



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2020 – 01:29 pm BST

PDB ID : 5J8B  
Title : Crystal structure of Elongation Factor 4 (EF-4/LepA) in complex with  
GDP-CP bound to the Thermus thermophilus 70S ribosome  
Authors : Gagnon, M.G.; Lin, J.; Steitz, T.A.  
Deposited on : 2016-04-07  
Resolution : 2.60 Å (reported)

This is a 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 : 2.11  
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) : 2.11

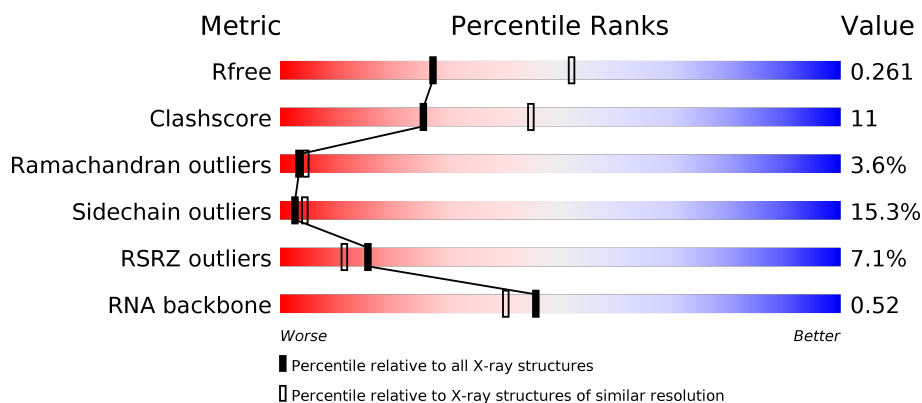
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>5%</div> <div>56%</div> <div>32%</div> <div>9%</div> <div>••</div> </div>
2	B	121	<div> <div>62%</div> <div>32%</div> <div>5%</div> <div>•</div> </div>
3	C	228	<div> <div>26%</div> <div>22%</div> <div>29%</div> <div>8%</div> <div>40%</div> </div>
4	D	276	<div> <div>68%</div> <div>25%</div> <div>7%</div> </div>





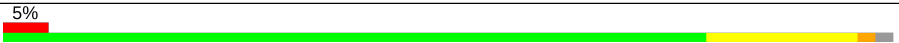
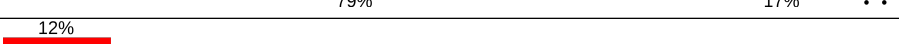




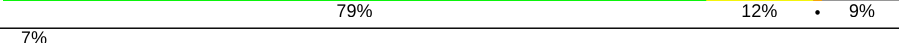











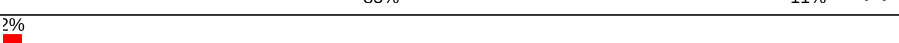


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Mol	Chain	Length	Quality of chain
5	E	206	
6	F	210	
7	G	182	
8	H	180	
9	J	173	
10	K	147	
11	N	140	
12	O	122	
13	P	150	
14	Q	141	
15	R	118	
16	S	112	
17	T	146	
18	U	118	
19	V	101	
20	W	113	
21	X	96	
22	Y	110	
23	Z	206	
24	0	85	
25	1	98	
26	2	72	
27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

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Mol	Chain	Length	Quality of chain
30	6	54	
31	7	49	
32	8	65	
33	9	37	
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	

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Mol	Chain	Length	Quality of chain
55	v	24	
56	w	76	
57	x	77	
58	y	76	
59	z	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
56	5MU	w	54	-	-	-	X
60	MG	A	3004	-	-	-	X
60	MG	A	3050	-	-	-	X
60	MG	A	3094	-	-	-	X
60	MG	A	3100	-	-	-	X
60	MG	A	3144	-	-	-	X
60	MG	A	3157	-	-	-	X
60	MG	A	3169	-	-	-	X
60	MG	A	3217	-	-	-	X
60	MG	A	3223	-	-	-	X
60	MG	A	3234	-	-	-	X
60	MG	A	3236	-	-	-	X
60	MG	A	3237	-	-	-	X
60	MG	A	3242	-	-	-	X
60	MG	A	3267	-	-	-	X
60	MG	A	3277	-	-	-	X
60	MG	A	3283	-	-	-	X
60	MG	A	3391	-	-	-	X
60	MG	A	3573	-	-	-	X
60	MG	A	3577	-	-	-	X
60	MG	A	3586	-	-	-	X
60	MG	A	3624	-	-	-	X
60	MG	B	201	-	-	-	X
60	MG	V	202	-	-	-	X
60	MG	a	1614	-	-	-	X
60	MG	a	1615	-	-	-	X
60	MG	a	1620	-	-	-	X
60	MG	a	1636	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	a	1638	-	-	-	X
60	MG	a	1643	-	-	-	X
60	MG	a	1665	-	-	-	X
60	MG	a	1666	-	-	-	X
60	MG	a	1718	-	-	-	X
60	MG	a	1785	-	-	-	X
60	MG	x	106	-	-	-	X

## 2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2874	Total	C	N	O	P	11	0	0
			61902	27550	11582	19897	2873			

- 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 L1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	P	3	Total	Mg	0	0
			3	3		
60	B	18	Total	Mg	0	0
			18	18		
60	6	2	Total	Mg	0	0
			2	2		
60	W	1	Total	Mg	0	0
			1	1		
60	N	1	Total	Mg	0	0
			1	1		
60	X	1	Total	Mg	0	0
			1	1		
60	f	1	Total	Mg	0	0
			1	1		
60	E	5	Total	Mg	0	0
			5	5		
60	V	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	A	644	Total 644	Mg 644	0	0
60	n	3	Total 3	Mg 3	0	0
60	5	2	Total 2	Mg 2	0	0
60	x	9	Total 9	Mg 9	0	0
60	R	2	Total 2	Mg 2	0	0
60	D	6	Total 6	Mg 6	0	0
60	e	1	Total 1	Mg 1	0	0
60	v	2	Total 2	Mg 2	0	0
60	Z	1	Total 1	Mg 1	0	0
60	a	188	Total 188	Mg 188	0	0
60	U	1	Total 1	Mg 1	0	0
60	9	1	Total 1	Mg 1	0	0
60	m	2	Total 2	Mg 2	0	0
60	0	4	Total 4	Mg 4	0	0
60	G	2	Total 2	Mg 2	0	0
60	Q	2	Total 2	Mg 2	0	0
60	d	1	Total 1	Mg 1	0	0
60	H	1	Total 1	Mg 1	0	0
60	7	1	Total 1	Mg 1	0	0
60	z	2	Total 2	Mg 2	0	0
60	8	1	Total 1	Mg 1	0	0

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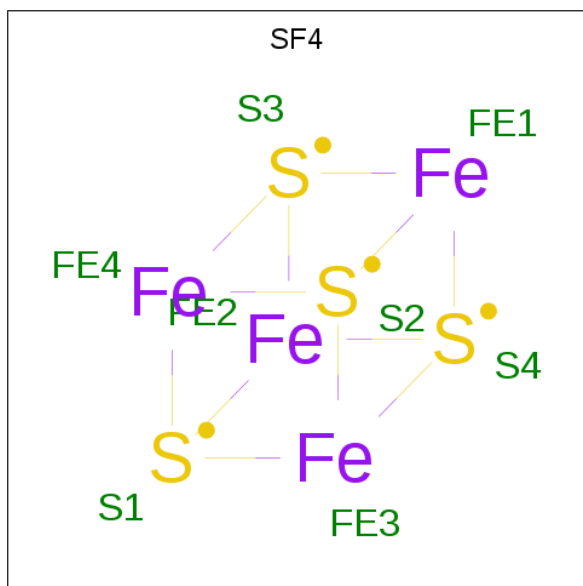
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	O	2	Total 2	Mg 2	0	0
60	l	1	Total 1	Mg 1	0	0
60	F	6	Total 6	Mg 6	0	0

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

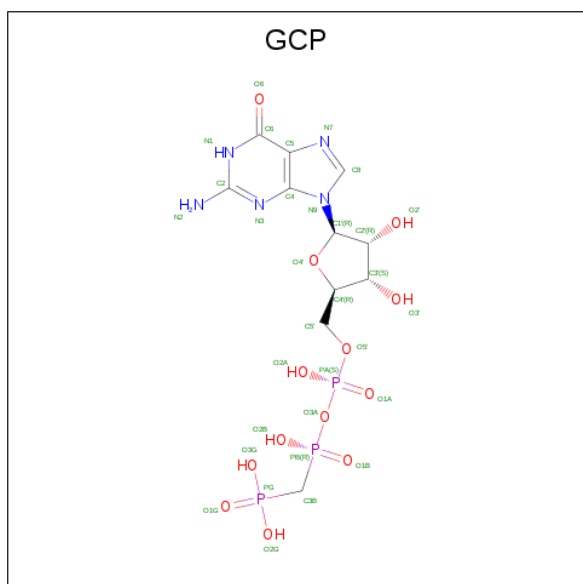
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	Y	1	Total 1	Zn 1	0	0
61	6	1	Total 1	Zn 1	0	0
61	4	1	Total 1	Zn 1	0	0
61	n	1	Total 1	Zn 1	0	0
61	5	1	Total 1	Zn 1	0	0
61	9	1	Total 1	Zn 1	0	0

