2-N3	-8.75	121.47	128.43
55	w	46	7MG	N3-C4-N9	8.18	137.42	126.91
33	x	55	PSU	N1-C2-N3	-7.94	122.11	128.43
55	w	55	PSU	N1-C2-N3	-7.49	122.48	128.43
55	w	39	PSU	N1-C2-N3	-7.42	122.53	128.43
33	x	54	5MU	C4-N3-C2	7.11	121.15	115.14
33	x	39	PSU	C4-N3-C2	7.07	121.11	115.14
55	w	54	5MU	C4-N3-C2	7.05	121.09	115.14
33	x	55	PSU	C4-N3-C2	6.67	120.77	115.14
33	x	32	PSU	C4-N3-C2	6.67	120.77	115.14
55	w	46	7MG	N7-C8-N9	-6.63	93.90	103.38
55	w	32	PSU	C4-N3-C2	6.60	120.71	115.14
55	w	39	PSU	C4-N3-C2	6.30	120.46	115.14
33	x	46	7MG	C5-C4-N3	-6.29	116.21	126.49
33	x	55	PSU	C5-C4-N3	-5.95	117.69	125.36
55	w	55	PSU	C4-N3-C2	5.58	119.85	115.14
33	x	46	7MG	C6-C5-C4	5.17	120.75	115.20
55	w	39	PSU	C5-C4-N3	-5.07	118.83	125.36
33	x	39	PSU	C5-C4-N3	-5.03	118.88	125.36
33	x	32	PSU	C5-C4-N3	-5.01	118.90	125.36
33	x	46	7MG	N7-C8-N9	-4.96	96.29	103.38
55	w	37	MIA	C5-C6-N1	-4.84	116.79	120.81
55	w	37	MIA	C16-C14-C13	-4.81	108.74	122.65
55	w	37	MIA	C12-C13-C14	-4.81	117.78	127.14
55	w	55	PSU	C5-C6-N1	-4.73	118.63	124.44
55	w	32	PSU	C5-C4-N3	-4.69	119.32	125.36
55	w	32	PSU	C6-N1-C2	4.65	123.03	115.36
55	w	46	7MG	C5-C4-N3	-4.65	118.90	126.49
55	w	32	PSU	C5-C6-N1	-4.63	118.75	124.44
55	w	55	PSU	C5-C4-N3	-4.58	119.45	125.36
33	x	55	PSU	C5-C6-N1	-4.40	119.04	124.44
33	x	32	PSU	C6-N1-C2	4.38	122.59	115.36
33	x	39	PSU	C5-C6-N1	-4.36	119.08	124.44
55	w	8	4SU	C2-N3-C4	4.33	121.43	115.15
55	w	76	F3O	N3-C2-N1	-4.28	121.99	128.68
33	x	32	PSU	C5-C6-N1	-4.25	119.22	124.44
55	w	55	PSU	C6-N1-C2	4.19	122.27	115.36
33	x	39	PSU	C6-N1-C2	4.19	122.27	115.36
55	w	76	F3O	O3'-C-CA	4.16	121.26	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	46	7MG	C6-N1-C2	4.11	122.46	115.93
33	x	46	7MG	C6-N1-C2	4.04	122.35	115.93
33	x	55	PSU	C6-N1-C2	3.93	121.85	115.36
33	x	8	4SU	C2-N3-C4	3.79	120.64	115.15
55	w	39	PSU	C6-N1-C2	3.39	120.94	115.36
55	w	76	F3O	C1'-N9-C4	-3.37	120.72	126.64
55	w	32	PSU	C5-C1'-C2'	-3.36	109.33	115.32
33	x	46	7MG	C5-C6-N1	-3.25	116.45	123.14
33	x	37	MIA	N3-C2-N1	-3.24	123.62	128.68
55	w	55	PSU	C5-C1'-C2'	-3.20	109.62	115.32
55	w	46	7MG	C5-C6-N1	-3.14	116.68	123.14
55	w	46	7MG	C8-N7-C5	3.10	117.00	108.94
55	w	8	4SU	C5-C4-N3	-3.04	119.77	123.83
33	x	46	7MG	C5-C4-N9	-2.89	102.39	106.44
33	x	8	4SU	C5-C4-N3	-2.81	120.06	123.83
55	w	46	7MG	C6-C5-C4	2.77	118.17	115.20
33	x	37	MIA	C4-C5-N7	-2.75	106.53	109.40
55	w	76	F3O	O3'-C-O	-2.75	118.81	123.94
33	x	32	PSU	O4'-C1'-C5	2.67	114.07	109.93
55	w	37	MIA	C4-C5-N7	-2.66	106.63	109.40
55	w	37	MIA	C2-N3-C4	2.65	118.97	115.32
33	x	46	7MG	C8-N7-C5	2.63	115.78	108.94
55	w	39	PSU	C5-C6-N1	-2.60	121.25	124.44
55	w	37	MIA	C15-C14-C13	-2.54	115.31	122.65
33	x	46	7MG	C2-N3-C4	2.43	120.61	113.89
55	w	46	7MG	C2-N3-C4	2.36	120.42	113.89
33	x	39	PSU	C5-C1'-C2'	-2.25	111.30	115.32
33	x	54	5MU	C5-C6-N1	-2.25	119.77	122.19
33	x	46	7MG	C4-N9-C1'	2.24	131.92	126.60
55	w	76	F3O	C3'-O3'-C	-2.18	114.05	117.78
33	x	46	7MG	N2-C2-N3	2.12	120.55	117.25
33	x	46	7MG	CM7-N7-C5	2.07	131.97	124.01
33	x	39	PSU	O4'-C1'-C5	2.06	113.12	109.93
33	x	55	PSU	O4'-C1'-C2'	2.04	107.97	104.66
55	w	39	PSU	C4-C5-C1'	2.04	124.97	121.12

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	x	37	MIA	C3'-C4'-C5'-O5'
33	x	54	5MU	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
33	x	54	5MU	C3'-C4'-C5'-O5'
33	x	32	PSU	O4'-C4'-C5'-O5'
55	w	37	MIA	C5-C6-N6-C12
55	w	37	MIA	N1-C6-N6-C12
55	w	37	MIA	C12-C13-C14-C16
55	w	76	F3O	C4'-C5'-O5'-P
33	x	46	7MG	C4'-C5'-O5'-P
33	x	54	5MU	O4'-C4'-C5'-O5'
33	x	32	PSU	C3'-C4'-C5'-O5'
33	x	39	PSU	C3'-C4'-C5'-O5'
33	x	37	MIA	O4'-C4'-C5'-O5'
33	x	39	PSU	O4'-C4'-C5'-O5'
55	w	76	F3O	CA-C-O3'-C3'
55	w	76	F3O	O3'-C-CA-N
55	w	76	F3O	CA-CB-CG-CD2
55	w	76	F3O	CA-CB-CG-CD1
55	w	76	F3O	O3'-C-CA-CB
33	x	46	7MG	C2'-C1'-N9-C8
55	w	37	MIA	C4'-C5'-O5'-P
33	x	46	7MG	O4'-C1'-N9-C8
33	x	37	MIA	C4'-C5'-O5'-P
55	w	46	7MG	C2'-C1'-N9-C8
33	x	46	7MG	C3'-C4'-C5'-O5'

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	SF4	d	501	37	0,12,12	0.00	-	-		
61	GDP	y	703	58	24,30,30	1.31	2 (8%)	31,47,47	1.95	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	d	501	37	-	-	0/6/5/5
61	GDP	y	703	58	-	1/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

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

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	y	703	GDP	C2-N3-C4	5.76	121.93	115.36
61	y	703	GDP	C5-C6-N1	-3.86	118.15	123.43
61	y	703	GDP	C6-N1-C2	3.43	121.37	115.93
61	y	703	GDP	C4-C5-N7	-3.36	105.90	109.40
61	y	703	GDP	C3'-C2'-C1'	3.28	105.91	100.98
61	y	703	GDP	N3-C2-N1	-2.81	123.47	127.22
61	y	703	GDP	PA-O3A-PB	-2.40	124.59	132.83
61	y	703	GDP	C6-C5-C4	-2.38	118.52	120.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

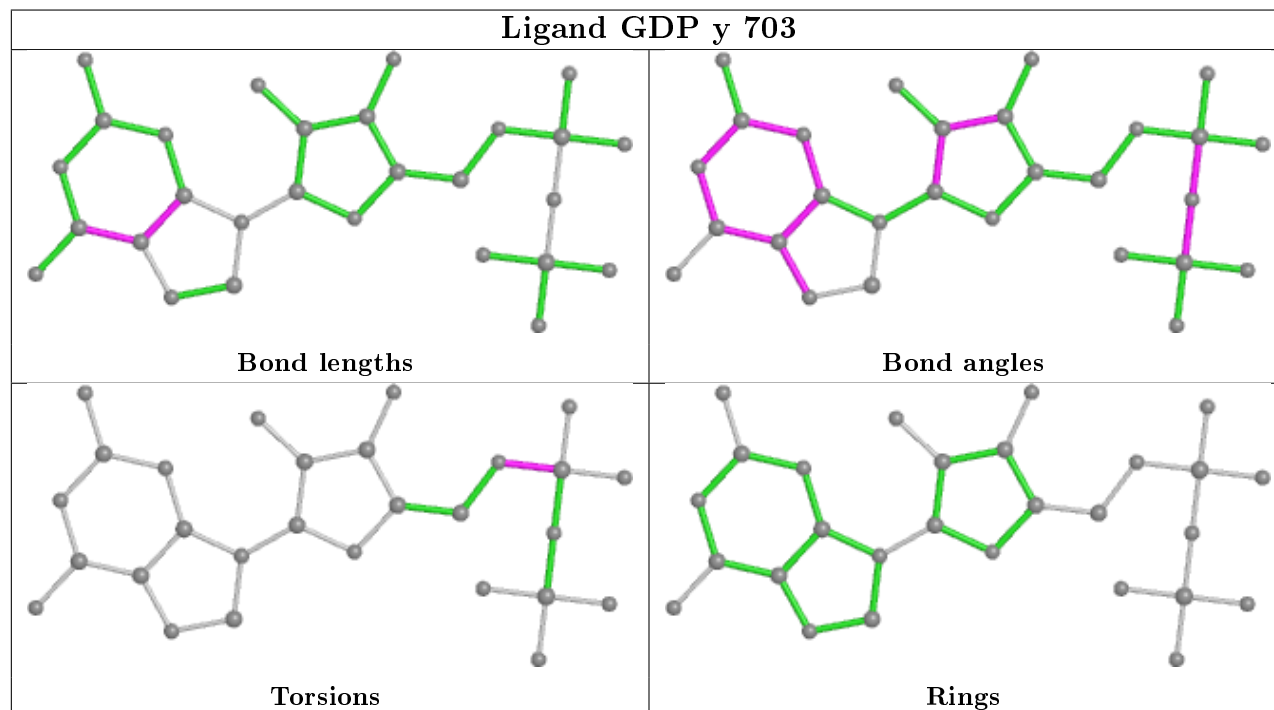
Mol	Chain	Res	Type	Atoms
61	y	703	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

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

All (648) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	J	51	LEU	23.3
9	K	52	ILE	16.9
1	A	2178	C	15.9
1	A	2145	C	13.3
1	A	2165	G	13.2
1	A	1509	C	12.3
1	A	2179	C	10.7
33	x	34	G	10.7
1	A	2114	A	10.6
33	x	30	G	10.3
57	y	13	SER	10.2
1	A	2182	G	10.1
8	J	50	ARG	10.0
57	y	599	ALA	10.0
8	J	53	VAL	9.9
9	K	48	MET	9.9
1	A	2146	C	9.8
9	K	10	LEU	9.6
57	y	310	SER	9.6
33	x	35	A	9.1
8	J	89	ALA	9.0
1	A	2166	G	8.9
1	A	2104	G	8.9
1	A	2169	A	8.8
57	y	600	VAL	8.8
8	J	7	VAL	8.7
1	A	2164	C	8.7
1	A	2116	G	8.7
57	y	209	GLN	8.6
33	x	31	A	8.6
1	A	2159	G	8.5
33	x	36	A	8.5
9	K	51	ALA	8.2
33	x	56	C	8.2