- Molecule 62 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

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



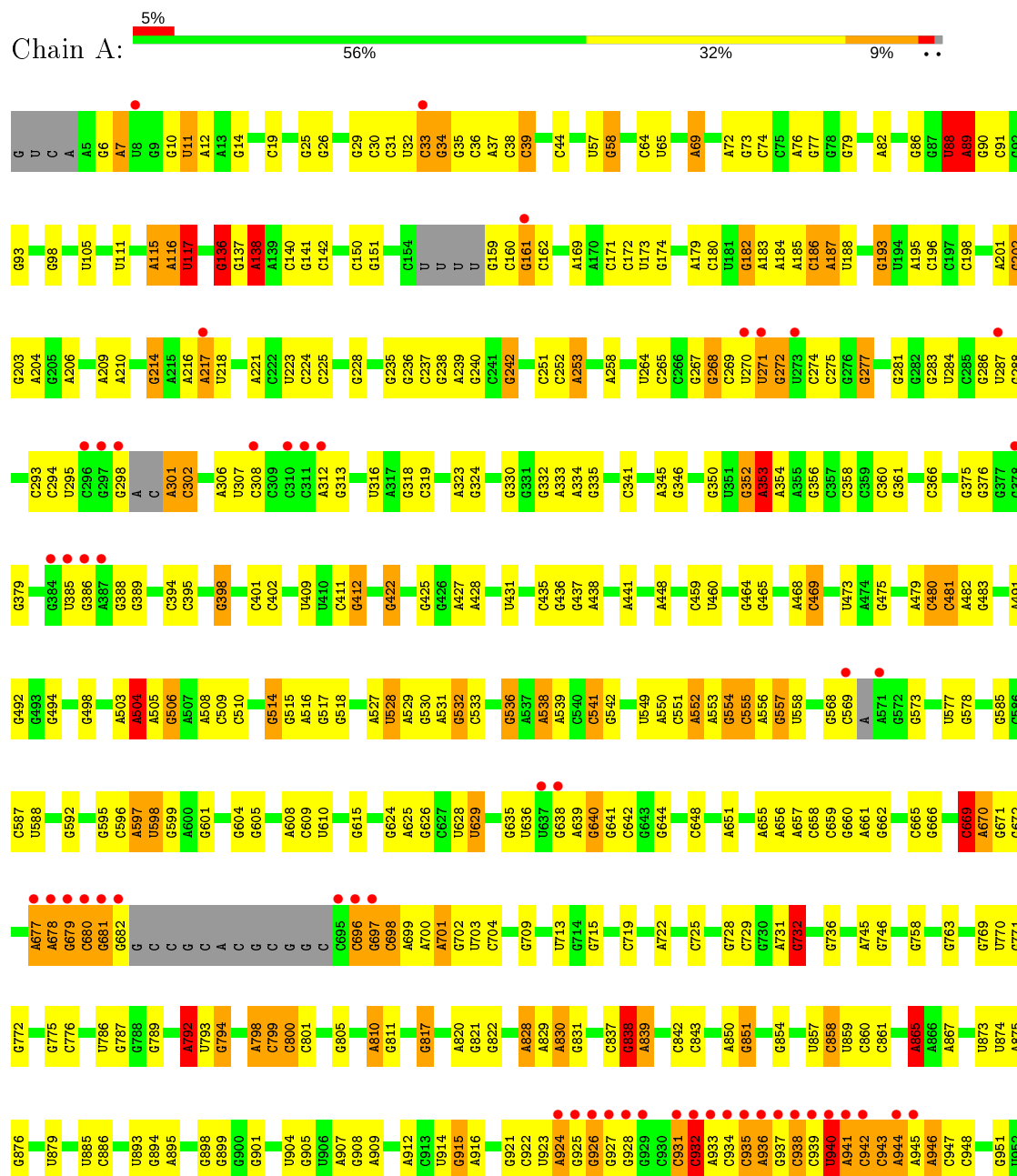
*Continued from previous page...*

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

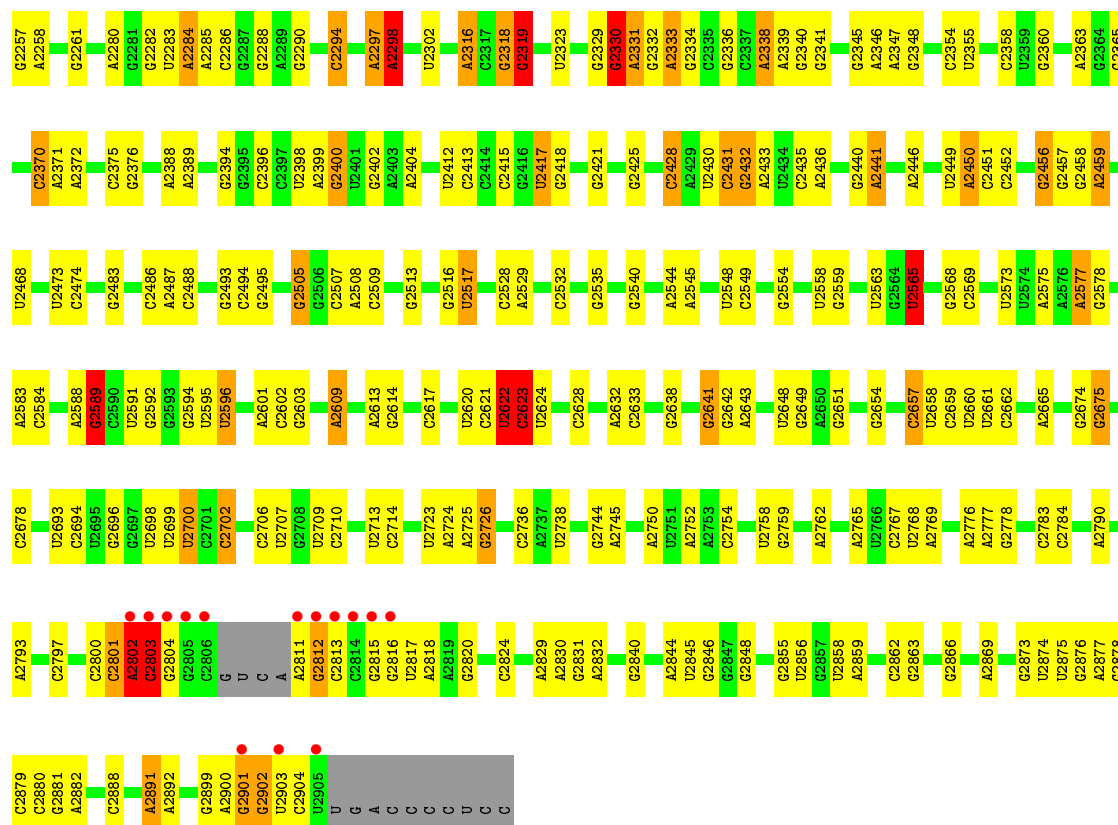
### 3 Residue-property plots

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

#### • Molecule 1: 23S Ribosomal RNA

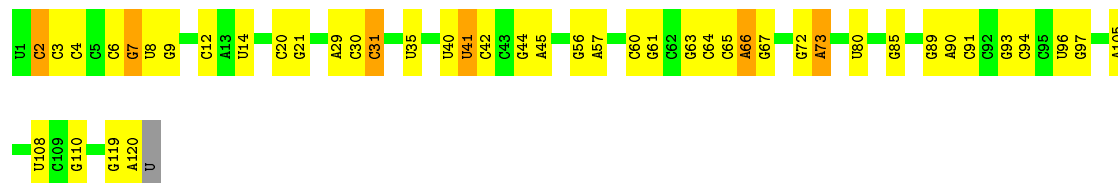


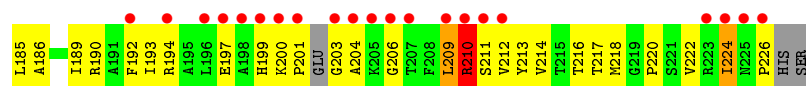




### • Molecule 2: 5S Ribosomal RNA

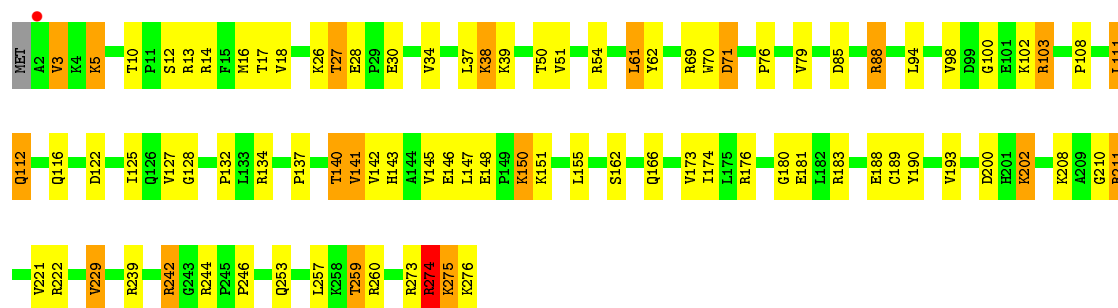
Chain B: 62% 32% 5%





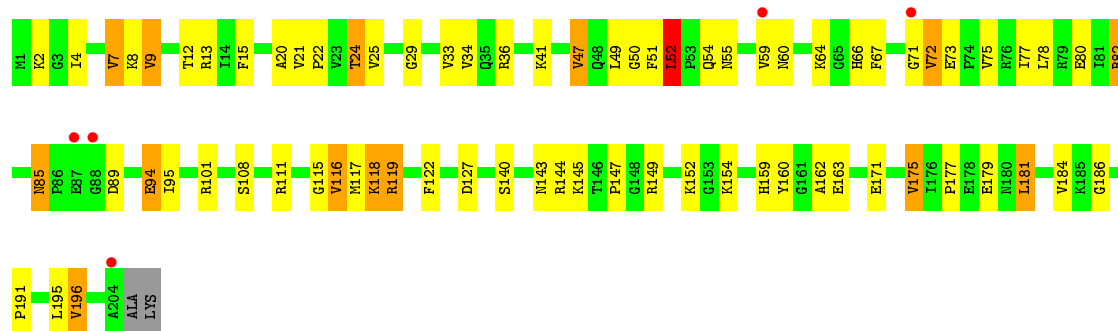
• Molecule 4: 50S ribosomal protein L2

Chain D: 68% 25% 7%



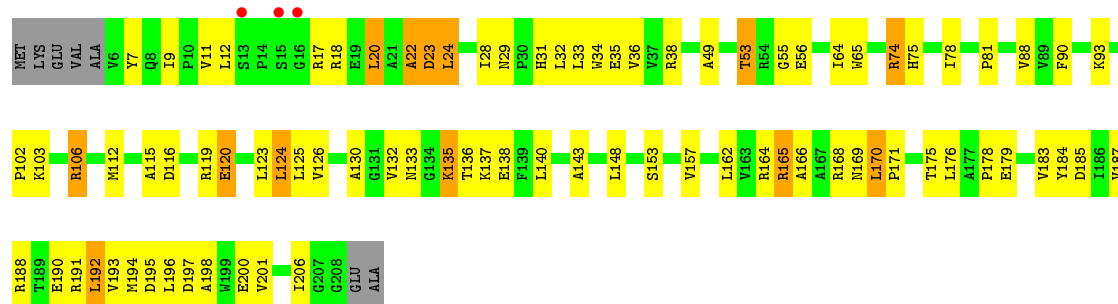
• Molecule 5: 50S ribosomal protein L3

Chain E: 2% 63% 29% 7%



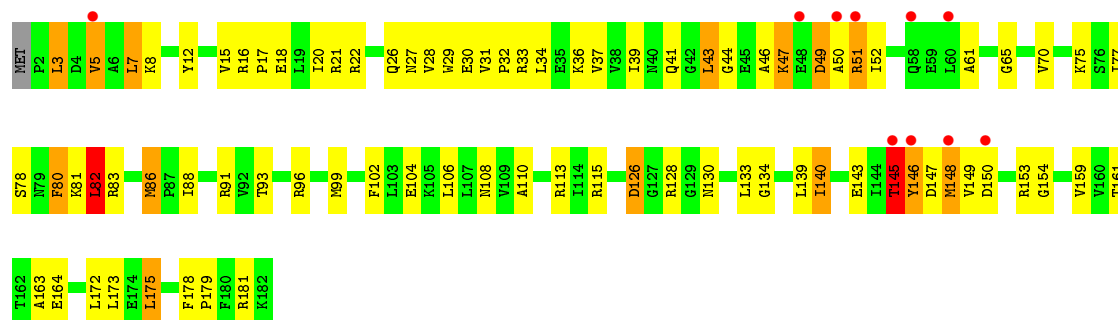
• Molecule 6: 50S ribosomal protein L4

Chain F: % 56% 34% 6%

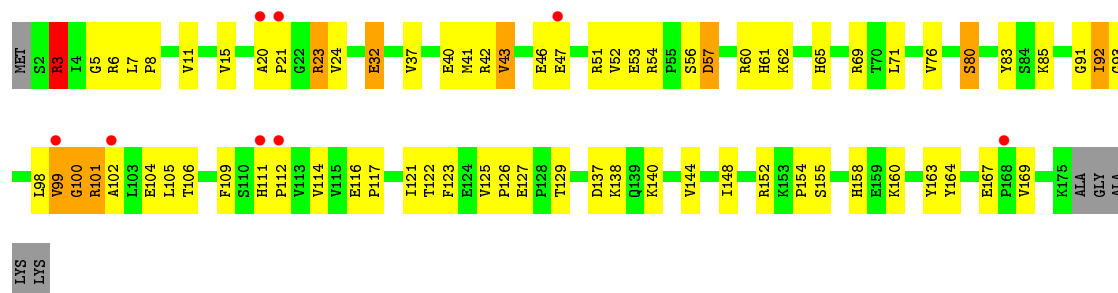


• Molecule 7: 50S ribosomal protein L5

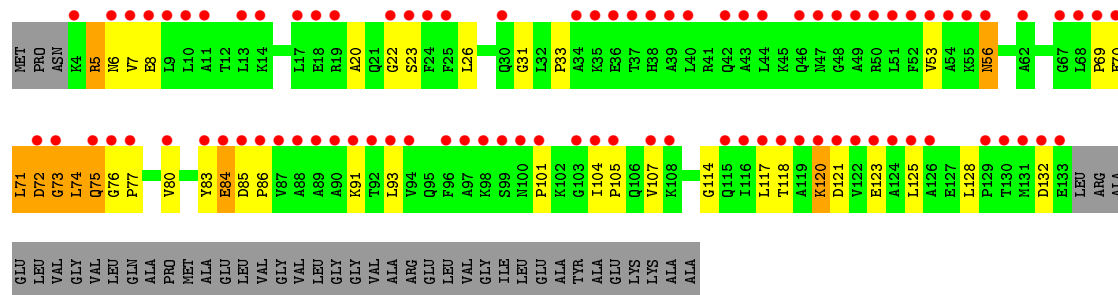
Chain G: 5% 54% 36% 8%



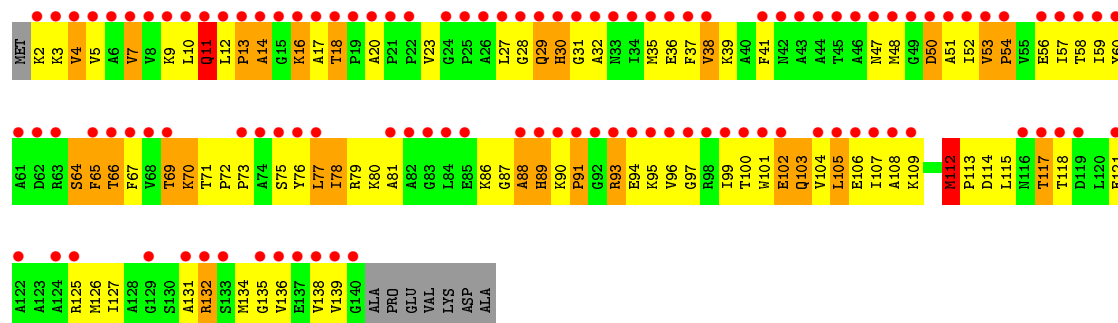
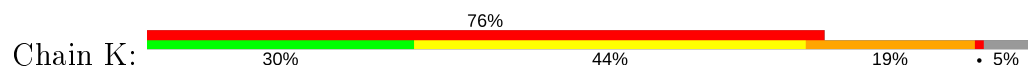
• Molecule 8: 50S ribosomal protein L6



• Molecule 9: 50S ribosomal protein L10

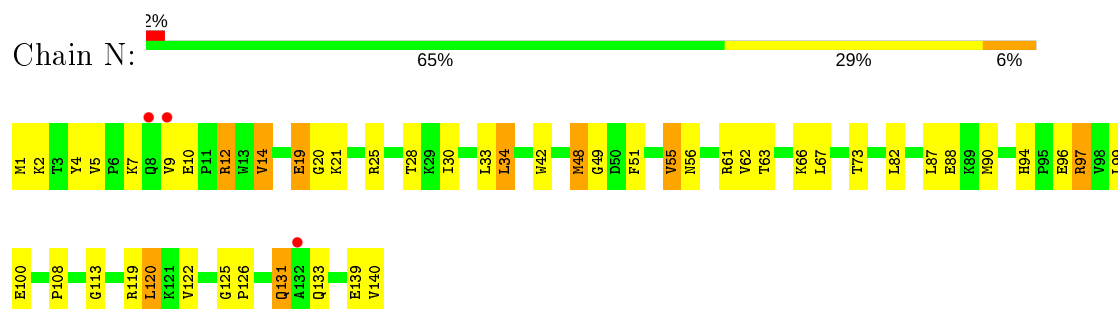


• Molecule 10: 50S ribosomal protein L11

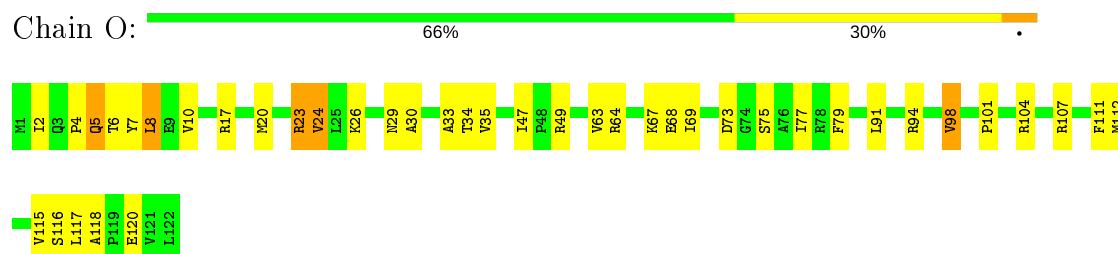




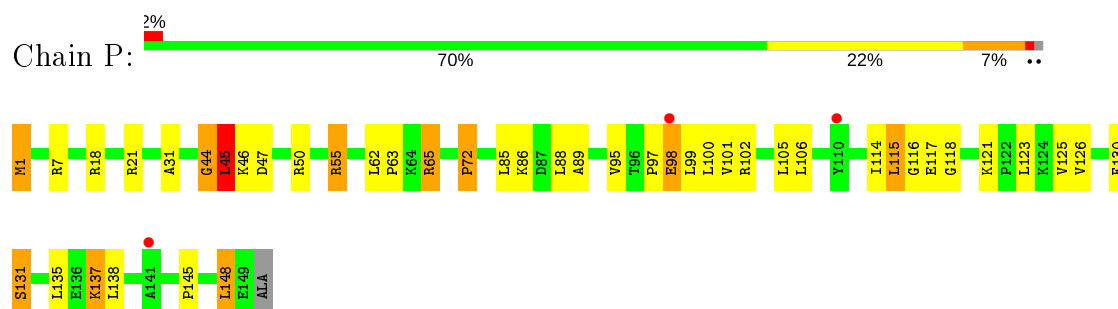
- Molecule 11: 50S ribosomal protein L13



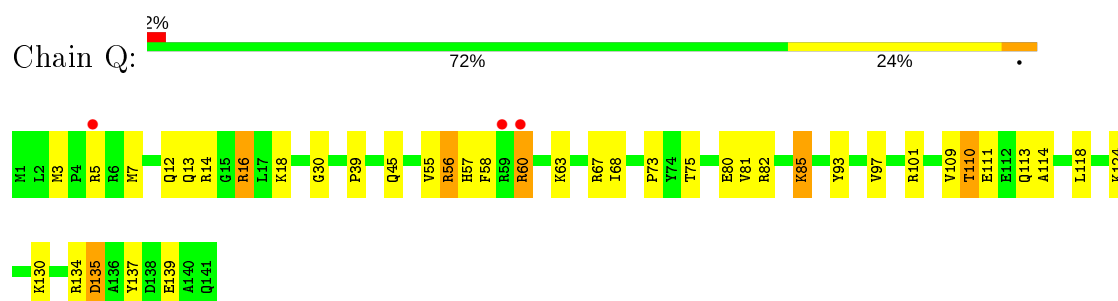
- Molecule 12: 50S ribosomal protein L14



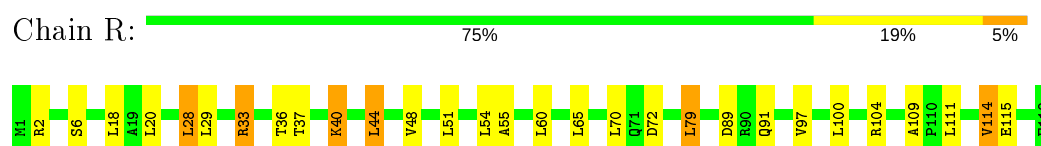
- Molecule 13: 50S ribosomal protein L15