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Mol	Chain	Res	Type	RSRZ
9	K	9	LYS	8.2
9	K	8	VAL	8.0
33	x	26	A	8.0
33	x	33	U	7.9
33	x	61	C	7.9
9	K	47	ASN	7.9
57	y	539	ALA	7.8
33	x	64	A	7.7
1	A	2105	C	7.7
1	A	2177	C	7.6
9	K	13	PRO	7.5
9	K	95	LYS	7.2
1	A	2152	G	7.0
57	y	299	PRO	7.0
1	A	2181	G	7.0
57	y	543	GLY	7.0
19	W	112	GLY	6.9
57	y	264	LEU	6.9
57	y	217	LEU	6.9
1	A	2107	C	6.9
8	J	49	ALA	6.8
1	A	2125	G	6.8
1	A	2170	A	6.7
33	x	5	G	6.7
1	A	2154	G	6.7
9	K	22	PRO	6.5
1	A	2173	A	6.5
57	y	554	LEU	6.4
33	x	11	C	6.4
1	A	2155	G	6.4
9	K	96	VAL	6.4
57	y	266	ALA	6.3
40	g	79	ARG	6.3
57	y	462	ASP	6.3
1	A	2133	G	6.3
33	x	1	G	6.2
57	y	517	ALA	6.2
9	K	2	LYS	6.2
9	K	12	LEU	6.2
33	x	13	C	6.1
1	A	2121	G	6.1
1	A	2112	G	6.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	D	276	LYS	6.1
1	A	2106	G	6.1
33	x	28	G	6.1
33	x	29	G	6.0
57	y	542	GLY	6.0
9	K	16	LYS	6.0
33	x	3	C	6.0
57	y	371	ALA	6.0
1	A	2151	G	5.9
57	y	309	ASP	5.9
33	x	44	G	5.9
33	x	62	C	5.9
57	y	138	ILE	5.9
33	x	53	G	5.9
33	x	20	U	5.8
1	A	2120	G	5.8
57	y	156	LEU	5.8
1	A	2138	C	5.8
1	A	614(B)	G	5.8
9	K	107	ILE	5.8
57	y	77	VAL	5.8
57	y	225	GLY	5.7
1	A	2141	G	5.7
8	J	88	ALA	5.7
1	A	2176	A	5.7
9	K	123	ALA	5.7
33	x	19	G	5.7
57	y	416	THR	5.7
57	y	92	GLU	5.6
9	K	57	ILE	5.6
57	y	513	ALA	5.6
33	x	63	G	5.5
1	A	2142	C	5.5
1	A	2123	G	5.5
1	A	2137	C	5.5
57	y	208	TYR	5.5
33	x	57	G	5.5
40	g	156	TRP	5.5
57	y	435	LEU	5.4
33	x	65	G	5.4
57	y	16	ALA	5.4
57	y	529	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	2126	A	5.4
10	N	140	VAL	5.3
33	x	60	U	5.3
9	K	62	ASP	5.3
9	K	66	THR	5.3
33	x	76	A	5.2
9	K	54	PRO	5.2
57	y	205	TYR	5.2
8	J	54	ALA	5.2
1	A	2143	C	5.2
9	K	45	THR	5.2
57	y	329	ALA	5.2
57	y	525	ALA	5.2
33	x	43	C	5.2
57	y	370	ILE	5.2
8	J	90	ALA	5.1
1	A	2167	U	5.1
33	x	52	G	5.1
8	J	62	ALA	5.1
57	y	414	ILE	5.1
57	y	494	VAL	5.1
9	K	120	LEU	5.0
33	x	70	G	5.0
57	y	397	PRO	5.0
57	y	590	VAL	5.0
8	J	116	ILE	5.0
9	K	41	PHE	5.0
57	y	504	LEU	5.0
8	J	37	THR	5.0
33	x	2	C	5.0
9	K	93	ARG	5.0
1	A	2109	U	5.0
1	A	2161	C	5.0
33	x	10	G	5.0
57	y	265	VAL	5.0
1	A	2122	U	4.9
57	y	313	TYR	4.9
9	K	7	VAL	4.9
57	y	204	VAL	4.9
33	x	71	G	4.9
57	y	222	VAL	4.9
33	x	47	U	4.9

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Mol	Chain	Res	Type	RSRZ
9	K	92	GLY	4.9
1	A	2128	C	4.8
57	y	368	SER	4.8
9	K	97	GLY	4.8
33	x	67	C	4.8
1	A	2127	G	4.8
1	A	2162	G	4.8
57	y	538	GLN	4.8
33	x	18	G	4.7
33	x	22	G	4.7
1	A	2117	A	4.7
12	P	95	VAL	4.7
1	A	2160	G	4.7
33	x	12	U	4.7
8	J	83	TYR	4.6
24	1	2	SER	4.6
12	P	114	ILE	4.6
9	K	68	VAL	4.6
9	K	3	LYS	4.6
57	y	369	LEU	4.6
57	y	601	LEU	4.6
9	K	61	ALA	4.6
57	y	302	PHE	4.6
57	y	547	ALA	4.5
57	y	272	HIS	4.5
56	v	12	A	4.5
33	x	6	G	4.5
57	y	596	ALA	4.5
57	y	32	LEU	4.5
57	y	218	PHE	4.5
1	A	2131	G	4.4
1	A	2174	C	4.4
12	P	85	LEU	4.4
33	x	48	C	4.4
9	K	67	PHE	4.4
1	A	2134	A	4.4
50	q	98	LEU	4.4
57	y	64	VAL	4.4
9	K	110	GLN	4.3
33	x	27	G	4.3
33	x	58	A	4.3
57	y	492	VAL	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	2113	U	4.3
1	A	2144	U	4.3
9	K	134	MET	4.3
57	y	79	HIS	4.3
33	x	4	C	4.3
57	y	493	ASN	4.3
57	y	602	SER	4.3
12	P	88	LEU	4.2
33	x	45	U	4.2
57	y	496	VAL	4.2
9	K	44	ALA	4.2
1	A	2190	G	4.2
48	o	20	GLY	4.2
57	y	568	THR	4.2
33	x	23	A	4.2
57	y	29	ILE	4.2
57	y	330	LEU	4.2
8	J	23	SER	4.1
33	x	38	A	4.1
8	J	118	THR	4.1
33	x	68	C	4.1
8	J	8	GLU	4.0
8	J	94	VAL	4.0
57	y	541	ILE	4.0
57	y	433	GLY	4.0
1	A	2139	C	4.0
33	x	69	G	4.0
9	K	127	ILE	4.0
1	A	2153	G	4.0
9	K	35	MET	3.9
6	G	2	PRO	3.9
57	y	374	PRO	3.9
8	J	61	LEU	3.9
57	y	91	TYR	3.9
1	A	2119	A	3.9
57	y	520	ILE	3.9
57	y	516	MET	3.9
57	y	530	ARG	3.9
57	y	583	ARG	3.9
9	K	14	ALA	3.9
57	y	544	LYS	3.8
57	y	497	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
8	J	52	PHE	3.8
43	j	85	LEU	3.8
9	K	65	PHE	3.8
33	x	14	A	3.8
57	y	563	TYR	3.8
1	A	2175	C	3.8
33	x	21	A	3.8
1	A	1175	U	3.7
1	A	2148	G	3.7
57	y	471	SER	3.7
7	H	26	VAL	3.7
57	y	312	ASP	3.7
9	K	80	LYS	3.7
57	y	452	TYR	3.7
57	y	33	THR	3.7
1	A	2136	C	3.7
1	A	2140	C	3.7
33	x	51	U	3.7
9	K	94	GLU	3.7
8	J	85	ASP	3.7
57	y	445	GLN	3.6
57	y	503	ALA	3.6
57	y	495	LEU	3.6
33	x	25	C	3.6
1	A	652(F)	G	3.6
3	D	275	LYS	3.6
57	y	-5	GLU	3.6
8	J	4	LYS	3.6
9	K	25	PRO	3.6
30	7	46	VAL	3.6
57	y	581	LYS	3.6
33	x	15	G	3.6
1	A	2168	G	3.6
57	y	489	LEU	3.6
57	y	242	VAL	3.6
9	K	49	GLY	3.5
57	y	350	GLY	3.5
53	t	101	GLY	3.5
57	y	279	THR	3.5
57	y	198	ALA	3.5
9	K	37	PHE	3.5
34	a	204	U	3.5

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Mol	Chain	Res	Type	RSRZ
9	K	17	ALA	3.5
1	A	2163	C	3.5
9	K	18	THR	3.5
57	y	207	ALA	3.5
33	x	72	C	3.5
1	A	271(K)	U	3.4
1	A	1420	U	3.4
57	y	526	GLU	3.4
57	y	448	VAL	3.4
57	y	163	ALA	3.4
57	y	286	PRO	3.4
33	x	73	A	3.4
32	9	37	GLY	3.4
57	y	444	ALA	3.4
57	y	531	GLN	3.4
57	y	400	THR	3.4
7	H	2	SER	3.4
40	g	80	VAL	3.4
9	K	83	GLY	3.3
57	y	487	GLY	3.3
1	A	2147	G	3.3
57	y	274	VAL	3.3
21	Y	1	MET	3.3
9	K	21	PRO	3.3
57	y	349	LEU	3.3
1	A	2101	G	3.3
57	y	552	LYS	3.3
57	y	440	TYR	3.3
7	H	47	GLU	3.3
57	y	561	LYS	3.3
57	y	11	ASN	3.3
57	y	9	ILE	3.3
9	K	63	ARG	3.3
1	A	1046	A	3.2
8	J	14	LYS	3.2
22	Z	57	ILE	3.2
8	J	63	LEU	3.2
1	A	2102	U	3.2
1	A	2793	G	3.2
57	y	399	PRO	3.2
20	X	1	MET	3.2
8	J	97	ALA	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
12	P	121	LYS	3.2
37	d	182	LYS	3.2
8	J	24	PHE	3.2
8	J	75	GLN	3.1
57	y	457	ALA	3.1
57	y	280	ILE	3.1
12	P	83	VAL	3.1
1	A	652(B)	A	3.1
57	y	132	ILE	3.1
1	A	2110	G	3.1
57	y	446	LYS	3.1
57	y	236	GLU	3.1
1	A	2156	G	3.1
26	3	2	PRO	3.1
8	J	17	LEU	3.0
19	W	65	LEU	3.0
8	J	78	SER	3.0
57	y	524	LEU	3.0
9	K	138	VAL	3.0
9	K	58	THR	3.0
15	S	20	ARG	3.0
57	y	93	VAL	3.0
50	q	99	SER	3.0
57	y	523	LYS	3.0
57	y	131	ILE	3.0
9	K	85	GLU	3.0
57	y	72	ASP	3.0
19	W	111	HIS	3.0
57	y	558	VAL	3.0
12	P	127	ALA	3.0
39	f	97	PHE	3.0
33	x	40	C	3.0
57	y	67	THR	3.0
21	Y	39	VAL	2.9
9	K	91	PRO	2.9
57	y	-2	ARG	2.9
57	y	99	ALA	2.9
57	y	-1	LEU	2.9
9	K	27	LEU	2.9
46	m	120	LYS	2.9
1	A	2135	A	2.9
57	y	537	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
57	y	473	GLY	2.9
57	y	1	GLU	2.9
57	y	75	GLU	2.9
9	K	55	VAL	2.9
57	y	166	ALA	2.9
12	P	126	VAL	2.9
57	y	12	PHE	2.9
34	a	1030(B)	C	2.9
33	x	50	U	2.9
57	y	164	ILE	2.9
9	K	121	GLU	2.9
1	A	652(S)	C	2.8
1	A	2118	U	2.8
1	A	2132	U	2.8
57	y	551	VAL	2.8
15	S	37	ALA	2.8
57	y	267	ALA	2.8
9	K	64	SER	2.8
1	A	2124	G	2.8
9	K	115	LEU	2.8
57	y	540	ALA	2.8
57	y	586	ALA	2.8
1	A	2189	U	2.8
57	y	519	ALA	2.8
57	y	591	GLU	2.8
57	y	486	PRO	2.8
57	y	461	TYR	2.8
12	P	87	ASP	2.8
57	y	499	GLU	2.8
1	A	2115	G	2.8
9	K	59	ILE	2.8
14	R	118	GLU	2.7
9	K	133	SER	2.7
57	y	597	PHE	2.7
57	y	134	VAL	2.7
57	y	250	LEU	2.7
16	T	115	ARG	2.7
1	A	2103	C	2.7
57	y	426	GLN	2.7
6	G	48	GLU	2.7
12	P	130	PHE	2.7
33	x	74	C	2.7