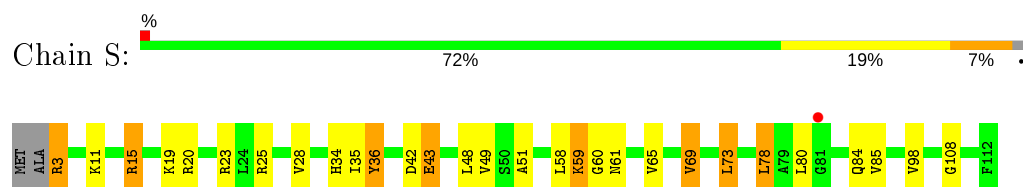
- Molecule 14: 50S ribosomal protein L16



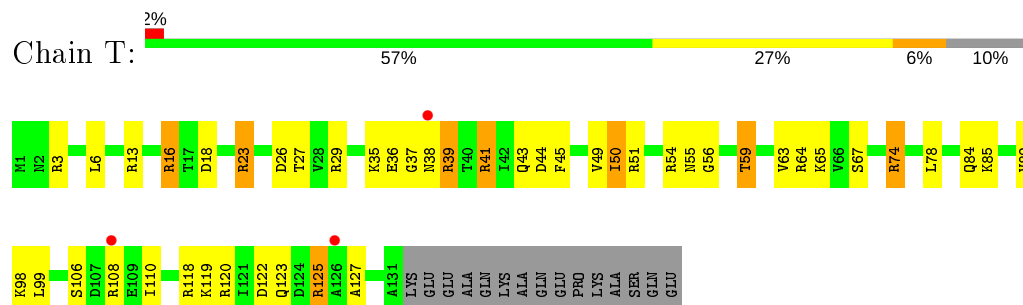
- Molecule 15: 50S ribosomal protein L17



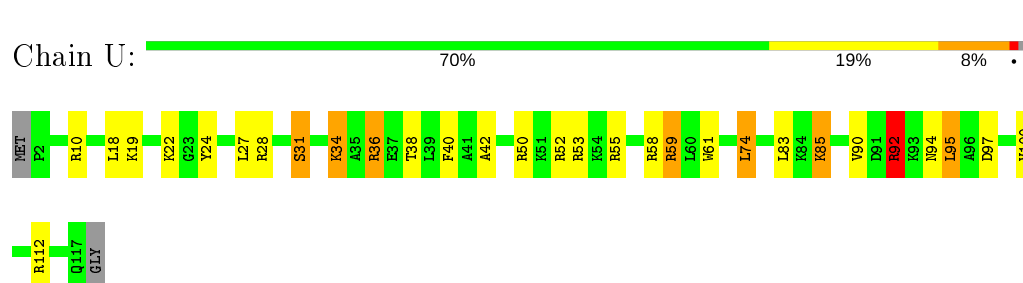
- Molecule 16: 50S ribosomal protein L18



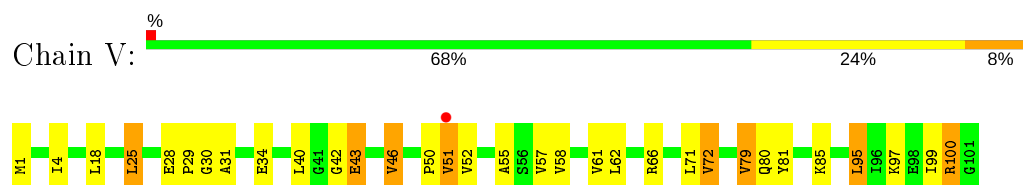
- Molecule 17: 50S ribosomal protein L19



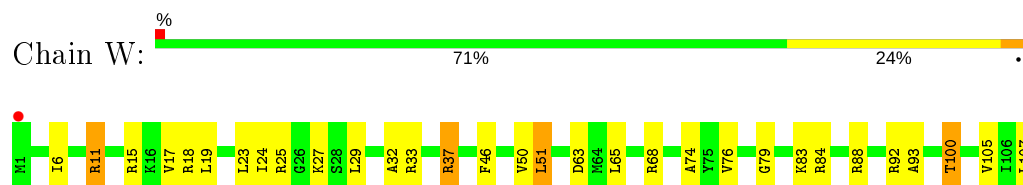
- Molecule 18: 50S ribosomal protein L20



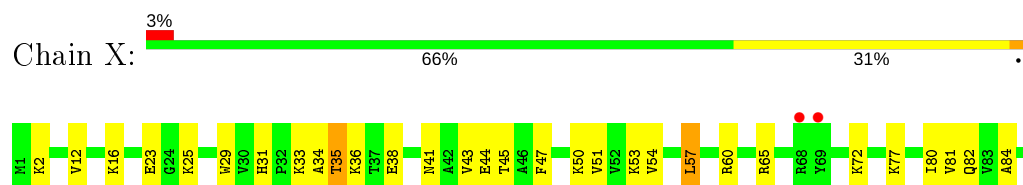
- Molecule 19: 50S ribosomal protein L21



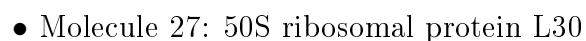
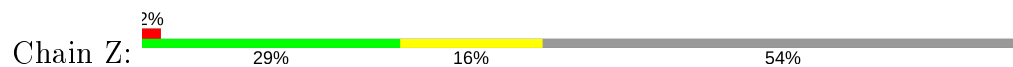
- Molecule 20: 50S ribosomal protein L22

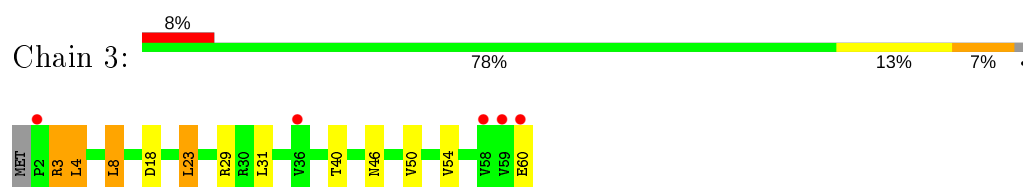


- Molecule 21: 50S ribosomal protein L23

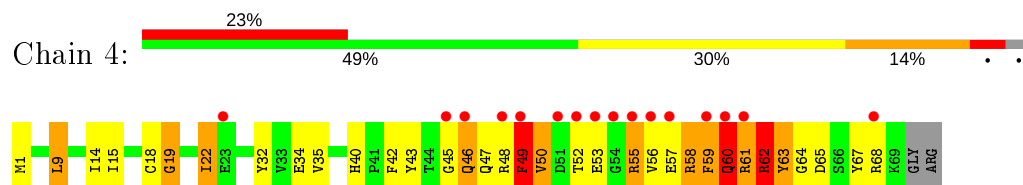


- Chain Y: 

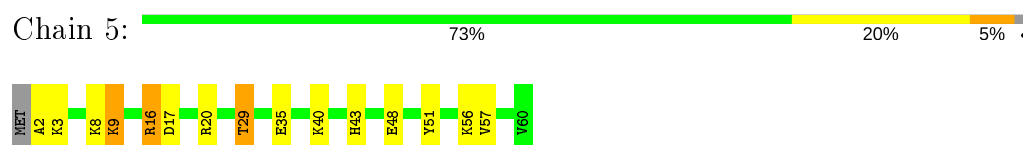




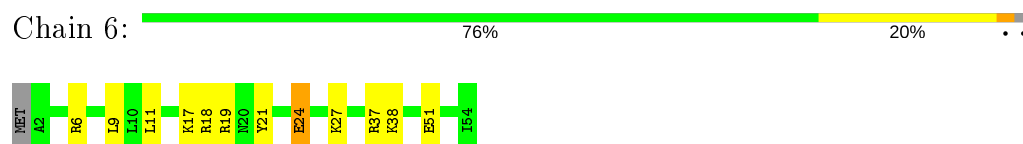
- Molecule 28: 50S ribosomal protein L31



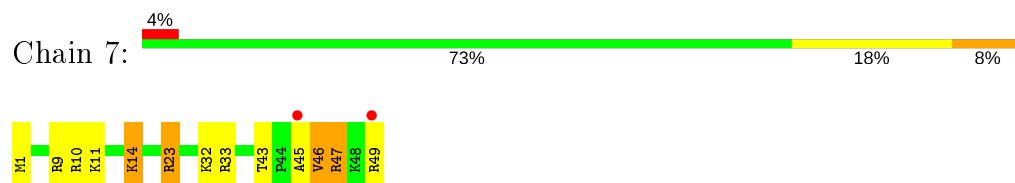
- Molecule 29: 50S ribosomal protein L32



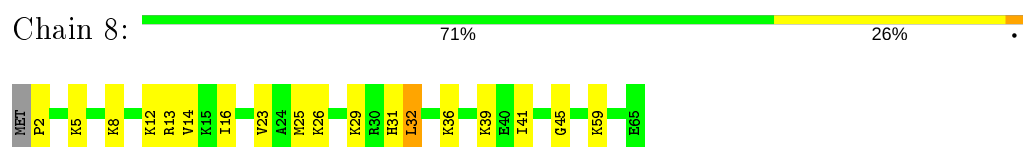
- Molecule 30: 50S ribosomal protein L33



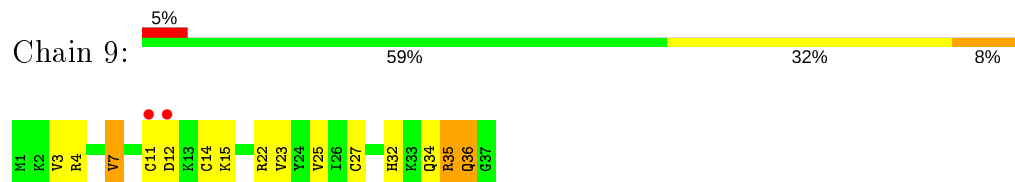
- Molecule 31: 50S ribosomal protein L34



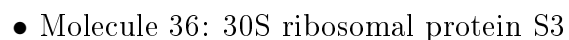
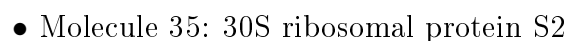
- Molecule 32: 50S ribosomal protein L35