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Mol	Chain	Res	Type	RSRZ
28	5	60	VAL	2.7
39	f	98	LEU	2.7
57	y	598	LEU	2.7
9	K	74	ALA	2.7
57	y	-6	ALA	2.7
12	P	86	LYS	2.7
57	y	288	PRO	2.7
49	p	39	TYR	2.7
1	A	652(D)	C	2.7
1	A	2180	U	2.7
43	j	73	ASP	2.7
57	y	396	LEU	2.7
1	A	2129	C	2.7
8	J	110	GLY	2.7
27	4	55	ARG	2.7
1	A	614(A)	U	2.6
9	K	137	GLU	2.6
9	K	53	VAL	2.6
8	J	84	GLU	2.6
34	a	1030(C)	G	2.6
51	r	31	LEU	2.6
57	y	535	VAL	2.6
8	J	19	ARG	2.6
56	v	13	A	2.6
1	A	34	C	2.6
1	A	652(T)	C	2.6
9	K	114	ASP	2.6
9	K	135	GLY	2.6
9	K	140	GLY	2.6
8	J	124	ALA	2.6
35	b	129	GLU	2.6
57	y	85	GLY	2.6
8	J	77	PRO	2.6
9	K	30	HIS	2.6
9	K	86	LYS	2.6
22	Z	140	ASP	2.6
27	4	51	ASP	2.6
57	y	518	ARG	2.6
57	y	14	ILE	2.6
8	J	111	LEU	2.6
57	y	105	LEU	2.6
7	H	33	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
33	x	59	U	2.6
21	Y	35	TYR	2.6
57	y	514	TYR	2.6
57	y	534	GLU	2.5
9	K	90	LYS	2.5
35	b	38	GLY	2.5
9	K	50	ASP	2.5
33	x	49	C	2.5
6	G	49	ASP	2.5
12	P	120	ALA	2.5
7	H	77	LYS	2.5
57	y	173	GLY	2.5
12	P	137	LYS	2.5
1	A	2185	C	2.5
1	A	1176	G	2.5
1	A	2108	C	2.5
1	A	2183	C	2.5
23	0	48	GLY	2.5
57	y	203	SER	2.5
21	Y	55	TYR	2.5
33	x	41	C	2.5
33	x	9	A	2.5
57	y	363	ARG	2.5
8	J	76	GLY	2.5
9	K	84	LEU	2.5
51	r	85	LEU	2.5
57	y	500	VAL	2.5
7	H	48	GLY	2.5
57	y	505	THR	2.5
8	J	18	GLU	2.4
57	y	488	ASP	2.4
57	y	589	LYS	2.4
8	J	74	LEU	2.4
23	0	62	LEU	2.4
8	J	87	VAL	2.4
9	K	136	VAL	2.4
50	q	69	LYS	2.4
21	Y	48	ALA	2.4
1	A	2157	G	2.4
35	b	37	ASN	2.4
30	7	49	ARG	2.4
57	y	415	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2897	U	2.4
12	P	1	MET	2.4
8	J	10	LEU	2.4
9	K	34	ILE	2.4
51	r	78	LEU	2.4
57	y	450	LEU	2.4
57	y	509	HIS	2.4
15	S	3	ARG	2.4
12	P	92	GLU	2.4
33	x	42	C	2.4
57	y	546	ILE	2.4
8	J	57	THR	2.4
5	F	33	LEU	2.4
1	A	652(E)	G	2.4
37	d	44	GLY	2.4
57	y	165	PHE	2.4
57	y	562	CYS	2.4
1	A	2150	U	2.4
44	k	19	ALA	2.4
57	y	124	ALA	2.4
26	3	8	LEU	2.4
38	e	142	LEU	2.4
8	J	133	GLU	2.3
57	y	210	GLY	2.3
57	y	278	ASP	2.3
9	K	69	THR	2.3
23	0	47	PRO	2.3
9	K	46	ALA	2.3
12	P	91	PHE	2.3
57	y	443	GLY	2.3
45	l	18	VAL	2.3
35	b	232	PRO	2.3
57	y	434	ARG	2.3
33	x	24	G	2.3
57	y	298	LYS	2.3
1	A	2172	U	2.3
8	J	69	PRO	2.3
57	y	334	PRO	2.3
57	y	115	ALA	2.3
57	y	475	ALA	2.3
57	y	549	ALA	2.3
23	0	74	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
12	P	148	LEU	2.3
22	Z	117	LEU	2.3
57	y	170	THR	2.3
57	y	257	GLU	2.3
9	K	75	SER	2.3
57	y	276	VAL	2.3
4	E	195	LEU	2.3
43	j	86	MET	2.3
8	J	25	PHE	2.3
26	3	60	GLU	2.3
57	y	439	ASN	2.3
4	E	114	ALA	2.3
8	J	117	LEU	2.3
23	0	78	TYR	2.3
33	x	7	A	2.3
9	K	102	GLU	2.3
34	a	1021	G	2.3
57	y	259	GLY	2.2
46	m	48	LEU	2.2
57	y	171	GLY	2.2
7	H	32	GLU	2.2
57	y	481	GLN	2.2
21	Y	50	ARG	2.2
57	y	71	LYS	2.2
1	A	2184	G	2.2
54	u	18	TYR	2.2
48	o	89	GLY	2.2
57	y	109	ALA	2.2
57	y	351	LEU	2.2
35	b	130	ARG	2.2
32	9	23	VAL	2.2
1	A	2188	C	2.2
8	J	36	GLU	2.2
24	1	20	ARG	2.2
57	y	469	SER	2.2
22	Z	62	PRO	2.2
57	y	158	LEU	2.2
57	y	121	PHE	2.2
57	y	402	ILE	2.2
1	A	229	A	2.2
8	J	15	GLU	2.2
21	Y	71	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
57	y	297	ALA	2.2
4	E	159	HIS	2.2
9	K	111	LYS	2.2
40	g	78	ARG	2.2
57	y	571	LYS	2.2
57	y	326	ASN	2.1
21	Y	34	LYS	2.1
11	O	97	ARG	2.1
20	X	9	LEU	2.1
50	q	27	PHE	2.1
12	P	94	GLU	2.1
36	c	126	ARG	2.1
57	y	234	GLY	2.1
57	y	372	THR	2.1
57	y	-22	LEU	2.1
57	y	201	PHE	2.1
8	J	73	GLY	2.1
21	Y	17	SER	2.1
12	P	115	LEU	2.1
15	S	7	TYR	2.1
57	y	258	ALA	2.1
57	y	528	ILE	2.1
8	J	86	PRO	2.1
32	9	15	LYS	2.1
12	P	15	ARG	2.1
51	r	20	ALA	2.1
57	y	255	ALA	2.1
7	H	174	GLY	2.1
22	Z	27	VAL	2.1
8	J	99	SER	2.1
6	G	50	ALA	2.1
7	H	145	ALA	2.1
12	P	79	ARG	2.1
12	P	125	VAL	2.1
57	y	490	VAL	2.1
57	y	232	SER	2.1
44	k	31	THR	2.1
49	p	19	ILE	2.1
57	y	420	TYR	2.1
19	W	1	MET	2.1
27	4	56	VAL	2.1
50	q	97	SER	2.1

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Mol	Chain	Res	Type	RSRZ
9	K	26	ALA	2.1
9	K	124	ALA	2.1
40	g	85	TYR	2.1
33	x	66	U	2.1
57	y	305	LEU	2.0
7	H	136	ILE	2.0
57	y	277	GLY	2.0
3	D	181	GLU	2.0
6	G	182	LYS	2.0
14	R	97	VAL	2.0
8	J	66	LEU	2.0
15	S	17	ARG	2.0
4	E	113	PHE	2.0
57	y	412	LEU	2.0
49	p	8	ARG	2.0
9	K	131	ALA	2.0
22	Z	145	GLU	2.0
7	H	164	TYR	2.0
7	H	76	VAL	2.0
21	Y	92	ASN	2.0
3	D	271	ILE	2.0
40	g	81	GLY	2.0
44	k	109	VAL	2.0
57	y	246	THR	2.0
32	9	2	LYS	2.0
48	o	34	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	5MU	x	54	21/22	0.20	0.65	275,282,283,285	0
33	4SU	x	8	20/21	0.32	0.42	263,275,277,277	0
33	PSU	x	55	20/21	0.33	0.83	274,285,289,293	0
33	7MG	x	46	24/25	0.34	0.36	275,282,285,287	0
33	PSU	x	32	20/21	0.41	0.63	188,202,216,216	0
33	MIA	x	37	22/30	0.50	0.78	204,221,237,241	0
33	PSU	x	39	20/21	0.73	0.33	175,193,200,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	F3O	w	76	33/34	0.92	0.26	50,60,79,81	0
55	7MG	w	46	24/25	0.92	0.18	59,76,103,118	0
55	PSU	w	55	20/21	0.93	0.17	75,83,85,86	0
55	4SU	w	8	20/21	0.95	0.14	56,58,64,64	0
55	MIA	w	37	29/30	0.95	0.17	46,55,61,64	0
55	PSU	w	39	20/21	0.96	0.14	41,50,55,56	0
55	5MU	w	54	21/22	0.96	0.14	67,77,82,84	0
55	PSU	w	32	20/21	0.97	0.12	40,46,49,51	0