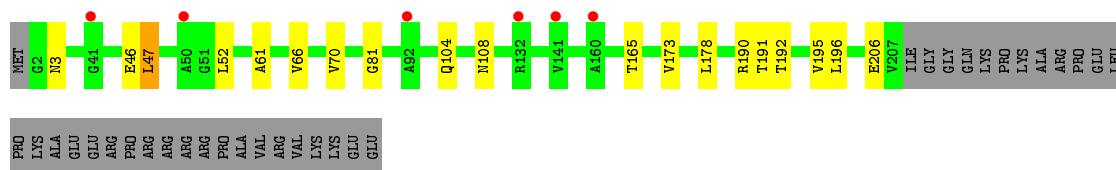


- Molecule 33: 50S ribosomal protein L36

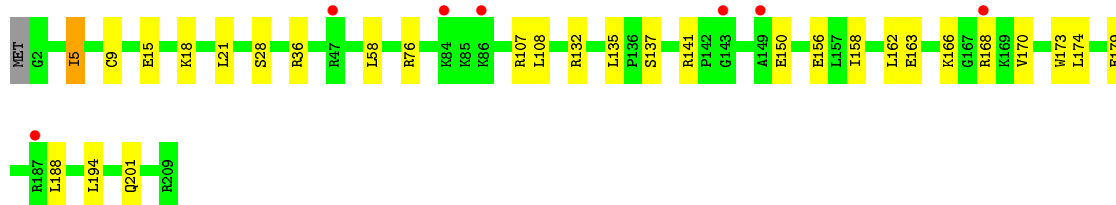
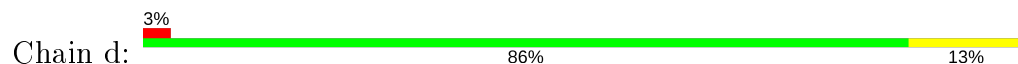


- Molecule 34: 16S Ribosomal RNA

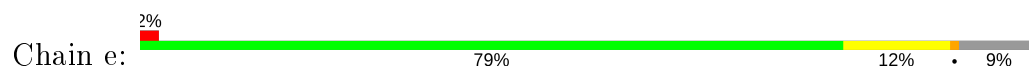




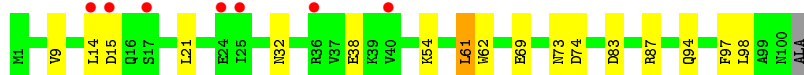
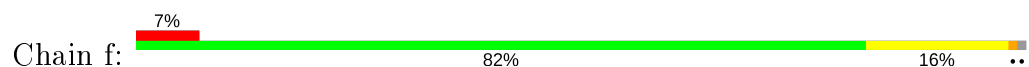
- Molecule 37: 30S ribosomal protein S4



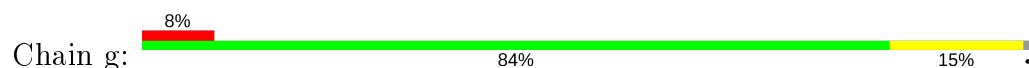
- Molecule 38: 30S ribosomal protein S5



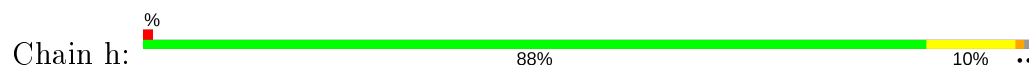
- Molecule 39: 30S ribosomal protein S6



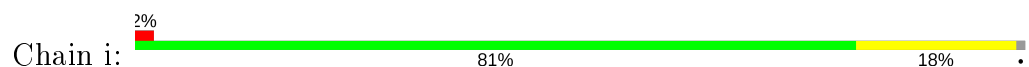
- Molecule 40: 30S ribosomal protein S7

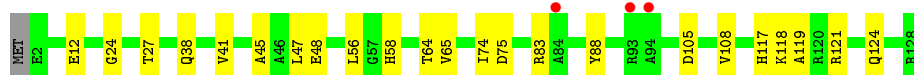


- Molecule 41: 30S ribosomal protein S8



- Molecule 42: 30S ribosomal protein S9

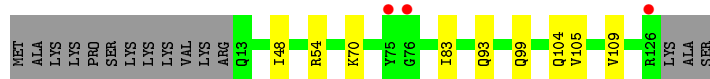
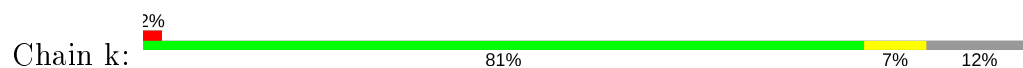




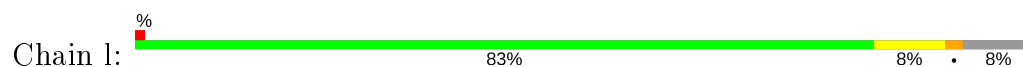
- Molecule 43: 30S ribosomal protein S10



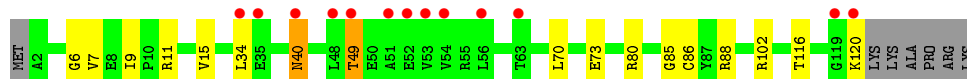
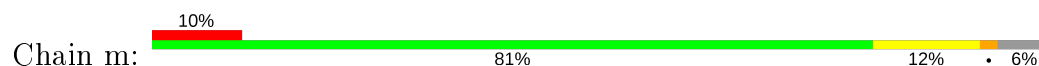
- Molecule 44: 30S ribosomal protein S11



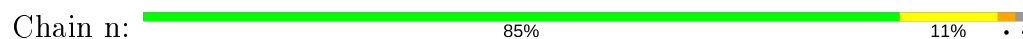
- Molecule 45: 30S ribosomal protein S12



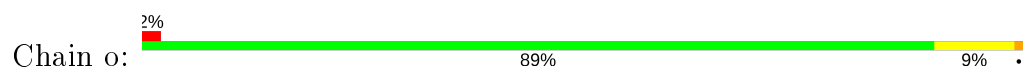
- Molecule 46: 30S ribosomal protein S13



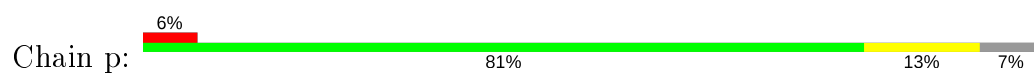
- Molecule 47: 30S ribosomal protein S14 type Z



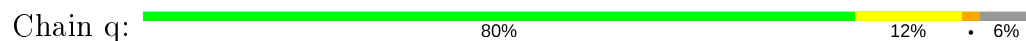
- Molecule 48: 30S ribosomal protein S15



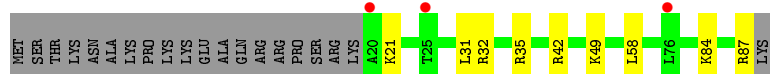
- Molecule 49: 30S ribosomal protein S16



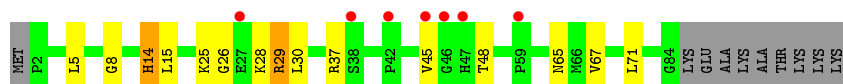
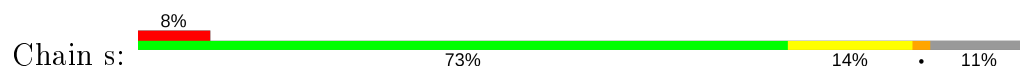
- Molecule 50: 30S ribosomal protein S17



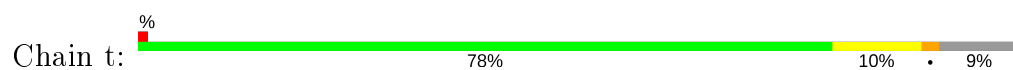
- Molecule 51: 30S ribosomal protein S18



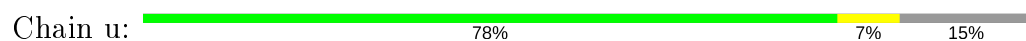
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein Thx

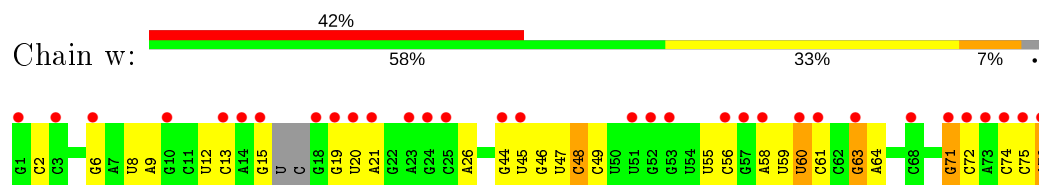


- Molecule 55: mRNA

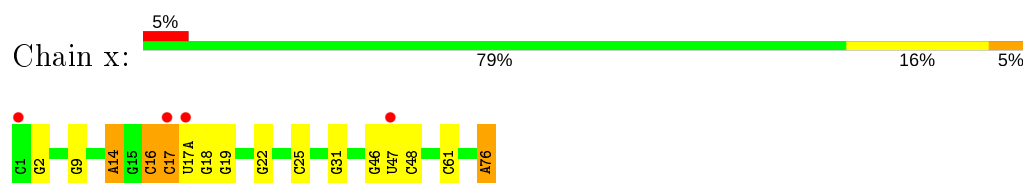




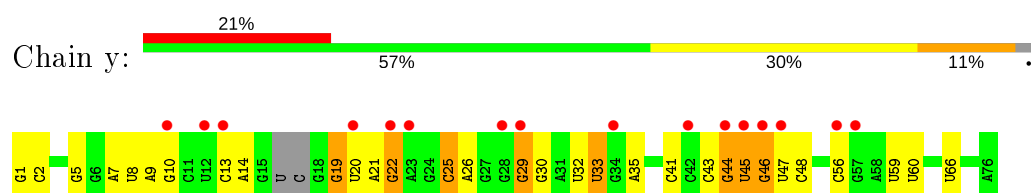
- Molecule 56: A-site tRNA



- Molecule 57: P-site tRNA



- Molecule 58: E-site tRNA



- Molecule 59: GDPCP fused to the N-terminus of the 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, $\alpha$ , $\beta$ , $\gamma$	213.12Å 271.72Å 436.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.60 49.52 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.52-2.60) 98.7 (49.52-2.59)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, $R_{free}$	0.192 , 0.261 0.192 , 0.261	Depositor DCC
$R_{free}$ test set	38580 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	155465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