## 6.3 Carbohydrates [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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3608	1/1	0.29	0.47	108,108,108,108	0
58	MG	A	3157	1/1	0.34	0.24	118,118,118,118	0
58	MG	A	3435	1/1	0.37	0.38	95,95,95,95	0
58	MG	a	3390	1/1	0.44	0.44	45,45,45,45	0
58	MG	x	3001	1/1	0.50	0.28	237,237,237,237	0
58	MG	U	203	1/1	0.54	0.47	67,67,67,67	0
58	MG	x	3003	1/1	0.55	1.33	215,215,215,215	0
58	MG	A	3282	1/1	0.56	0.44	66,66,66,66	0
58	MG	D	302	1/1	0.58	0.29	74,74,74,74	0
58	MG	A	3056	1/1	0.59	0.42	68,68,68,68	0
58	MG	A	3265	1/1	0.60	0.18	61,61,61,61	0
58	MG	B	215	1/1	0.61	0.12	114,114,114,114	0
58	MG	A	3011	1/1	0.61	0.47	79,79,79,79	0
58	MG	0	101	1/1	0.62	0.39	73,73,73,73	0
58	MG	a	3323	1/1	0.62	0.49	69,69,69,69	0
58	MG	B	214	1/1	0.62	1.50	83,83,83,83	0
58	MG	A	3253	1/1	0.63	0.30	66,66,66,66	0
58	MG	B	216	1/1	0.63	0.12	86,86,86,86	0
58	MG	A	3161	1/1	0.63	0.45	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	B	209	1/1	0.65	0.27	70,70,70,70	0
58	MG	A	3216	1/1	0.66	0.38	62,62,62,62	0
58	MG	A	3160	1/1	0.66	0.49	61,61,61,61	0
58	MG	A	3093	1/1	0.66	0.32	81,81,81,81	0
58	MG	A	3068	1/1	0.66	0.27	56,56,56,56	0
58	MG	A	3354	1/1	0.67	0.24	101,101,101,101	0
58	MG	A	3577	1/1	0.67	0.20	72,72,72,72	0
58	MG	B	213	1/1	0.67	0.11	81,81,81,81	0
58	MG	A	3334	1/1	0.67	0.13	84,84,84,84	0
58	MG	G	202	1/1	0.68	0.24	67,67,67,67	0
58	MG	A	3002	1/1	0.68	0.34	50,50,50,50	0
58	MG	A	3165	1/1	0.68	1.03	60,60,60,60	0
58	MG	A	3560	1/1	0.68	0.26	79,79,79,79	0
58	MG	A	3572	1/1	0.68	0.38	70,70,70,70	0
58	MG	A	3213	1/1	0.69	0.46	67,67,67,67	0
58	MG	a	3455	1/1	0.69	0.10	67,67,67,67	0
58	MG	a	3391	1/1	0.69	0.15	72,72,72,72	0
58	MG	A	3319	1/1	0.70	0.23	31,31,31,31	0
58	MG	A	3132	1/1	0.70	0.78	48,48,48,48	0
58	MG	A	3554	1/1	0.71	0.21	74,74,74,74	0
58	MG	A	3054	1/1	0.71	0.27	71,71,71,71	0
58	MG	A	3084	1/1	0.71	0.20	57,57,57,57	0
58	MG	A	3226	1/1	0.72	0.43	68,68,68,68	0
58	MG	B	208	1/1	0.72	0.11	74,74,74,74	0
58	MG	A	3044	1/1	0.72	0.38	72,72,72,72	0
58	MG	A	3408	1/1	0.72	0.12	98,98,98,98	0
58	MG	a	3388	1/1	0.73	0.23	59,59,59,59	0
58	MG	A	3603	1/1	0.74	0.35	82,82,82,82	0
58	MG	a	3316	1/1	0.74	0.24	54,54,54,54	0
58	MG	a	3392	1/1	0.74	0.14	65,65,65,65	0
58	MG	A	3254	1/1	0.74	0.37	67,67,67,67	0
58	MG	A	3152	1/1	0.74	0.43	68,68,68,68	0
58	MG	a	3472	1/1	0.75	0.17	61,61,61,61	0
58	MG	A	3410	1/1	0.75	0.20	51,51,51,51	0
58	MG	A	3058	1/1	0.75	0.51	57,57,57,57	0
58	MG	A	3619	1/1	0.76	0.28	78,78,78,78	0
58	MG	B	210	1/1	0.76	0.22	68,68,68,68	0
58	MG	A	3113	1/1	0.76	0.31	63,63,63,63	0
58	MG	A	3087	1/1	0.76	0.29	58,58,58,58	0
58	MG	A	3075	1/1	0.76	0.17	67,67,67,67	0
58	MG	N	201	1/1	0.76	0.39	57,57,57,57	0
58	MG	A	3220	1/1	0.76	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3231	1/1	0.76	0.39	48,48,48,48	0
58	MG	a	3369	1/1	0.76	0.24	60,60,60,60	0
58	MG	A	3025	1/1	0.77	0.20	60,60,60,60	0
58	MG	a	3440	1/1	0.77	0.14	69,69,69,69	0
58	MG	A	3108	1/1	0.77	0.35	54,54,54,54	0
58	MG	A	3284	1/1	0.77	0.29	67,67,67,67	0
58	MG	A	3052	1/1	0.78	0.38	59,59,59,59	0
58	MG	A	3066	1/1	0.78	0.19	56,56,56,56	0
58	MG	x	3002	1/1	0.78	1.22	101,101,101,101	0
58	MG	A	3564	1/1	0.78	0.21	75,75,75,75	0
58	MG	a	3480	1/1	0.78	0.27	77,77,77,77	0
58	MG	A	3182	1/1	0.78	0.32	53,53,53,53	0
58	MG	A	3263	1/1	0.78	0.33	55,55,55,55	0
58	MG	A	3095	1/1	0.78	0.40	63,63,63,63	0
58	MG	a	3352	1/1	0.79	0.25	59,59,59,59	0
58	MG	P	201	1/1	0.79	0.54	54,54,54,54	0
58	MG	A	3032	1/1	0.79	0.32	50,50,50,50	0
58	MG	A	3209	1/1	0.79	0.18	71,71,71,71	0
58	MG	A	3607	1/1	0.80	0.17	90,90,90,90	0
58	MG	A	3617	1/1	0.80	0.19	65,65,65,65	0
58	MG	6	101	1/1	0.80	0.32	64,64,64,64	0
58	MG	a	3436	1/1	0.80	0.26	66,66,66,66	0
58	MG	A	3294	1/1	0.80	0.37	44,44,44,44	0
58	MG	A	3240	1/1	0.80	0.24	79,79,79,79	0
58	MG	A	3297	1/1	0.80	0.24	67,67,67,67	0
58	MG	A	3073	1/1	0.80	0.45	56,56,56,56	0
58	MG	A	3339	1/1	0.80	0.17	68,68,68,68	0
58	MG	A	3375	1/1	0.80	0.12	55,55,55,55	0
58	MG	A	3293	1/1	0.80	0.33	51,51,51,51	0
58	MG	A	3245	1/1	0.80	0.29	56,56,56,56	0
58	MG	A	3040	1/1	0.80	0.28	58,58,58,58	0
58	MG	A	3570	1/1	0.80	0.17	57,57,57,57	0
58	MG	A	3270	1/1	0.80	0.25	61,61,61,61	0
58	MG	A	3305	1/1	0.80	0.29	70,70,70,70	0
58	MG	A	3059	1/1	0.80	0.34	66,66,66,66	0
58	MG	A	3101	1/1	0.80	0.32	74,74,74,74	0
58	MG	A	3568	1/1	0.81	0.20	83,83,83,83	0
58	MG	B	217	1/1	0.81	0.27	67,67,67,67	0
58	MG	A	3236	1/1	0.81	0.56	67,67,67,67	0
58	MG	A	3174	1/1	0.81	0.32	59,59,59,59	0
58	MG	a	3371	1/1	0.81	0.25	65,65,65,65	0
58	MG	A	3067	1/1	0.81	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	B	207	1/1	0.81	0.26	103,103,103,103	0
58	MG	A	3287	1/1	0.81	0.26	54,54,54,54	0
58	MG	A	3259	1/1	0.81	0.09	74,74,74,74	0
58	MG	V	201	1/1	0.81	0.15	53,53,53,53	0
58	MG	A	3569	1/1	0.81	0.45	85,85,85,85	0
58	MG	A	3273	1/1	0.81	0.43	77,77,77,77	0
58	MG	A	3635	1/1	0.81	0.62	69,69,69,69	0
58	MG	A	3255	1/1	0.81	0.33	57,57,57,57	0
58	MG	A	3247	1/1	0.82	0.43	66,66,66,66	0
58	MG	A	3185	1/1	0.82	0.36	63,63,63,63	0
58	MG	A	3598	1/1	0.82	0.14	74,74,74,74	0
58	MG	A	3112	1/1	0.82	0.37	66,66,66,66	0
58	MG	B	206	1/1	0.82	0.18	75,75,75,75	0
58	MG	A	3003	1/1	0.82	0.29	59,59,59,59	0
58	MG	A	3357	1/1	0.82	0.24	69,69,69,69	0
58	MG	a	3348	1/1	0.82	0.50	53,53,53,53	0
58	MG	A	3057	1/1	0.82	0.25	56,56,56,56	0
58	MG	A	3288	1/1	0.82	0.32	60,60,60,60	0
58	MG	A	3352	1/1	0.82	0.32	47,47,47,47	0
58	MG	D	305	1/1	0.82	0.18	37,37,37,37	0
58	MG	A	3565	1/1	0.82	0.15	67,67,67,67	0
58	MG	A	3162	1/1	0.82	0.18	71,71,71,71	0
58	MG	A	3171	1/1	0.82	0.18	37,37,37,37	0
58	MG	A	3243	1/1	0.83	0.56	58,58,58,58	0
58	MG	a	3377	1/1	0.83	0.23	85,85,85,85	0
58	MG	f	201	1/1	0.83	0.25	92,92,92,92	0
58	MG	A	3576	1/1	0.83	0.33	89,89,89,89	0
58	MG	A	3596	1/1	0.83	0.20	45,45,45,45	0
58	MG	a	3484	1/1	0.83	0.24	67,67,67,67	0
58	MG	A	3426	1/1	0.83	0.28	55,55,55,55	0
58	MG	A	3029	1/1	0.83	0.18	52,52,52,52	0
58	MG	A	3122	1/1	0.83	0.20	35,35,35,35	0
58	MG	A	3114	1/1	0.83	1.03	57,57,57,57	0
58	MG	A	3045	1/1	0.83	0.22	68,68,68,68	0
58	MG	A	3405	1/1	0.83	0.15	61,61,61,61	0
58	MG	A	3563	1/1	0.83	0.19	73,73,73,73	0
58	MG	A	3434	1/1	0.83	0.23	56,56,56,56	0
58	MG	A	3175	1/1	0.83	0.38	46,46,46,46	0
58	MG	A	3117	1/1	0.83	1.10	50,50,50,50	0
58	MG	A	3034	1/1	0.83	0.20	71,71,71,71	0
58	MG	A	3124	1/1	0.83	0.14	54,54,54,54	0
58	MG	a	3393	1/1	0.83	0.52	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3481	1/1	0.83	0.32	65,65,65,65	0
58	MG	A	3120	1/1	0.83	0.76	52,52,52,52	0
58	MG	a	3327	1/1	0.84	0.12	62,62,62,62	0
58	MG	A	3573	1/1	0.84	0.20	70,70,70,70	0
58	MG	A	3121	1/1	0.84	0.18	62,62,62,62	0
58	MG	A	3360	1/1	0.84	0.21	60,60,60,60	0
58	MG	a	3329	1/1	0.84	0.16	46,46,46,46	0
58	MG	7	102	1/1	0.84	1.31	66,66,66,66	0
58	MG	A	3388	1/1	0.84	0.15	47,47,47,47	0
58	MG	R	201	1/1	0.84	0.54	67,67,67,67	0
58	MG	a	3425	1/1	0.84	0.26	47,47,47,47	0
58	MG	A	3102	1/1	0.84	0.13	59,59,59,59	0
58	MG	A	3328	1/1	0.84	0.20	62,62,62,62	0
58	MG	a	3332	1/1	0.84	0.16	45,45,45,45	0
58	MG	A	3246	1/1	0.84	0.24	49,49,49,49	0
58	MG	A	3181	1/1	0.84	0.10	35,35,35,35	0
58	MG	v	101	1/1	0.84	0.53	89,89,89,89	0
58	MG	A	3001	1/1	0.85	0.34	70,70,70,70	0
58	MG	A	3601	1/1	0.85	0.20	45,45,45,45	0
58	MG	A	3514	1/1	0.85	0.14	34,34,34,34	0
58	MG	0	102	1/1	0.85	0.10	61,61,61,61	0
58	MG	A	3085	1/1	0.85	0.34	52,52,52,52	0
58	MG	a	3400	1/1	0.85	0.31	61,61,61,61	0
58	MG	A	3383	1/1	0.85	0.24	55,55,55,55	0
58	MG	a	3403	1/1	0.85	0.16	61,61,61,61	0
58	MG	P	202	1/1	0.85	0.27	86,86,86,86	0
58	MG	A	3615	1/1	0.85	0.24	50,50,50,50	0
58	MG	A	3549	1/1	0.85	0.47	75,75,75,75	0
58	MG	A	3589	1/1	0.85	0.25	46,46,46,46	0
58	MG	a	3434	1/1	0.85	0.24	54,54,54,54	0
58	MG	F	305	1/1	0.85	0.25	59,59,59,59	0
58	MG	A	3009	1/1	0.85	0.30	50,50,50,50	0
58	MG	A	3244	1/1	0.85	0.20	59,59,59,59	0
58	MG	A	3376	1/1	0.85	0.12	67,67,67,67	0
58	MG	y	701	1/1	0.85	0.26	68,68,68,68	0
58	MG	a	3426	1/1	0.85	0.13	69,69,69,69	0
58	MG	A	3276	1/1	0.85	0.07	73,73,73,73	0
58	MG	a	3450	1/1	0.85	0.08	55,55,55,55	0
58	MG	A	3451	1/1	0.85	0.18	82,82,82,82	0
58	MG	A	3298	1/1	0.85	0.17	58,58,58,58	0
58	MG	a	3428	1/1	0.85	0.27	46,46,46,46	0
58	MG	A	3614	1/1	0.85	0.16	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3039	1/1	0.85	0.82	59,59,59,59	0
58	MG	A	3081	1/1	0.85	0.28	61,61,61,61	0
58	MG	A	3135	1/1	0.85	0.46	54,54,54,54	0
58	MG	A	3436	1/1	0.85	0.18	87,87,87,87	0
58	MG	A	3239	1/1	0.85	0.33	56,56,56,56	0
58	MG	A	3018	1/1	0.85	0.24	49,49,49,49	0
58	MG	A	3110	1/1	0.86	0.26	42,42,42,42	0
58	MG	a	3306	1/1	0.86	0.68	55,55,55,55	0
58	MG	A	3109	1/1	0.86	0.26	52,52,52,52	0
58	MG	A	3520	1/1	0.86	0.21	80,80,80,80	0
58	MG	a	3373	1/1	0.86	0.24	63,63,63,63	0
58	MG	a	3328	1/1	0.86	0.25	60,60,60,60	0
58	MG	a	3419	1/1	0.86	0.24	72,72,72,72	0
58	MG	a	3458	1/1	0.86	0.26	62,62,62,62	0
58	MG	a	3396	1/1	0.86	0.11	42,42,42,42	0
58	MG	A	3275	1/1	0.86	0.16	63,63,63,63	0
58	MG	A	3600	1/1	0.86	0.26	64,64,64,64	0
58	MG	A	3141	1/1	0.86	0.23	55,55,55,55	0
58	MG	A	3461	1/1	0.86	0.51	59,59,59,59	0
58	MG	7	103	1/1	0.86	0.26	57,57,57,57	0
58	MG	A	3353	1/1	0.86	0.18	79,79,79,79	0
58	MG	A	3370	1/1	0.86	0.16	64,64,64,64	0
58	MG	A	3148	1/1	0.86	0.38	60,60,60,60	0
58	MG	A	3498	1/1	0.86	0.18	76,76,76,76	0
58	MG	a	3451	1/1	0.86	0.13	49,49,49,49	0
58	MG	A	3532	1/1	0.86	0.42	66,66,66,66	0
58	MG	a	3360	1/1	0.86	0.35	40,40,40,40	0
58	MG	5	101	1/1	0.86	0.58	69,69,69,69	0
58	MG	Q	203	1/1	0.86	0.21	45,45,45,45	0
58	MG	V	202	1/1	0.87	0.74	51,51,51,51	0
58	MG	a	3410	1/1	0.87	0.37	45,45,45,45	0
58	MG	A	3309	1/1	0.87	0.25	52,52,52,52	0
58	MG	A	3042	1/1	0.87	0.16	92,92,92,92	0
58	MG	a	3358	1/1	0.87	0.36	70,70,70,70	0
58	MG	A	3278	1/1	0.87	0.46	64,64,64,64	0
58	MG	A	3606	1/1	0.87	0.19	55,55,55,55	0