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

<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, ZN, MIA, SF4, MG, GCP, 5MC, 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	0.69	11/69327 (0.0%)	1.23	339/108217 (0.3%)
2	B	0.51	0/2878	1.00	1/4490 (0.0%)
3	C	0.36	0/1044	0.66	1/1413 (0.1%)
4	D	0.50	0/2186	0.73	1/2944 (0.0%)
5	E	0.45	0/1592	0.69	0/2149
6	F	0.46	0/1619	0.62	0/2193
7	G	0.38	0/1450	0.64	1/1959 (0.1%)
8	H	0.42	0/1356	0.63	0/1834
9	J	0.32	0/640	0.55	0/889
10	K	0.43	0/1044	0.65	1/1416 (0.1%)
11	N	0.41	0/1144	0.63	0/1543
12	O	0.49	0/943	0.68	1/1269 (0.1%)
13	P	0.47	0/1152	0.74	1/1533 (0.1%)
14	Q	0.46	0/1143	0.58	0/1527
15	R	0.38	0/982	0.66	0/1312
16	S	0.40	0/887	0.63	0/1180
17	T	0.43	0/1105	0.65	0/1477
18	U	0.46	0/977	0.69	2/1301 (0.2%)
19	V	0.48	0/782	0.68	1/1049 (0.1%)
20	W	0.46	0/897	0.63	0/1205
21	X	0.43	0/764	0.65	1/1025 (0.1%)
22	Y	0.43	0/819	0.66	1/1095 (0.1%)
23	Z	0.38	0/801	0.59	0/1079
24	0	0.43	0/599	0.64	0/798
25	1	0.52	0/762	0.74	1/1014 (0.1%)
26	2	0.38	0/590	0.58	0/781
27	3	0.38	0/474	0.69	1/635 (0.2%)
28	4	0.40	0/570	0.64	0/768
29	5	0.44	0/473	0.71	0/639
30	6	0.46	0/460	0.64	0/613
31	7	0.46	0/438	0.71	0/575
32	8	0.47	0/519	0.67	0/684

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	K	0	1
19	V	0	1
26	2	0	1
28	4	0	1
37	d	0	1
39	f	0	1
42	i	0	2

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

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	71	G	C6-N1	-10.59	1.32	1.39
56	w	71	G	N1-C2	-10.38	1.29	1.37
57	x	14	A	N7-C5	-8.86	1.33	1.39
1	A	353	A	N9-C4	-7.12	1.33	1.37
1	A	1091	A	C5-C6	-7.12	1.34	1.41
57	x	14	A	C8-N7	-7.08	1.26	1.31
1	A	2298	A	N9-C4	-6.99	1.33	1.37
36	c	173	VAL	C-N	-6.97	1.21	1.34
34	a	953	A	N9-C4	-6.84	1.33	1.37
1	A	1187	A	N9-C4	-6.75	1.33	1.37
1	A	1066	A	N9-C4	-6.07	1.34	1.37
1	A	552	A	N9-C4	-6.03	1.34	1.37
1	A	1744	A	N9-C4	-5.48	1.34	1.37
1	A	989	A	N9-C4	-5.46	1.34	1.37
34	a	1108	U	P-O5'	5.41	1.65	1.59
57	x	14	A	N9-C4	5.38	1.41	1.37
1	A	353	A	N3-C4	-5.36	1.31	1.34
1	A	1955	C	N3-C4	-5.31	1.30	1.33
57	x	14	A	C6-N6	5.24	1.38	1.33
56	w	2	C	N3-C4	-5.08	1.30	1.33
1	A	1853	G	N3-C4	-5.02	1.31	1.35