58	MG	A	3197	1/1	0.87	0.29	40,40,40,40	0
58	MG	A	3272	1/1	0.87	0.33	62,62,62,62	0
58	MG	A	3072	1/1	0.87	0.33	43,43,43,43	0
58	MG	A	3119	1/1	0.87	0.27	50,50,50,50	0
58	MG	A	3145	1/1	0.87	0.09	48,48,48,48	0
58	MG	A	3097	1/1	0.87	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	a	3341	1/1	0.87	0.28	60,60,60,60	0
58	MG	A	3212	1/1	0.87	0.15	55,55,55,55	0
58	MG	A	3104	1/1	0.87	0.21	64,64,64,64	0
58	MG	A	3350	1/1	0.87	0.10	63,63,63,63	0
58	MG	A	3544	1/1	0.87	0.17	55,55,55,55	0
58	MG	a	3362	1/1	0.87	0.15	73,73,73,73	0
58	MG	a	3418	1/1	0.87	0.12	67,67,67,67	0
58	MG	A	3373	1/1	0.87	0.08	64,64,64,64	0
58	MG	A	3014	1/1	0.87	0.14	39,39,39,39	0
58	MG	A	3237	1/1	0.87	0.17	51,51,51,51	0
58	MG	a	3409	1/1	0.87	0.10	74,74,74,74	0
58	MG	A	3490	1/1	0.87	0.25	47,47,47,47	0
58	MG	a	3368	1/1	0.87	0.23	44,44,44,44	0
58	MG	A	3092	1/1	0.87	0.38	67,67,67,67	0
58	MG	w	101	1/1	0.87	0.79	60,60,60,60	0
58	MG	A	3586	1/1	0.87	0.28	55,55,55,55	0
58	MG	A	3215	1/1	0.88	0.19	66,66,66,66	0
58	MG	A	3562	1/1	0.88	0.18	59,59,59,59	0
58	MG	Z	301	1/1	0.88	0.17	66,66,66,66	0
58	MG	a	3314	1/1	0.88	0.20	60,60,60,60	0
58	MG	a	3468	1/1	0.88	0.18	69,69,69,69	0
58	MG	A	3574	1/1	0.88	0.16	57,57,57,57	0
58	MG	A	3624	1/1	0.88	0.15	52,52,52,52	0
58	MG	a	3340	1/1	0.88	0.43	81,81,81,81	0
58	MG	A	3419	1/1	0.88	0.13	74,74,74,74	0
58	MG	A	3089	1/1	0.88	0.19	47,47,47,47	0
58	MG	A	3285	1/1	0.88	0.24	50,50,50,50	0
58	MG	A	3126	1/1	0.88	0.21	60,60,60,60	0
58	MG	A	3464	1/1	0.88	0.25	49,49,49,49	0
58	MG	A	3129	1/1	0.88	0.24	48,48,48,48	0
58	MG	A	3502	1/1	0.88	0.25	56,56,56,56	0
58	MG	A	3118	1/1	0.88	0.87	52,52,52,52	0
58	MG	A	3103	1/1	0.88	0.29	56,56,56,56	0
58	MG	a	3321	1/1	0.88	0.18	48,48,48,48	0
58	MG	A	3064	1/1	0.88	0.38	50,50,50,50	0
58	MG	A	3430	1/1	0.88	0.14	44,44,44,44	0
58	MG	A	3030	1/1	0.88	0.36	64,64,64,64	0
58	MG	a	3413	1/1	0.88	0.14	54,54,54,54	0
58	MG	a	3359	1/1	0.88	0.14	65,65,65,65	0
58	MG	A	3286	1/1	0.88	0.16	62,62,62,62	0
58	MG	A	3086	1/1	0.88	0.19	50,50,50,50	0
58	MG	A	3223	1/1	0.88	0.30	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3516	1/1	0.88	0.21	55,55,55,55	0
58	MG	A	3013	1/1	0.88	0.22	52,52,52,52	0
58	MG	A	3355	1/1	0.88	0.13	84,84,84,84	0
58	MG	A	3433	1/1	0.88	0.09	64,64,64,64	0
58	MG	A	3134	1/1	0.88	0.43	67,67,67,67	0
58	MG	a	3423	1/1	0.88	0.40	66,66,66,66	0
58	MG	a	3421	1/1	0.88	0.11	61,61,61,61	0
58	MG	A	3347	1/1	0.88	0.18	75,75,75,75	0
58	MG	A	3264	1/1	0.88	0.33	65,65,65,65	0
58	MG	A	3551	1/1	0.88	0.20	63,63,63,63	0
58	MG	a	3474	1/1	0.88	0.16	64,64,64,64	0
58	MG	A	3543	1/1	0.88	0.14	71,71,71,71	0
58	MG	A	3326	1/1	0.88	0.17	69,69,69,69	0
58	MG	A	3268	1/1	0.88	0.26	58,58,58,58	0
58	MG	A	3010	1/1	0.89	0.20	41,41,41,41	0
58	MG	A	3611	1/1	0.89	0.20	52,52,52,52	0
58	MG	A	3173	1/1	0.89	0.18	57,57,57,57	0
58	MG	A	3525	1/1	0.89	0.14	54,54,54,54	0
58	MG	A	3507	1/1	0.89	0.17	46,46,46,46	0
58	MG	A	3079	1/1	0.89	0.46	63,63,63,63	0
58	MG	a	3303	1/1	0.89	0.17	58,58,58,58	0
58	MG	A	3060	1/1	0.89	0.26	81,81,81,81	0
58	MG	A	3465	1/1	0.89	0.15	68,68,68,68	0
58	MG	a	3346	1/1	0.89	0.14	50,50,50,50	0
58	MG	A	3602	1/1	0.89	0.11	73,73,73,73	0
58	MG	A	3585	1/1	0.89	0.18	47,47,47,47	0
58	MG	A	3367	1/1	0.89	0.48	51,51,51,51	0
58	MG	a	3313	1/1	0.89	0.20	61,61,61,61	0
58	MG	A	3020	1/1	0.89	0.16	50,50,50,50	0
58	MG	A	3616	1/1	0.89	0.32	59,59,59,59	0
58	MG	A	3555	1/1	0.89	0.17	69,69,69,69	0
58	MG	A	3005	1/1	0.89	0.37	40,40,40,40	0
58	MG	A	3346	1/1	0.89	0.24	68,68,68,68	0
58	MG	A	3605	1/1	0.89	0.24	70,70,70,70	0
58	MG	A	3423	1/1	0.89	0.21	59,59,59,59	0
58	MG	A	3374	1/1	0.89	0.15	58,58,58,58	0
58	MG	A	3250	1/1	0.89	0.21	58,58,58,58	0
58	MG	A	3335	1/1	0.89	0.09	56,56,56,56	0
58	MG	A	3281	1/1	0.89	0.14	57,57,57,57	0
58	MG	a	3310	1/1	0.89	0.10	52,52,52,52	0
58	MG	a	3385	1/1	0.89	0.12	33,33,33,33	0
58	MG	A	3252	1/1	0.89	0.27	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3397	1/1	0.89	0.16	36,36,36,36	0
58	MG	A	3366	1/1	0.89	0.11	58,58,58,58	0
58	MG	A	3478	1/1	0.89	0.11	65,65,65,65	0
58	MG	A	3198	1/1	0.89	0.22	55,55,55,55	0
58	MG	a	3334	1/1	0.89	0.35	43,43,43,43	0
58	MG	A	3186	1/1	0.89	0.16	90,90,90,90	0
58	MG	a	3330	1/1	0.89	0.57	63,63,63,63	0
58	MG	A	3224	1/1	0.89	0.45	51,51,51,51	0
58	MG	A	3343	1/1	0.89	0.14	69,69,69,69	0
58	MG	A	3467	1/1	0.89	0.35	52,52,52,52	0
58	MG	l	201	1/1	0.89	0.48	61,61,61,61	0
58	MG	A	3330	1/1	0.89	0.34	55,55,55,55	0
58	MG	E	304	1/1	0.89	0.21	55,55,55,55	0
58	MG	a	3315	1/1	0.89	0.21	60,60,60,60	0
58	MG	A	3053	1/1	0.89	0.45	61,61,61,61	0
58	MG	a	3361	1/1	0.89	0.15	73,73,73,73	0
58	MG	a	3335	1/1	0.89	0.37	37,37,37,37	0
58	MG	a	3366	1/1	0.89	0.24	38,38,38,38	0
58	MG	a	3350	1/1	0.89	0.12	73,73,73,73	0
58	MG	A	3050	1/1	0.89	0.12	39,39,39,39	0
58	MG	D	303	1/1	0.89	0.93	49,49,49,49	0
58	MG	A	3322	1/1	0.90	0.24	61,61,61,61	0
58	MG	A	3511	1/1	0.90	0.17	99,99,99,99	0
58	MG	a	3459	1/1	0.90	0.26	91,91,91,91	0
58	MG	A	3312	1/1	0.90	0.23	59,59,59,59	0
58	MG	X	101	1/1	0.90	0.22	72,72,72,72	0
58	MG	A	3023	1/1	0.90	0.30	48,48,48,48	0
58	MG	A	3150	1/1	0.90	0.14	74,74,74,74	0
58	MG	A	3571	1/1	0.90	0.38	89,89,89,89	0
58	MG	A	3062	1/1	0.90	0.26	42,42,42,42	0
58	MG	A	3242	1/1	0.90	0.11	63,63,63,63	0
58	MG	A	3479	1/1	0.90	0.18	43,43,43,43	0
58	MG	A	3139	1/1	0.90	0.59	62,62,62,62	0
58	MG	A	3533	1/1	0.90	0.18	47,47,47,47	0
58	MG	a	3325	1/1	0.90	0.83	55,55,55,55	0
58	MG	A	3063	1/1	0.90	0.16	62,62,62,62	0
58	MG	G	201	1/1	0.90	0.17	71,71,71,71	0
58	MG	A	3308	1/1	0.90	0.13	56,56,56,56	0
58	MG	A	3512	1/1	0.90	0.15	51,51,51,51	0
58	MG	E	301	1/1	0.90	0.79	56,56,56,56	0
58	MG	A	3078	1/1	0.90	0.35	47,47,47,47	0
58	MG	A	3207	1/1	0.90	0.17	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3046	1/1	0.90	0.18	55,55,55,55	0
58	MG	A	3235	1/1	0.90	0.14	48,48,48,48	0
58	MG	Q	202	1/1	0.90	0.98	51,51,51,51	0
58	MG	A	3431	1/1	0.90	0.35	69,69,69,69	0
58	MG	A	3199	1/1	0.90	0.15	42,42,42,42	0
58	MG	A	3074	1/1	0.90	0.16	42,42,42,42	0
58	MG	A	3107	1/1	0.90	1.43	75,75,75,75	0
58	MG	A	3037	1/1	0.90	0.27	61,61,61,61	0
58	MG	A	3304	1/1	0.90	0.18	39,39,39,39	0
58	MG	a	3324	1/1	0.90	0.47	40,40,40,40	0
58	MG	A	3008	1/1	0.90	0.98	80,80,80,80	0
58	MG	F	301	1/1	0.90	0.31	71,71,71,71	0
58	MG	A	3269	1/1	0.90	0.23	54,54,54,54	0
58	MG	A	3386	1/1	0.90	0.17	59,59,59,59	0
58	MG	A	3251	1/1	0.90	0.14	35,35,35,35	0
58	MG	A	3106	1/1	0.90	0.40	57,57,57,57	0
58	MG	A	3493	1/1	0.90	0.37	33,33,33,33	0
58	MG	a	3383	1/1	0.90	0.21	56,56,56,56	0
58	MG	a	3380	1/1	0.90	0.22	57,57,57,57	0
58	MG	a	3357	1/1	0.90	0.12	48,48,48,48	0
58	MG	Q	205	1/1	0.90	0.18	55,55,55,55	0
58	MG	A	3260	1/1	0.90	0.10	68,68,68,68	0
58	MG	B	211	1/1	0.90	0.34	61,61,61,61	0
58	MG	A	3143	1/1	0.90	0.27	60,60,60,60	0
58	MG	A	3463	1/1	0.90	0.25	46,46,46,46	0
58	MG	A	3131	1/1	0.90	0.29	53,53,53,53	0
58	MG	A	3277	1/1	0.90	0.52	71,71,71,71	0
58	MG	A	3291	1/1	0.90	0.12	60,60,60,60	0
58	MG	A	3299	1/1	0.90	0.19	64,64,64,64	0
58	MG	A	3448	1/1	0.90	0.45	48,48,48,48	0
58	MG	A	3517	1/1	0.90	0.25	51,51,51,51	0
58	MG	A	3262	1/1	0.91	0.08	63,63,63,63	0
58	MG	a	3353	1/1	0.91	0.16	48,48,48,48	0
58	MG	A	3261	1/1	0.91	0.23	61,61,61,61	0
58	MG	A	3177	1/1	0.91	0.18	65,65,65,65	0
58	MG	A	3578	1/1	0.91	0.24	64,64,64,64	0
58	MG	A	3069	1/1	0.91	0.23	46,46,46,46	0
58	MG	A	3491	1/1	0.91	0.26	72,72,72,72	0
58	MG	A	3142	1/1	0.91	0.10	84,84,84,84	0
58	MG	A	3406	1/1	0.91	0.14	56,56,56,56	0
58	MG	A	3248	1/1	0.91	0.61	57,57,57,57	0
58	MG	F	304	1/1	0.91	0.27	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3290	1/1	0.91	0.23	49,49,49,49	0
58	MG	a	3336	1/1	0.91	0.29	62,62,62,62	0
58	MG	A	3414	1/1	0.91	0.28	31,31,31,31	0
58	MG	Q	204	1/1	0.91	0.62	56,56,56,56	0
58	MG	a	3454	1/1	0.91	0.24	39,39,39,39	0
58	MG	A	3515	1/1	0.91	0.29	48,48,48,48	0
58	MG	A	3471	1/1	0.91	0.33	56,56,56,56	0
58	MG	A	3444	1/1	0.91	0.34	48,48,48,48	0
58	MG	a	3486	1/1	0.91	0.19	38,38,38,38	0
58	MG	A	3043	1/1	0.91	0.16	59,59,59,59	0
58	MG	D	304	1/1	0.91	0.36	74,74,74,74	0
58	MG	A	3048	1/1	0.91	0.20	43,43,43,43	0
58	MG	A	3356	1/1	0.91	0.24	57,57,57,57	0
58	MG	A	3168	1/1	0.91	0.41	48,48,48,48	0
58	MG	A	3051	1/1	0.91	0.24	43,43,43,43	0
58	MG	a	3370	1/1	0.91	0.18	66,66,66,66	0
58	MG	A	3061	1/1	0.91	0.22	54,54,54,54	0
58	MG	A	3580	1/1	0.91	0.24	67,67,67,67	0
58	MG	a	3407	1/1	0.91	0.35	82,82,82,82	0
58	MG	A	3031	1/1	0.91	0.18	70,70,70,70	0
58	MG	A	3403	1/1	0.91	0.15	40,40,40,40	0
58	MG	A	3411	1/1	0.91	0.23	47,47,47,47	0
58	MG	A	3432	1/1	0.91	0.20	58,58,58,58	0
58	MG	a	3405	1/1	0.91	0.19	70,70,70,70	0
58	MG	A	3631	1/1	0.91	0.24	87,87,87,87	0
58	MG	A	3266	1/1	0.91	0.39	61,61,61,61	0
58	MG	W	201	1/1	0.91	1.28	77,77,77,77	0
58	MG	a	3433	1/1	0.91	0.12	32,32,32,32	0
58	MG	A	3452	1/1	0.91	0.27	53,53,53,53	0
58	MG	a	3376	1/1	0.91	0.20	46,46,46,46	0
58	MG	a	3308	1/1	0.91	0.21	41,41,41,41	0
58	MG	A	3546	1/1	0.91	0.32	53,53,53,53	0
58	MG	a	3319	1/1	0.91	0.38	39,39,39,39	0
58	MG	A	3019	1/1	0.92	0.28	49,49,49,49	0
58	MG	A	3036	1/1	0.92	0.11	74,74,74,74	0
58	MG	A	3581	1/1	0.92	0.14	55,55,55,55	0
58	MG	a	3424	1/1	0.92	0.11	43,43,43,43	0
58	MG	a	3339	1/1	0.92	0.24	50,50,50,50	0
58	MG	A	3591	1/1	0.92	0.13	66,66,66,66	0
58	MG	a	3326	1/1	0.92	0.21	48,48,48,48	0
58	MG	A	3590	1/1	0.92	0.13	59,59,59,59	0
58	MG	A	3159	1/1	0.92	0.13	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3398	1/1	0.92	0.26	43,43,43,43	0
58	MG	A	3613	1/1	0.92	0.17	52,52,52,52	0
58	MG	A	3341	1/1	0.92	0.33	57,57,57,57	0
58	MG	A	3487	1/1	0.92	0.23	60,60,60,60	0
58	MG	a	3364	1/1	0.92	0.43	56,56,56,56	0
58	MG	A	3441	1/1	0.92	0.14	73,73,73,73	0
58	MG	A	3504	1/1	0.92	0.37	38,38,38,38	0
58	MG	A	3227	1/1	0.92	0.44	43,43,43,43	0
58	MG	A	3365	1/1	0.92	0.14	51,51,51,51	0
58	MG	A	3136	1/1	0.92	0.39	49,49,49,49	0
58	MG	A	3004	1/1	0.92	0.22	55,55,55,55	0
58	MG	A	3497	1/1	0.92	0.26	50,50,50,50	0
58	MG	A	3505	1/1	0.92	0.18	68,68,68,68	0
58	MG	A	3204	1/1	0.92	0.25	43,43,43,43	0
58	MG	A	3201	1/1	0.92	0.20	63,63,63,63	0
58	MG	a	3461	1/1	0.92	0.15	44,44,44,44	0
58	MG	A	3575	1/1	0.92	0.09	70,70,70,70	0
58	MG	A	3508	1/1	0.92	0.13	46,46,46,46	0
58	MG	A	3323	1/1	0.92	0.15	42,42,42,42	0
58	MG	A	3567	1/1	0.92	0.17	47,47,47,47	0
58	MG	A	3099	1/1	0.92	0.20	34,34,34,34	0
58	MG	A	3146	1/1	0.92	0.27	56,56,56,56	0
58	MG	A	3076	1/1	0.92	0.19	41,41,41,41	0
58	MG	A	3345	1/1	0.92	0.19	44,44,44,44	0
58	MG	e	201	1/1	0.92	0.15	69,69,69,69	0
58	MG	A	3407	1/1	0.92	0.10	38,38,38,38	0
58	MG	A	3006	1/1	0.92	0.60	57,57,57,57	0
58	MG	A	3425	1/1	0.92	0.23	62,62,62,62	0
58	MG	A	3594	1/1	0.92	0.19	37,37,37,37	0
58	MG	A	3232	1/1	0.92	0.30	36,36,36,36	0
58	MG	A	3625	1/1	0.92	0.19	84,84,84,84	0
58	MG	A	3466	1/1	0.92	0.08	67,67,67,67	0
58	MG	A	3196	1/1	0.92	0.18	44,44,44,44	0
58	MG	A	3415	1/1	0.92	0.27	42,42,42,42	0
58	MG	A	3138	1/1	0.92	0.21	77,77,77,77	0
58	MG	A	3393	1/1	0.92	0.32	57,57,57,57	0
58	MG	A	3627	1/1	0.92	0.14	91,91,91,91	0
58	MG	E	303	1/1	0.92	0.19	41,41,41,41	0
58	MG	a	3462	1/1	0.92	0.13	74,74,74,74	0
58	MG	A	3217	1/1	0.92	0.39	50,50,50,50	0
58	MG	a	3420	1/1	0.92	0.17	62,62,62,62	0
58	MG	F	302	1/1	0.92	0.81	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3130	1/1	0.92	0.47	43,43,43,43	0
58	MG	A	3336	1/1	0.92	0.22	36,36,36,36	0
58	MG	A	3214	1/1	0.92	0.41	52,52,52,52	0
58	MG	A	3482	1/1	0.92	0.09	67,67,67,67	0
58	MG	A	3361	1/1	0.92	0.12	84,84,84,84	0
58	MG	A	3158	1/1	0.93	0.50	97,97,97,97	0
58	MG	A	3111	1/1	0.93	0.51	61,61,61,61	0
58	MG	a	3437	1/1	0.93	0.15	54,54,54,54	0
58	MG	a	3345	1/1	0.93	0.22	47,47,47,47	0
58	MG	a	3331	1/1	0.93	0.24	55,55,55,55	0
58	MG	a	3356	1/1	0.93	0.22	49,49,49,49	0
58	MG	A	3016	1/1	0.93	0.14	49,49,49,49	0
58	MG	A	3313	1/1	0.93	0.17	44,44,44,44	0
58	MG	A	3595	1/1	0.93	0.15	63,63,63,63	0
58	MG	A	3621	1/1	0.93	0.30	59,59,59,59	0
58	MG	a	3349	1/1	0.93	0.37	47,47,47,47	0
58	MG	a	3354	1/1	0.93	0.13	51,51,51,51	0
58	MG	A	3428	1/1	0.93	0.15	36,36,36,36	0
58	MG	A	3325	1/1	0.93	0.28	52,52,52,52	0
58	MG	A	3271	1/1	0.93	0.16	57,57,57,57	0
61	GDP	y	703	28/28	0.93	0.15	91,120,142,146	0
58	MG	a	3401	1/1	0.93	0.38	44,44,44,44	0
58	MG	a	3481	1/1	0.93	0.27	46,46,46,46	0
58	MG	A	3392	1/1	0.93	0.22	47,47,47,47	0
58	MG	A	3610	1/1	0.93	0.22	61,61,61,61	0
58	MG	A	3221	1/1	0.93	0.49	58,58,58,58	0
58	MG	A	3584	1/1	0.93	0.25	62,62,62,62	0
58	MG	a	3470	1/1	0.93	0.15	56,56,56,56	0
58	MG	F	303	1/1	0.93	0.11	36,36,36,36	0
58	MG	A	3542	1/1	0.93	0.66	60,60,60,60	0
58	MG	A	3080	1/1	0.93	0.31	54,54,54,54	0
58	MG	a	3445	1/1	0.93	0.20	66,66,66,66	0
58	MG	A	3449	1/1	0.93	0.23	51,51,51,51	0
58	MG	w	105	1/1	0.93	0.23	29,29,29,29	0
58	MG	A	3442	1/1	0.93	0.19	56,56,56,56	0
58	MG	A	3301	1/1	0.93	0.17	57,57,57,57	0
58	MG	9	101	1/1	0.93	0.30	57,57,57,57	0
58	MG	A	3082	1/1	0.93	0.64	53,53,53,53	0
58	MG	A	3024	1/1	0.93	0.15	63,63,63,63	0
58	MG	a	3463	1/1	0.93	0.21	45,45,45,45	0
58	MG	A	3327	1/1	0.93	0.14	49,49,49,49	0
58	MG	U	201	1/1	0.93	0.38	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3125	1/1	0.93	0.29	31,31,31,31	0
58	MG	A	3091	1/1	0.93	0.21	63,63,63,63	0
58	MG	a	3435	1/1	0.93	0.19	57,57,57,57	0
58	MG	A	3203	1/1	0.93	0.19	53,53,53,53	0
58	MG	A	3137	1/1	0.93	0.48	59,59,59,59	0
58	MG	a	3429	1/1	0.93	0.14	49,49,49,49	0
58	MG	a	3427	1/1	0.93	0.26	50,50,50,50	0
58	MG	A	3202	1/1	0.93	0.37	50,50,50,50	0
58	MG	A	3211	1/1	0.93	0.47	55,55,55,55	0
58	MG	a	3333	1/1	0.93	0.16	51,51,51,51	0
58	MG	A	3506	1/1	0.93	0.13	49,49,49,49	0
58	MG	A	3484	1/1	0.93	0.14	50,50,50,50	0
58	MG	A	3007	1/1	0.93	0.27	46,46,46,46	0
58	MG	0	103	1/1	0.93	0.19	61,61,61,61	0
58	MG	A	3154	1/1	0.93	0.18	60,60,60,60	0
58	MG	A	3404	1/1	0.93	0.20	57,57,57,57	0
58	MG	a	3408	1/1	0.93	0.12	55,55,55,55	0
58	MG	A	3027	1/1	0.93	0.24	44,44,44,44	0
58	MG	A	3469	1/1	0.93	0.12	54,54,54,54	0
58	MG	A	3140	1/1	0.93	0.16	57,57,57,57	0
58	MG	A	3153	1/1	0.93	0.22	82,82,82,82	0
58	MG	a	3431	1/1	0.93	0.10	41,41,41,41	0
58	MG	A	3096	1/1	0.93	0.23	58,58,58,58	0
58	MG	A	3439	1/1	0.93	0.18	58,58,58,58	0
58	MG	a	3301	1/1	0.93	0.23	49,49,49,49	0
58	MG	a	3411	1/1	0.93	0.16	53,53,53,53	0
58	MG	8	101	1/1	0.93	0.12	66,66,66,66	0
58	MG	A	3454	1/1	0.93	0.50	51,51,51,51	0
58	MG	A	3172	1/1	0.93	0.32	31,31,31,31	0
58	MG	A	3022	1/1	0.93	0.28	33,33,33,33	0
58	MG	a	3384	1/1	0.94	0.14	49,49,49,49	0
58	MG	A	3427	1/1	0.94	0.16	62,62,62,62	0
58	MG	A	3342	1/1	0.94	0.16	61,61,61,61	0
58	MG	B	204	1/1	0.94	0.15	85,85,85,85	0
58	MG	A	3552	1/1	0.94	0.18	64,64,64,64	0
58	MG	a	3422	1/1	0.94	0.32	50,50,50,50	0
58	MG	a	3337	1/1	0.94	0.26	50,50,50,50	0
58	MG	A	3315	1/1	0.94	0.27	56,56,56,56	0
58	MG	A	3210	1/1	0.94	0.20	56,56,56,56	0
58	MG	a	3477	1/1	0.94	0.12	68,68,68,68	0
58	MG	a	3342	1/1	0.94	0.46	50,50,50,50	0
58	MG	U	202	1/1	0.94	0.35	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	a	3469	1/1	0.94	0.38	42,42,42,42	0
58	MG	Q	201	1/1	0.94	0.50	51,51,51,51	0
58	MG	A	3401	1/1	0.94	0.11	37,37,37,37	0
58	MG	A	3382	1/1	0.94	0.24	36,36,36,36	0
58	MG	A	3311	1/1	0.94	0.28	52,52,52,52	0
58	MG	A	3065	1/1	0.94	0.25	74,74,74,74	0
59	ZN	5	102	1/1	0.94	0.08	70,70,70,70	0
58	MG	A	3289	1/1	0.94	0.15	43,43,43,43	0
58	MG	A	3316	1/1	0.94	0.30	47,47,47,47	0
58	MG	A	3167	1/1	0.94	0.54	65,65,65,65	0
58	MG	a	3442	1/1	0.94	0.08	45,45,45,45	0
58	MG	A	3545	1/1	0.94	0.23	64,64,64,64	0
58	MG	A	3333	1/1	0.94	0.08	62,62,62,62	0
58	MG	a	3304	1/1	0.94	0.10	55,55,55,55	0
58	MG	A	3026	1/1	0.94	0.09	55,55,55,55	0
58	MG	A	3629	1/1	0.94	0.20	70,70,70,70	0
58	MG	A	3450	1/1	0.94	0.17	57,57,57,57	0
58	MG	w	103	1/1	0.94	0.18	38,38,38,38	0
58	MG	A	3524	1/1	0.94	0.12	53,53,53,53	0
58	MG	A	3456	1/1	0.94	0.29	47,47,47,47	0
58	MG	A	3295	1/1	0.94	0.27	30,30,30,30	0
58	MG	A	3402	1/1	0.94	0.09	50,50,50,50	0
58	MG	A	3363	1/1	0.94	0.18	30,30,30,30	0
58	MG	A	3446	1/1	0.94	0.29	39,39,39,39	0
58	MG	a	3320	1/1	0.94	0.14	39,39,39,39	0
58	MG	A	3486	1/1	0.94	0.23	40,40,40,40	0
58	MG	a	3351	1/1	0.94	0.18	36,36,36,36	0
58	MG	R	202	1/1	0.94	0.29	53,53,53,53	0
58	MG	G	203	1/1	0.94	0.09	69,69,69,69	0
58	MG	a	3302	1/1	0.94	0.25	58,58,58,58	0
58	MG	A	3047	1/1	0.94	0.19	39,39,39,39	0
58	MG	a	3467	1/1	0.94	0.16	62,62,62,62	0
58	MG	A	3331	1/1	0.94	0.12	54,54,54,54	0
58	MG	a	3441	1/1	0.94	0.19	62,62,62,62	0
58	MG	A	3149	1/1	0.94	0.18	53,53,53,53	0
58	MG	A	3472	1/1	0.94	0.17	53,53,53,53	0
58	MG	A	3462	1/1	0.94	0.12	53,53,53,53	0
58	MG	A	3302	1/1	0.94	0.34	59,59,59,59	0
58	MG	E	302	1/1	0.94	0.13	35,35,35,35	0
58	MG	A	3033	1/1	0.94	0.18	39,39,39,39	0
58	MG	A	3622	1/1	0.94	0.24	49,49,49,49	0
58	MG	A	3310	1/1	0.94	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	a	3363	1/1	0.94	0.24	43,43,43,43	0
58	MG	A	3147	1/1	0.94	0.22	64,64,64,64	0
58	MG	A	3241	1/1	0.94	0.15	42,42,42,42	0
58	MG	A	3531	1/1	0.94	0.07	91,91,91,91	0
58	MG	A	3476	1/1	0.94	0.30	50,50,50,50	0
58	MG	a	3387	1/1	0.94	0.08	55,55,55,55	0
58	MG	A	3028	1/1	0.94	0.27	66,66,66,66	0
58	MG	a	3457	1/1	0.94	0.33	41,41,41,41	0
58	MG	a	3476	1/1	0.94	0.10	50,50,50,50	0
58	MG	A	3279	1/1	0.94	0.14	55,55,55,55	0
58	MG	A	3379	1/1	0.94	0.25	50,50,50,50	0
58	MG	A	3558	1/1	0.94	0.15	73,73,73,73	0
58	MG	A	3371	1/1	0.94	0.11	53,53,53,53	0
58	MG	A	3380	1/1	0.94	0.20	52,52,52,52	0
58	MG	A	3489	1/1	0.94	0.12	55,55,55,55	0
58	MG	A	3628	1/1	0.94	0.16	87,87,87,87	0
58	MG	a	3446	1/1	0.94	0.18	68,68,68,68	0
58	MG	A	3529	1/1	0.94	0.25	56,56,56,56	0
58	MG	A	3041	1/1	0.94	0.24	42,42,42,42	0
58	MG	a	3466	1/1	0.94	0.18	60,60,60,60	0
58	MG	m	201	1/1	0.94	0.20	35,35,35,35	0
58	MG	A	3258	1/1	0.94	0.21	43,43,43,43	0
58	MG	a	3372	1/1	0.94	0.30	47,47,47,47	0
58	MG	a	3485	1/1	0.94	0.25	51,51,51,51	0
58	MG	A	3620	1/1	0.94	0.31	49,49,49,49	0
58	MG	A	3477	1/1	0.95	0.14	65,65,65,65	0
58	MG	A	3359	1/1	0.95	0.13	45,45,45,45	0
58	MG	A	3453	1/1	0.95	0.15	44,44,44,44	0
58	MG	A	3618	1/1	0.95	0.29	45,45,45,45	0
58	MG	A	3180	1/1	0.95	0.65	44,44,44,44	0
58	MG	A	3098	1/1	0.95	0.16	48,48,48,48	0
58	MG	a	3389	1/1	0.95	0.11	38,38,38,38	0
58	MG	A	3133	1/1	0.95	0.49	44,44,44,44	0
58	MG	A	3035	1/1	0.95	0.09	47,47,47,47	0
59	ZN	4	501	1/1	0.95	0.06	117,117,117,117	0
58	MG	A	3475	1/1	0.95	0.07	55,55,55,55	0
58	MG	A	3539	1/1	0.95	0.14	52,52,52,52	0
58	MG	A	3559	1/1	0.95	0.22	46,46,46,46	0
58	MG	A	3228	1/1	0.95	0.19	62,62,62,62	0
58	MG	A	3300	1/1	0.95	0.17	60,60,60,60	0
58	MG	A	3105	1/1	0.95	0.11	35,35,35,35	0
58	MG	A	3344	1/1	0.95	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	a	3386	1/1	0.95	0.47	41,41,41,41	0
58	MG	A	3550	1/1	0.95	0.13	58,58,58,58	0
58	MG	A	3200	1/1	0.95	0.18	44,44,44,44	0
58	MG	A	3088	1/1	0.95	0.15	63,63,63,63	0
58	MG	A	3623	1/1	0.95	0.20	52,52,52,52	0
58	MG	A	3280	1/1	0.95	0.28	32,32,32,32	0
58	MG	A	3206	1/1	0.95	0.14	65,65,65,65	0
58	MG	A	3218	1/1	0.95	0.45	32,32,32,32	0
58	MG	A	3189	1/1	0.95	0.31	37,37,37,37	0
58	MG	a	3416	1/1	0.95	0.25	61,61,61,61	0
58	MG	A	3351	1/1	0.95	0.20	38,38,38,38	0
58	MG	A	3222	1/1	0.95	0.20	33,33,33,33	0
58	MG	A	3274	1/1	0.95	0.47	45,45,45,45	0
58	MG	A	3420	1/1	0.95	0.20	31,31,31,31	0
58	MG	A	3384	1/1	0.95	0.23	51,51,51,51	0
58	MG	7	101	1/1	0.95	0.72	48,48,48,48	0
58	MG	A	3314	1/1	0.95	0.24	54,54,54,54	0
58	MG	a	3365	1/1	0.95	0.74	45,45,45,45	0
58	MG	a	3430	1/1	0.95	0.08	65,65,65,65	0
58	MG	A	3205	1/1	0.95	0.12	43,43,43,43	0
58	MG	A	3303	1/1	0.95	0.07	55,55,55,55	0
58	MG	a	3464	1/1	0.95	0.07	44,44,44,44	0
58	MG	A	3394	1/1	0.95	0.20	30,30,30,30	0
58	MG	B	212	1/1	0.95	0.18	75,75,75,75	0
58	MG	A	3208	1/1	0.95	0.27	40,40,40,40	0
58	MG	B	201	1/1	0.95	0.33	51,51,51,51	0