All (572) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	71	G	N3-C2-N2	23.02	136.02	119.90
56	w	71	G	C5-C6-O6	22.98	142.39	128.60
56	w	2	C	N1-C2-O2	21.56	131.84	118.90
56	w	71	G	N1-C2-N2	-21.15	97.16	116.20
1	A	1091	A	N9-C4-C5	-17.30	98.88	105.80
56	w	71	G	N1-C6-O6	-15.20	110.78	119.90
1	A	1091	A	C8-N9-C4	15.05	111.82	105.80
1	A	39	C	C2-N3-C4	14.70	127.25	119.90
57	x	14	A	C4-C5-C6	14.37	124.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	2	C	C2-N3-C4	14.36	127.08	119.90
57	x	14	A	C5-N7-C8	14.31	111.06	103.90
34	a	361	U	C5-C6-N1	-12.83	116.28	122.70
58	y	46	G	C4-N9-C1'	12.63	142.92	126.50
1	A	1775	G	C4-C5-N7	12.58	115.83	110.80
56	w	2	C	N3-C2-O2	-12.28	113.31	121.90
1	A	1066	A	C2-N3-C4	-12.23	104.49	110.60
58	y	22	G	C5-C6-O6	-12.12	121.33	128.60
56	w	2	C	C5-C6-N1	11.97	126.99	121.00
58	y	46	G	C8-N9-C1'	-11.80	111.66	127.00
1	A	39	C	N3-C4-C5	11.73	126.59	121.90
57	x	14	A	C5-C6-N1	-11.62	111.89	117.70
56	w	71	G	C6-N1-C2	11.53	132.02	125.10
1	A	536	G	O4'-C1'-N9	11.30	117.24	108.20
1	A	2298	A	C2-N3-C4	-11.26	104.97	110.60
1	A	2221	C	C5-C6-N1	10.94	126.47	121.00
56	w	71	G	C2-N3-C4	-10.74	106.53	111.90
1	A	1091	A	C4-C5-N7	10.48	115.94	110.70
1	A	1125	C	N3-C2-O2	-10.35	114.66	121.90
58	y	22	G	N1-C6-O6	9.94	125.87	119.90
1	A	117	U	O5'-P-OP1	-9.94	96.76	105.70
34	a	1037	C	O4'-C1'-N1	9.93	116.14	108.20
56	w	2	C	C6-N1-C2	-9.78	116.39	120.30
1	A	2018	G	O5'-P-OP2	-9.74	96.93	105.70
58	y	46	G	N1-C2-N2	-9.72	107.45	116.20
1	A	1187	A	C2-N3-C4	-9.70	105.75	110.60
57	x	76	A	N1-C2-N3	9.64	134.12	129.30
1	A	1066	A	N1-C2-N3	9.61	134.11	129.30
1	A	985	A	O5'-P-OP1	-9.61	97.06	105.70
56	w	71	G	C5-C6-N1	-9.40	106.80	111.50
1	A	2221	C	C6-N1-C2	-9.30	116.58	120.30
57	x	22	G	C5-N7-C8	-9.27	99.66	104.30
1	A	1957	A	O4'-C1'-N9	9.24	115.59	108.20
57	x	17	C	N1-C2-O2	9.12	124.38	118.90
1	A	1125	C	N1-C2-O2	9.12	124.37	118.90
34	a	1313	G	O4'-C1'-N9	9.10	115.48	108.20
58	y	22	G	C6-C5-N7	-8.98	125.01	130.40
1	A	1091	A	N1-C6-N6	8.95	123.97	118.60
58	y	46	G	O4'-C1'-N9	8.94	115.36	108.20
1	A	799	C	O5'-P-OP1	-8.92	97.67	105.70
1	A	1742	G	O5'-P-OP2	-8.89	97.70	105.70
58	y	46	G	N3-C4-N9	8.88	131.33	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1109	U	C2-N1-C1'	8.84	128.31	117.70
34	a	511	G	O5'-P-OP2	-8.76	97.81	105.70
1	A	1248	A	O4'-C1'-N9	8.74	115.19	108.20
1	A	353	A	N1-C2-N3	8.71	133.65	129.30
1	A	989	A	C5-N7-C8	-8.66	99.57	103.90
34	a	1109	U	C5-C6-N1	8.66	127.03	122.70
34	a	1261	A	N7-C8-N9	8.64	118.12	113.80
1	A	1877	A	O4'-C1'-N9	8.62	115.10	108.20
1	A	1125	C	C6-N1-C2	-8.61	116.86	120.30
34	a	1480	A	C5-N7-C8	-8.60	99.60	103.90
58	y	45	U	N3-C2-O2	-8.59	116.19	122.20
1	A	2297	A	N7-C8-N9	8.57	118.09	113.80
1	A	1775	G	N9-C4-C5	-8.56	101.97	105.40
1	A	2330	G	N3-C4-C5	8.53	132.86	128.60
1	A	2221	C	C2-N1-C1'	8.52	128.17	118.80
1	A	2297	A	C5-N7-C8	-8.47	99.67	103.90
56	w	2	C	C2-N1-C1'	8.47	128.11	118.80
1	A	1775	G	C5-N7-C8	-8.38	100.11	104.30
34	a	1007	C	C2-N1-C1'	8.37	128.01	118.80
57	x	17	C	C2-N1-C1'	8.36	127.99	118.80
1	A	353	A	C2-N3-C4	-8.34	106.43	110.60
1	A	1589	C	C2-N1-C1'	8.32	127.95	118.80
34	a	961	A	O5'-P-OP1	-8.28	98.25	105.70
1	A	253	A	C5-N7-C8	-8.25	99.78	103.90
1	A	2457	G	N1-C6-O6	-8.24	114.96	119.90
1	A	2330	G	N3-C4-N9	-8.16	121.10	126.00
1	A	1589	C	N1-C2-O2	8.14	123.78	118.90
34	a	262	G	N3-C4-N9	-8.11	121.13	126.00
34	a	953	A	C5-N7-C8	-8.11	99.85	103.90
57	x	46	G	C6-N1-C2	-8.09	120.24	125.10
1	A	1187	A	N3-C4-N9	-8.08	120.94	127.40
56	w	76	A	N7-C8-N9	8.00	117.80	113.80
1	A	1091	A	C6-N1-C2	8.00	123.40	118.60
34	a	570	C	C6-N1-C2	7.99	123.50	120.30
1	A	2013	G	P-O3'-C3'	7.99	129.29	119.70
1	A	989	A	N1-C6-N6	7.95	123.37	118.60
1	A	865	A	O5'-P-OP1	-7.85	98.63	105.70
58	y	46	G	N3-C4-C5	-7.81	124.69	128.60
1	A	2189	G	C6-C5-N7	-7.80	125.72	130.40
58	y	22	G	C4-C5-N7	7.79	113.92	110.80
1	A	1187	A	N3-C4-C5	7.76	132.23	126.80
1	A	2565	U	O5'-P-OP1	-7.74	98.73	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1091	A	O4'-C1'-N9	-7.72	102.02	108.20
58	y	22	G	N3-C4-N9	7.72	130.63	126.00
34	a	262	G	N3-C4-C5	7.69	132.45	128.60
34	a	1263	U	N1-C2-O2	7.66	128.16	122.80
58	y	45	U	N1-C2-O2	7.60	128.12	122.80
57	x	14	A	C4-C5-N7	-7.58	106.91	110.70
1	A	1091	A	N1-C2-N3	-7.57	125.52	129.30
1	A	2297	A	C8-N9-C4	-7.53	102.79	105.80
1	A	1066	A	C5-N7-C8	-7.53	100.14	103.90
58	y	46	G	N1-C2-N3	7.50	128.40	123.90
57	x	76	A	C2-N3-C4	-7.50	106.85	110.60
57	x	76	A	C5-N7-C8	-7.45	100.17	103.90
7	G	82	LEU	CA-CB-CG	7.43	132.38	115.30
57	x	76	A	C6-C5-N7	-7.42	127.11	132.30
34	a	1480	A	N7-C8-N9	7.40	117.50	113.80
57	x	17	C	N3-C2-O2	-7.37	116.74	121.90
1	A	1662	C	O5'-P-OP1	-7.37	99.07	105.70
55	v	13	A	C5-N7-C8	-7.35	100.22	103.90
1	A	1066	A	N7-C8-N9	7.34	117.47	113.80
57	x	76	A	O4'-C1'-N9	7.34	114.07	108.20
1	A	2249	G	N3-C4-N9	7.33	130.40	126.00
1	A	994	G	O5'-P-OP1	-7.33	99.11	105.70
1	A	2298	A	N3-C4-C5	7.33	131.93	126.80
34	a	1007	C	N1-C2-O2	7.24	123.24	118.90
58	y	46	G	C6-C5-N7	-7.24	126.06	130.40
56	w	2	C	C4-C5-C6	-7.22	113.79	117.40
1	A	990	G	N1-C6-O6	-7.16	115.61	119.90
1	A	893	U	C5-C6-N1	-7.14	119.13	122.70
1	A	1248	A	N1-C6-N6	7.14	122.88	118.60
56	w	72	C	N1-C2-O2	7.13	123.18	118.90
1	A	1699	G	N3-C4-C5	-7.12	125.04	128.60
34	a	1261	A	C5-N7-C8	-7.11	100.35	103.90
1	A	1764	U	O4'-C1'-N1	7.10	113.88	108.20
57	x	22	G	N7-C8-N9	7.10	116.65	113.10
34	a	1261	A	C8-N9-C4	-7.08	102.97	105.80
1	A	2221	C	N1-C2-O2	7.08	123.15	118.90
1	A	940	U	C2-N1-C1'	7.02	126.13	117.70
1	A	1812	C	C6-N1-C2	-7.00	117.50	120.30
1	A	977	A	C5-N7-C8	-7.00	100.40	103.90
1	A	989	A	C4-C5-N7	7.00	114.20	110.70
34	a	939	U	O5'-P-OP2	-6.99	99.41	105.70
2	B	41	U	C5-C6-N1	-6.98	119.21	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1761	G	C5-C6-O6	-6.96	124.42	128.60
1	A	1693	G	O4'-C1'-N9	-6.95	102.64	108.20
34	a	317	A	O5'-P-OP2	-6.94	99.46	105.70
34	a	1389	U	O5'-P-OP2	-6.93	99.46	105.70
1	A	552	A	C2-N3-C4	-6.84	107.18	110.60
1	A	838	G	O4'-C1'-N9	-6.84	102.73	108.20
1	A	2457	G	C5-C6-O6	6.83	132.70	128.60
1	A	2882	A	O4'-C1'-N9	6.82	113.66	108.20
34	a	1006	C	C2-N1-C1'	6.74	126.22	118.80
1	A	792	A	O4'-C1'-N9	6.73	113.59	108.20
56	w	60	U	N3-C2-O2	-6.73	117.49	122.20
34	a	1209	A	C5-N7-C8	-6.70	100.55	103.90
34	a	1019	G	C4-N9-C1'	6.70	135.21	126.50
58	y	22	G	N9-C4-C5	-6.67	102.73	105.40
56	w	2	C	C5-C4-N4	6.66	124.86	120.20
1	A	2657	C	O5'-P-OP2	-6.64	99.72	105.70
34	a	732	C	P-O3'-C3'	6.64	127.66	119.70
1	A	186	C	N1-C2-O2	-6.63	114.92	118.90
1	A	353	A	N3-C4-N9	-6.62	122.10	127.40
34	a	1263	U	C2-N1-C1'	6.62	125.64	117.70
57	x	17	C	O5'-P-OP1	-6.62	99.74	105.70
1	A	1424	A	O4'-C1'-N9	-6.62	102.91	108.20
57	x	14	A	C8-N9-C1'	-6.62	115.78	127.70
1	A	253	A	C4-C5-N7	6.61	114.00	110.70
58	y	44	G	C5-C6-O6	-6.60	124.64	128.60
1	A	2189	G	C4-N9-C1'	6.60	135.08	126.50
1	A	1976	U	C2-N1-C1'	-6.59	109.79	117.70
34	a	850	A	O4'-C1'-N9	6.58	113.47	108.20
1	A	1853	G	N3-C2-N2	-6.58	115.30	119.90
1	A	1744	A	C2-N3-C4	-6.55	107.33	110.60
1	A	1699	G	C8-N9-C4	-6.54	103.78	106.40
1	A	1154	C	C5-C6-N1	6.54	124.27	121.00
1	A	2189	G	N3-C4-N9	6.54	129.92	126.00
1	A	2075	A	C8-N9-C4	6.54	108.41	105.80
1	A	656	A	C8-N9-C4	6.52	108.41	105.80
1	A	2592	G	O4'-C1'-N9	6.52	113.42	108.20
1	A	552	A	C5-N7-C8	-6.51	100.64	103.90
1	A	1430	G	O4'-C1'-N9	6.50	113.40	108.20
1	A	1775	G	C5-C6-O6	-6.50	124.70	128.60
1	A	893	U	C2-N1-C1'	-6.49	109.91	117.70
34	a	361	U	C4-C5-C6	6.49	123.59	119.70
1	A	732	G	N9-C4-C5	-6.49	102.80	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1006	G	N1-C6-O6	-6.49	116.01	119.90
34	a	954	G	N1-C6-O6	6.47	123.78	119.90
57	x	14	A	C4-N9-C1'	6.47	137.95	126.30
1	A	2577	A	O4'-C1'-N9	6.46	113.37	108.20
1	A	2458	G	C4-N9-C1'	-6.45	118.11	126.50
34	a	262	G	C5-N7-C8	-6.44	101.08	104.30
1	A	138	A	N7-C8-N9	6.44	117.02	113.80
57	x	17	C	O5'-P-OP2	6.42	118.41	110.70
1	A	977	A	O4'-C1'-N9	6.42	113.34	108.20
1	A	11	U	C2-N1-C1'	6.38	125.36	117.70
56	w	76	A	C8-N9-C4	-6.38	103.25	105.80
57	x	76	A	C4-C5-N7	6.37	113.89	110.70
57	x	76	A	N7-C8-N9	6.37	116.99	113.80
1	A	2803	C	N1-C2-O2	-6.35	115.09	118.90
34	a	1268	A	C5-N7-C8	-6.34	100.73	103.90
34	a	1209	A	N7-C8-N9	6.34	116.97	113.80
34	a	1340	U	C5-C6-N1	-6.34	119.53	122.70