58	MG	a	3456	1/1	0.95	0.19	59,59,59,59	0
58	MG	a	3311	1/1	0.95	0.20	51,51,51,51	0
58	MG	A	3368	1/1	0.95	0.23	47,47,47,47	0
58	MG	A	3474	1/1	0.95	0.13	51,51,51,51	0
58	MG	w	106	1/1	0.95	0.17	45,45,45,45	0
58	MG	A	3083	1/1	0.95	0.07	37,37,37,37	0
58	MG	A	3390	1/1	0.95	0.24	46,46,46,46	0
58	MG	A	3348	1/1	0.95	0.19	71,71,71,71	0
58	MG	B	218	1/1	0.95	0.22	74,74,74,74	0
58	MG	A	3582	1/1	0.95	0.14	63,63,63,63	0
58	MG	a	3444	1/1	0.95	0.16	53,53,53,53	0
58	MG	l	202	1/1	0.95	0.33	61,61,61,61	0
58	MG	A	3455	1/1	0.95	0.22	73,73,73,73	0
58	MG	A	3604	1/1	0.95	0.35	64,64,64,64	0
58	MG	a	3414	1/1	0.95	0.20	50,50,50,50	0
58	MG	A	3257	1/1	0.95	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3151	1/1	0.95	0.29	43,43,43,43	0
58	MG	A	3553	1/1	0.95	0.08	40,40,40,40	0
58	MG	A	3123	1/1	0.95	0.17	51,51,51,51	0
58	MG	A	3634	1/1	0.95	0.14	56,56,56,56	0
58	MG	A	3164	1/1	0.95	0.19	51,51,51,51	0
58	MG	a	3375	1/1	0.96	0.57	41,41,41,41	0
58	MG	A	3534	1/1	0.96	0.36	45,45,45,45	0
58	MG	A	3527	1/1	0.96	0.20	63,63,63,63	0
58	MG	A	3155	1/1	0.96	0.28	44,44,44,44	0
58	MG	A	3307	1/1	0.96	0.21	45,45,45,45	0
58	MG	A	3412	1/1	0.96	0.22	45,45,45,45	0
58	MG	A	3566	1/1	0.96	0.11	40,40,40,40	0
58	MG	a	3404	1/1	0.96	0.44	38,38,38,38	0
58	MG	A	3548	1/1	0.96	0.14	40,40,40,40	0
58	MG	A	3561	1/1	0.96	0.14	54,54,54,54	0
58	MG	A	3501	1/1	0.96	0.26	46,46,46,46	0
58	MG	A	3540	1/1	0.96	0.22	55,55,55,55	0
58	MG	A	3267	1/1	0.96	0.28	59,59,59,59	0
58	MG	A	3385	1/1	0.96	0.19	57,57,57,57	0
58	MG	A	3422	1/1	0.96	0.18	52,52,52,52	0
58	MG	A	3381	1/1	0.96	0.24	43,43,43,43	0
58	MG	a	3399	1/1	0.96	0.18	36,36,36,36	0
58	MG	A	3166	1/1	0.96	0.30	57,57,57,57	0
58	MG	A	3557	1/1	0.96	0.33	60,60,60,60	0
58	MG	A	3156	1/1	0.96	0.08	86,86,86,86	0
58	MG	A	3234	1/1	0.96	0.36	48,48,48,48	0
58	MG	A	3163	1/1	0.96	0.16	34,34,34,34	0
58	MG	A	3522	1/1	0.96	0.17	51,51,51,51	0
58	MG	A	3473	1/1	0.96	0.15	46,46,46,46	0
58	MG	A	3128	1/1	0.96	0.19	45,45,45,45	0
58	MG	a	3452	1/1	0.96	0.11	52,52,52,52	0
58	MG	a	3367	1/1	0.96	0.25	30,30,30,30	0
58	MG	A	3115	1/1	0.96	0.12	48,48,48,48	0
58	MG	A	3071	1/1	0.96	0.22	41,41,41,41	0
58	MG	A	3070	1/1	0.96	0.11	57,57,57,57	0
58	MG	a	3378	1/1	0.96	0.24	39,39,39,39	0
58	MG	A	3324	1/1	0.96	0.21	43,43,43,43	0
58	MG	w	104	1/1	0.96	0.09	38,38,38,38	0
58	MG	A	3597	1/1	0.96	0.28	65,65,65,65	0
58	MG	a	3347	1/1	0.96	0.23	41,41,41,41	0
58	MG	A	3492	1/1	0.96	0.10	62,62,62,62	0
58	MG	A	3187	1/1	0.96	0.44	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3219	1/1	0.96	0.11	61,61,61,61	0
58	MG	A	3499	1/1	0.96	0.10	60,60,60,60	0
58	MG	B	203	1/1	0.96	0.07	56,56,56,56	0
58	MG	A	3587	1/1	0.96	0.25	48,48,48,48	0
58	MG	A	3468	1/1	0.96	0.13	48,48,48,48	0
58	MG	A	3190	1/1	0.96	0.30	38,38,38,38	0
58	MG	A	3445	1/1	0.96	0.08	51,51,51,51	0
58	MG	A	3500	1/1	0.96	0.29	40,40,40,40	0
58	MG	A	3318	1/1	0.96	0.32	60,60,60,60	0
58	MG	A	3541	1/1	0.96	0.26	56,56,56,56	0
58	MG	a	3309	1/1	0.96	0.81	37,37,37,37	0
58	MG	A	3292	1/1	0.96	0.24	54,54,54,54	0
58	MG	A	3496	1/1	0.96	0.17	47,47,47,47	0
58	MG	B	205	1/1	0.96	0.21	81,81,81,81	0
58	MG	A	3349	1/1	0.96	0.27	39,39,39,39	0
58	MG	A	3536	1/1	0.96	0.21	39,39,39,39	0
58	MG	A	3503	1/1	0.96	0.21	41,41,41,41	0
58	MG	a	3432	1/1	0.96	0.09	46,46,46,46	0
58	MG	A	3510	1/1	0.96	0.15	60,60,60,60	0
58	MG	A	3547	1/1	0.96	0.20	60,60,60,60	0
58	MG	A	3077	1/1	0.96	0.13	48,48,48,48	0
58	MG	A	3090	1/1	0.96	0.39	38,38,38,38	0
58	MG	a	3338	1/1	0.96	0.17	66,66,66,66	0
58	MG	A	3317	1/1	0.96	0.20	31,31,31,31	0
58	MG	A	3387	1/1	0.96	0.18	53,53,53,53	0
58	MG	A	3012	1/1	0.96	0.16	37,37,37,37	0
58	MG	a	3417	1/1	0.96	0.31	37,37,37,37	0
58	MG	A	3417	1/1	0.96	0.20	30,30,30,30	0
58	MG	A	3440	1/1	0.96	0.20	74,74,74,74	0
58	MG	R	203	1/1	0.96	0.25	44,44,44,44	0
58	MG	a	3475	1/1	0.96	0.38	38,38,38,38	0
58	MG	A	3556	1/1	0.96	0.15	55,55,55,55	0
58	MG	A	3116	1/1	0.96	0.34	50,50,50,50	0
58	MG	A	3321	1/1	0.96	0.09	41,41,41,41	0
58	MG	A	3599	1/1	0.96	0.22	57,57,57,57	0
58	MG	a	3344	1/1	0.96	0.12	51,51,51,51	0
58	MG	A	3358	1/1	0.96	0.18	63,63,63,63	0
58	MG	A	3632	1/1	0.96	0.27	63,63,63,63	0
58	MG	A	3470	1/1	0.97	0.17	43,43,43,43	0
58	MG	A	3593	1/1	0.97	0.30	41,41,41,41	0
58	MG	A	3169	1/1	0.97	0.30	57,57,57,57	0
58	MG	a	3465	1/1	0.97	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3372	1/1	0.97	0.17	59,59,59,59	0
58	MG	A	3229	1/1	0.97	0.13	46,46,46,46	0
58	MG	A	3535	1/1	0.97	0.22	49,49,49,49	0
58	MG	A	3364	1/1	0.97	0.16	61,61,61,61	0
59	ZN	Y	501	1/1	0.97	0.08	92,92,92,92	0
58	MG	A	3049	1/1	0.97	0.19	41,41,41,41	0
58	MG	A	3362	1/1	0.97	0.18	50,50,50,50	0
58	MG	A	3579	1/1	0.97	0.19	53,53,53,53	0
58	MG	a	3412	1/1	0.97	0.11	48,48,48,48	0
58	MG	A	3633	1/1	0.97	0.30	64,64,64,64	0
58	MG	a	3482	1/1	0.97	0.14	37,37,37,37	0
58	MG	A	3457	1/1	0.97	0.20	41,41,41,41	0
58	MG	a	3448	1/1	0.97	0.07	42,42,42,42	0
58	MG	a	3415	1/1	0.97	0.20	62,62,62,62	0
58	MG	A	3369	1/1	0.97	0.16	54,54,54,54	0
58	MG	A	3338	1/1	0.97	0.28	30,30,30,30	0
58	MG	a	3473	1/1	0.97	0.45	43,43,43,43	0
58	MG	A	3459	1/1	0.97	0.18	36,36,36,36	0
58	MG	A	3283	1/1	0.97	0.12	55,55,55,55	0
58	MG	A	3225	1/1	0.97	0.26	36,36,36,36	0
58	MG	a	3307	1/1	0.97	0.14	35,35,35,35	0
59	ZN	9	102	1/1	0.97	0.10	72,72,72,72	0
58	MG	a	3453	1/1	0.97	0.07	41,41,41,41	0
58	MG	a	3460	1/1	0.97	0.14	52,52,52,52	0
58	MG	A	3396	1/1	0.97	0.24	38,38,38,38	0
58	MG	A	3296	1/1	0.97	0.36	52,52,52,52	0
58	MG	A	3526	1/1	0.97	0.10	41,41,41,41	0
58	MG	A	3409	1/1	0.97	0.25	60,60,60,60	0
58	MG	A	3438	1/1	0.97	0.12	53,53,53,53	0
58	MG	A	3306	1/1	0.97	0.18	50,50,50,50	0
58	MG	a	3382	1/1	0.97	0.21	31,31,31,31	0
58	MG	D	301	1/1	0.97	0.29	41,41,41,41	0
58	MG	a	3355	1/1	0.97	0.20	39,39,39,39	0
58	MG	A	3538	1/1	0.97	0.16	40,40,40,40	0
58	MG	A	3519	1/1	0.97	0.30	30,30,30,30	0
58	MG	A	3100	1/1	0.97	0.13	45,45,45,45	0
58	MG	A	3458	1/1	0.97	0.32	27,27,27,27	0
58	MG	A	3389	1/1	0.97	0.25	30,30,30,30	0
58	MG	a	3439	1/1	0.97	0.21	48,48,48,48	0
58	MG	a	3381	1/1	0.97	0.18	55,55,55,55	0
58	MG	A	3612	1/1	0.97	0.05	53,53,53,53	0
58	MG	A	3485	1/1	0.97	0.22	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3178	1/1	0.97	0.23	31,31,31,31	0
58	MG	a	3478	1/1	0.97	0.14	48,48,48,48	0
58	MG	A	3055	1/1	0.97	0.12	45,45,45,45	0
58	MG	A	3340	1/1	0.97	0.23	65,65,65,65	0
58	MG	A	3509	1/1	0.97	0.25	51,51,51,51	0
58	MG	A	3337	1/1	0.97	0.27	44,44,44,44	0
58	MG	A	3144	1/1	0.97	0.32	38,38,38,38	0
58	MG	A	3400	1/1	0.97	0.09	35,35,35,35	0
58	MG	A	3630	1/1	0.97	0.18	43,43,43,43	0
58	MG	a	3449	1/1	0.97	0.21	50,50,50,50	0
58	MG	a	3443	1/1	0.97	0.06	46,46,46,46	0
58	MG	a	3398	1/1	0.97	0.39	27,27,27,27	0
58	MG	a	3317	1/1	0.97	0.31	26,26,26,26	0
58	MG	U	204	1/1	0.97	0.14	37,37,37,37	0
58	MG	A	3230	1/1	0.97	0.24	46,46,46,46	0
58	MG	A	3320	1/1	0.97	0.12	49,49,49,49	0
58	MG	a	3479	1/1	0.97	0.18	47,47,47,47	0
58	MG	a	3397	1/1	0.97	0.39	27,27,27,27	0
58	MG	A	3447	1/1	0.97	0.21	67,67,67,67	0
58	MG	a	3312	1/1	0.97	0.07	26,26,26,26	0
58	MG	O	201	1/1	0.97	0.09	38,38,38,38	0
59	ZN	6	102	1/1	0.97	0.09	70,70,70,70	0
58	MG	A	3583	1/1	0.97	0.10	55,55,55,55	0
58	MG	A	3609	1/1	0.97	0.14	39,39,39,39	0
58	MG	A	3424	1/1	0.97	0.27	57,57,57,57	0
58	MG	A	3437	1/1	0.97	0.20	28,28,28,28	0
58	MG	A	3494	1/1	0.97	0.17	42,42,42,42	0
58	MG	A	3391	1/1	0.97	0.21	30,30,30,30	0
58	MG	A	3592	1/1	0.97	0.09	67,67,67,67	0
58	MG	a	3322	1/1	0.97	0.09	50,50,50,50	0
58	MG	A	3488	1/1	0.97	0.31	50,50,50,50	0
58	MG	A	3626	1/1	0.97	0.14	51,51,51,51	0
58	MG	a	3471	1/1	0.97	0.27	49,49,49,49	0
58	MG	a	3447	1/1	0.98	0.41	36,36,36,36	0
58	MG	a	3487	1/1	0.98	0.32	35,35,35,35	0
58	MG	a	3379	1/1	0.98	0.21	30,30,30,30	0
58	MG	n	101	1/1	0.98	0.25	42,42,42,42	0
58	MG	A	3537	1/1	0.98	0.18	32,32,32,32	0
59	ZN	n	102	1/1	0.98	0.15	61,61,61,61	0
58	MG	a	3343	1/1	0.98	0.16	29,29,29,29	0
58	MG	A	3179	1/1	0.98	0.18	43,43,43,43	0
58	MG	A	3191	1/1	0.98	0.36	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3170	1/1	0.98	0.23	43,43,43,43	0
58	MG	A	3523	1/1	0.98	0.23	36,36,36,36	0
58	MG	y	702	1/1	0.98	0.18	75,75,75,75	0
58	MG	a	3395	1/1	0.98	0.30	32,32,32,32	0
58	MG	A	3413	1/1	0.98	0.25	51,51,51,51	0
58	MG	A	3483	1/1	0.98	0.18	55,55,55,55	0
58	MG	A	3176	1/1	0.98	0.10	35,35,35,35	0
58	MG	A	3233	1/1	0.98	0.17	53,53,53,53	0
58	MG	A	3249	1/1	0.98	0.11	31,31,31,31	0
58	MG	A	3443	1/1	0.98	0.14	39,39,39,39	0
58	MG	A	3518	1/1	0.98	0.04	65,65,65,65	0
58	MG	A	3377	1/1	0.98	0.17	44,44,44,44	0
58	MG	A	3015	1/1	0.98	0.20	43,43,43,43	0
58	MG	A	3184	1/1	0.98	0.39	40,40,40,40	0
58	MG	A	3418	1/1	0.98	0.38	32,32,32,32	0
58	MG	a	3318	1/1	0.98	0.24	41,41,41,41	0
58	MG	A	3399	1/1	0.98	0.28	29,29,29,29	0
58	MG	A	3528	1/1	0.98	0.09	51,51,51,51	0
58	MG	A	3421	1/1	0.98	0.18	40,40,40,40	0
58	MG	A	3183	1/1	0.98	0.19	54,54,54,54	0
58	MG	A	3188	1/1	0.98	0.32	44,44,44,44	0
58	MG	A	3256	1/1	0.98	0.15	55,55,55,55	0
58	MG	A	3460	1/1	0.98	0.20	44,44,44,44	0
58	MG	A	3238	1/1	0.98	0.27	45,45,45,45	0
58	MG	A	3429	1/1	0.98	0.24	30,30,30,30	0
58	MG	A	3332	1/1	0.98	0.20	39,39,39,39	0
58	MG	A	3195	1/1	0.98	0.23	41,41,41,41	0
58	MG	A	3480	1/1	0.98	0.15	35,35,35,35	0
58	MG	A	3416	1/1	0.98	0.21	41,41,41,41	0
58	MG	A	3495	1/1	0.98	0.25	40,40,40,40	0
58	MG	A	3021	1/1	0.98	0.18	34,34,34,34	0
58	MG	A	3329	1/1	0.98	0.14	40,40,40,40	0
58	MG	a	3374	1/1	0.98	0.41	30,30,30,30	0
58	MG	a	3394	1/1	0.98	0.19	32,32,32,32	0
58	MG	A	3127	1/1	0.98	0.14	73,73,73,73	0
58	MG	A	3194	1/1	0.98	0.34	34,34,34,34	0
58	MG	A	3588	1/1	0.98	0.17	40,40,40,40	0
58	MG	A	3530	1/1	0.99	0.25	38,38,38,38	0
58	MG	a	3305	1/1	0.99	0.19	46,46,46,46	0
58	MG	a	3402	1/1	0.99	0.19	43,43,43,43	0
58	MG	A	3017	1/1	0.99	0.11	63,63,63,63	0
58	MG	A	3193	1/1	0.99	0.22	38,38,38,38	0

*Continued on next page...*

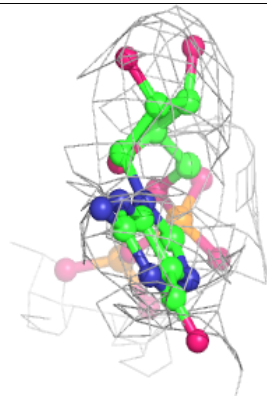
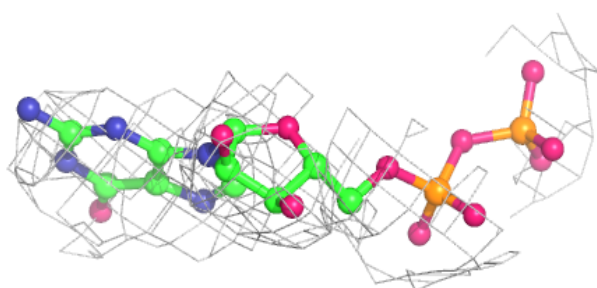
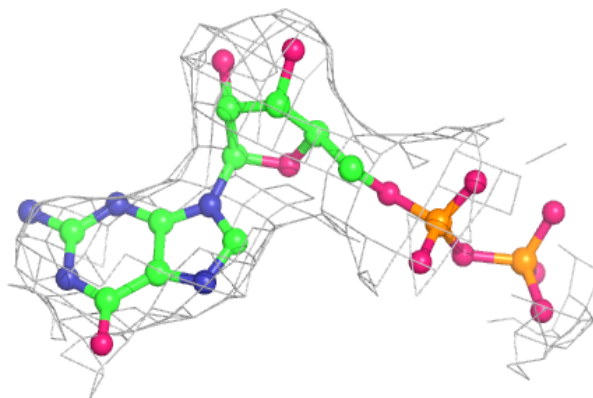
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A	3521	1/1	0.99	0.22	60,60,60,60	0
58	MG	a	3483	1/1	0.99	0.18	39,39,39,39	0
58	MG	A	3378	1/1	0.99	0.19	31,31,31,31	0
58	MG	A	3192	1/1	0.99	0.28	39,39,39,39	0
58	MG	A	3395	1/1	0.99	0.12	31,31,31,31	0
58	MG	a	3406	1/1	0.99	0.21	52,52,52,52	0
60	SF4	d	501	8/8	0.99	0.16	48,60,64,65	0
58	MG	A	3094	1/1	0.99	0.27	31,31,31,31	0
58	MG	A	3513	1/1	0.99	0.29	41,41,41,41	0
58	MG	a	3438	1/1	0.99	0.16	34,34,34,34	0
58	MG	w	102	1/1	0.99	0.30	49,49,49,49	0
58	MG	B	202	1/1	0.99	0.27	66,66,66,66	0
58	MG	A	3038	1/1	0.99	0.15	55,55,55,55	0

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

**Electron density around GDP y 703:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.