1	A	669	C	C5-C6-N1	6.33	124.17	121.00
1	A	1764	U	C2-N1-C1'	-6.33	110.11	117.70
56	w	71	G	C4-N9-C1'	6.33	134.72	126.50
34	a	1109	U	C6-N1-C2	-6.32	117.21	121.00
34	a	1141	C	C5-C6-N1	-6.32	117.84	121.00
1	A	940	U	N3-C2-O2	-6.32	117.78	122.20
34	a	1109	U	P-O3'-C3'	6.31	127.27	119.70
34	a	1239	U	N1-C2-O2	6.30	127.21	122.80
1	A	1604	A	N1-C2-N3	6.30	132.45	129.30
59	z	373	ALA	C-N-CD	-6.29	106.76	120.60
1	A	989	A	C2-N3-C4	-6.29	107.45	110.60
1	A	39	C	N3-C4-N4	-6.29	113.60	118.00
21	X	57	LEU	CA-CB-CG	6.29	129.76	115.30
34	a	1268	A	N7-C8-N9	6.25	116.93	113.80
56	w	2	C	N1-C2-N3	-6.25	114.82	119.20
10	K	112	MET	C-N-CD	6.24	141.51	128.40
1	A	940	U	N1-C2-O2	6.23	127.16	122.80
1	A	253	A	N7-C8-N9	6.23	116.92	113.80
1	A	1604	A	C2-N3-C4	-6.23	107.48	110.60
56	w	71	G	C8-N9-C1'	-6.22	118.92	127.00
1	A	1066	A	C8-N9-C4	-6.18	103.33	105.80
55	v	13	A	N7-C8-N9	6.18	116.89	113.80
1	A	2623	C	O5'-P-OP2	-6.18	100.14	105.70
34	a	1480	A	C4-C5-N7	6.17	113.78	110.70
1	A	214	G	O4'-C1'-N9	6.17	113.14	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2468	U	N3-C2-O2	-6.17	117.88	122.20
1	A	187	A	OP1-P-OP2	6.16	128.85	119.60
34	a	1497	A	C5-C6-N1	-6.16	114.62	117.70
1	A	1764	U	C6-N1-C1'	6.15	129.81	121.20
1	A	2189	G	C8-N9-C1'	-6.14	119.02	127.00
56	w	63	G	N7-C8-N9	6.14	116.17	113.10
1	A	837	C	N1-C2-O2	-6.14	115.22	118.90
34	a	1263	U	N3-C2-O2	-6.13	117.91	122.20
57	x	22	G	C4-C5-N7	6.13	113.25	110.80
1	A	553	A	O4'-C1'-N9	6.12	113.10	108.20
1	A	577	U	O4'-C1'-N1	6.11	113.09	108.20
34	a	1069	U	C2-N1-C1'	6.11	125.03	117.70
13	P	44	GLY	C-N-CA	6.10	136.96	121.70
34	a	1060	G	O5'-P-OP2	-6.10	100.21	105.70
1	A	1248	A	C2-N3-C4	-6.09	107.55	110.60
1	A	1773	C	O4'-C1'-N1	6.08	113.07	108.20
58	y	46	G	N3-C2-N2	6.07	124.15	119.90
1	A	1292	A	N1-C6-N6	6.07	122.24	118.60
1	A	2302	U	C5-C4-O4	6.06	129.54	125.90
18	U	74	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	839	A	N9-C4-C5	-6.06	103.38	105.80
34	a	1019	G	C8-N9-C1'	-6.06	119.12	127.00
1	A	2532	C	N1-C2-O2	-6.05	115.27	118.90
34	a	1203	G	N1-C6-O6	-6.04	116.27	119.90
1	A	1077	A	N1-C6-N6	6.04	122.23	118.60
34	a	1480	A	C8-N9-C4	-6.04	103.38	105.80
18	U	92	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	1066	A	N3-C4-N9	-6.03	122.58	127.40
1	A	2090	G	N1-C6-O6	6.01	123.50	119.90
58	y	45	U	C2-N1-C1'	6.01	124.91	117.70
1	A	1006	G	C5-C6-O6	6.00	132.20	128.60
1	A	990	G	C5-C6-O6	6.00	132.20	128.60
1	A	1744	A	N3-C4-N9	-6.00	122.60	127.40
1	A	1589	C	C5-C6-N1	5.99	124.00	121.00
34	a	856	G	N1-C6-O6	-5.99	116.31	119.90
34	a	1502	C	N1-C2-O2	-5.98	115.31	118.90
56	w	48	C	N1-C2-O2	5.97	122.48	118.90
57	x	14	A	N7-C8-N9	-5.97	110.81	113.80
1	A	1218	A	OP1-P-O3'	5.95	118.29	105.20
34	a	361	U	C2-N3-C4	-5.95	123.43	127.00
34	a	884	G	C5-C6-O6	-5.95	125.03	128.60
59	z	445	GLN	N-CA-C	-5.94	94.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1699	G	P-O3'-C3'	5.94	126.83	119.70
1	A	2802	A	C2-N3-C4	5.93	113.57	110.60
58	y	29	G	N3-C4-N9	5.93	129.56	126.00
1	A	541	C	C6-N1-C2	5.93	122.67	120.30
1	A	398	G	O4'-C1'-N9	5.91	112.93	108.20
1	A	1589	C	N3-C2-O2	-5.91	117.76	121.90
1	A	1018	G	O5'-P-OP2	-5.91	100.38	105.70
1	A	1097	C	C6-N1-C2	-5.91	117.94	120.30
1	A	552	A	C8-N9-C4	-5.90	103.44	105.80
1	A	1370	G	N1-C6-O6	-5.89	116.36	119.90
1	A	798	A	P-O3'-C3'	5.89	126.77	119.70
1	A	2341	G	N1-C6-O6	-5.89	116.36	119.90
34	a	1046	C	O5'-P-OP1	-5.89	100.40	105.70
1	A	725	C	C5-C6-N1	-5.88	118.06	121.00
34	a	1006	C	N1-C2-O2	5.88	122.43	118.90
1	A	552	A	N7-C8-N9	5.85	116.73	113.80
34	a	514	G	P-O3'-C3'	5.85	126.72	119.70
57	x	17	C	C6-N1-C1'	-5.85	113.78	120.80
58	y	10	G	N1-C6-O6	5.85	123.41	119.90
1	A	1589	C	C6-N1-C2	-5.84	117.96	120.30
1	A	2331	A	N1-C6-N6	5.84	122.11	118.60
1	A	1965	U	O5'-P-OP2	-5.84	100.44	105.70
1	A	1796	U	O5'-P-OP1	-5.84	100.45	105.70
1	A	551	C	C6-N1-C2	5.83	122.63	120.30
1	A	2189	G	C4-C5-N7	5.83	113.13	110.80
34	a	1007	C	C6-N1-C1'	-5.83	113.81	120.80
1	A	11	U	N1-C2-O2	5.82	126.87	122.80
1	A	1026	A	C8-N9-C4	5.82	108.13	105.80
1	A	2517	U	C5-C4-O4	-5.80	122.42	125.90
1	A	2297	A	N9-C1'-C2'	5.80	121.54	114.00
1	A	1091	A	N3-C4-C5	5.79	130.86	126.80
1	A	136	G	O4'-C1'-N9	5.79	112.83	108.20
1	A	789	G	O5'-P-OP2	-5.79	100.49	105.70
57	x	14	A	N1-C6-N6	5.79	122.08	118.60
1	A	2081	A	C8-N9-C4	5.79	108.12	105.80
1	A	794	G	N7-C8-N9	-5.79	110.21	113.10
1	A	2458	G	C6-C5-N7	5.79	133.87	130.40
34	a	489	G	N3-C4-C5	-5.79	125.70	128.60
58	y	45	U	C6-N1-C2	-5.78	117.53	121.00
1	A	893	U	N3-C4-O4	-5.78	115.36	119.40
1	A	1343	C	C6-N1-C2	-5.78	117.99	120.30
1	A	2402	G	O4'-C1'-N9	5.77	112.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2189	G	C5-C6-O6	-5.75	125.15	128.60
1	A	2221	C	C2-N3-C4	5.75	122.78	119.90
1	A	253	A	O4'-C1'-N9	5.75	112.80	108.20
1	A	851	G	C8-N9-C4	5.75	108.70	106.40
1	A	1868	C	C6-N1-C2	-5.74	118.00	120.30
1	A	136	G	C4-C5-N7	5.74	113.09	110.80
1	A	138	A	C5-N7-C8	-5.74	101.03	103.90
57	x	46	G	N3-C2-N2	-5.73	115.89	119.90
1	A	138	A	N1-C2-N3	5.72	132.16	129.30
34	a	750	A	C8-N9-C4	5.72	108.09	105.80
34	a	884	G	N1-C6-O6	5.72	123.33	119.90
1	A	1248	A	N9-C4-C5	-5.72	103.51	105.80
1	A	1985	G	N1-C6-O6	-5.72	116.47	119.90
58	y	33	U	O4'-C1'-N1	5.71	112.77	108.20
1	A	794	G	C4-N9-C1'	-5.71	119.08	126.50
1	A	2458	G	C8-N9-C1'	5.70	134.41	127.00
1	A	839	A	N1-C6-N6	5.70	122.02	118.60
34	a	1112	C	C6-N1-C2	-5.69	118.02	120.30
34	a	1037	C	C1'-O4'-C4'	-5.69	105.35	109.90
58	y	44	G	N1-C6-O6	5.69	123.31	119.90
34	a	732	C	C2-N1-C1'	5.69	125.06	118.80
34	a	1019	G	N3-C4-N9	5.69	129.41	126.00
34	a	1317	C	N1-C2-O2	5.68	122.31	118.90
1	A	89	A	N7-C8-N9	5.68	116.64	113.80
1	A	1589	C	C6-N1-C1'	-5.68	113.99	120.80
1	A	1951	G	C4-N9-C1'	-5.67	119.12	126.50
34	a	717	A	O4'-C1'-N9	5.67	112.74	108.20
1	A	1744	A	C5-N7-C8	-5.67	101.07	103.90
1	A	1853	G	N9-C4-C5	5.67	107.67	105.40
34	a	25	U	C5-C4-O4	-5.66	122.50	125.90
58	y	46	G	C4-C5-C6	5.65	122.19	118.80
34	a	489	G	C4-N9-C1'	5.65	133.84	126.50
1	A	2801	C	O4'-C1'-N1	5.64	112.72	108.20
1	A	2189	G	N1-C6-O6	5.64	123.29	119.90
58	y	1	G	C8-N9-C4	-5.64	104.14	106.40
3	C	62	VAL	CB-CA-C	5.64	122.12	111.40
34	a	1380	C	C6-N1-C2	-5.64	118.04	120.30
1	A	1248	A	C4-C5-N7	5.63	113.52	110.70
1	A	136	G	N7-C8-N9	5.63	115.91	113.10
1	A	1298	A	C2-N3-C4	5.63	113.41	110.60
57	x	25	C	C2-N3-C4	-5.63	117.09	119.90
1	A	2013	G	OP1-P-O3'	-5.62	92.83	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	640	G	N1-C6-O6	-5.62	116.53	119.90
1	A	986	G	OP2-P-O3'	5.62	117.56	105.20
1	A	1256	G	N9-C4-C5	-5.62	103.15	105.40
1	A	805	G	O5'-P-OP2	-5.62	100.65	105.70
1	A	1005	C	N1-C2-O2	-5.62	115.53	118.90
1	A	1820	C	P-O3'-C3'	5.61	126.43	119.70
34	a	1037	C	C5'-C4'-O4'	5.61	115.83	109.10
34	a	556	A	N9-C4-C5	5.60	108.04	105.80
1	A	977	A	C4-C5-N7	5.60	113.50	110.70
1	A	2001	G	N3-C4-N9	5.60	129.36	126.00
4	D	274	ARG	C-N-CA	5.60	135.69	121.70
1	A	198	C	N1-C2-O2	-5.59	115.55	118.90
1	A	732	G	N3-C4-N9	5.59	129.35	126.00
1	A	990	G	C6-C5-N7	5.58	133.75	130.40
1	A	2840	G	C8-N9-C4	5.58	108.63	106.40
1	A	989	A	C6-C5-N7	-5.58	128.40	132.30
1	A	2517	U	N3-C4-O4	5.58	123.30	119.40
1	A	2400	G	N3-C2-N2	-5.56	116.00	119.90
1	A	800	C	O5'-P-OP2	-5.56	100.70	105.70
1	A	801	C	N1-C2-O2	5.55	122.23	118.90
1	A	989	A	O5'-P-OP1	5.55	117.36	110.70
1	A	2609	A	O5'-P-OP2	-5.55	100.71	105.70
12	O	8	LEU	CA-CB-CG	5.55	128.06	115.30
56	w	76	A	C5-N7-C8	-5.55	101.13	103.90
34	a	1048	U	O4'-C1'-N1	5.54	112.63	108.20
1	A	1773	C	C5-C4-N4	5.54	124.08	120.20
34	a	1007	C	N3-C2-O2	-5.54	118.02	121.90
1	A	1091	A	N7-C8-N9	-5.54	111.03	113.80
34	a	1019	G	C6-C5-N7	-5.53	127.08	130.40
45	l	52	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	839	A	C5-C6-N6	-5.52	119.28	123.70
1	A	1357	U	N3-C2-O2	-5.52	118.33	122.20
1	A	2458	G	N3-C4-N9	-5.52	122.69	126.00
1	A	138	A	C8-N9-C4	-5.52	103.59	105.80
59	z	292	PRO	CA-C-N	5.52	127.23	116.20
1	A	989	A	N9-C1'-C2'	5.51	121.17	114.00
34	a	1007	C	C6-N1-C2	-5.51	118.09	120.30
1	A	817	G	C5-C6-O6	-5.51	125.29	128.60
1	A	1359	C	C6-N1-C2	-5.51	118.09	120.30
1	A	2413	C	N1-C2-O2	5.51	122.21	118.90
34	a	1141	C	C4-C5-C6	5.51	120.15	117.40
56	w	12	U	C5-C4-O4	-5.50	122.60	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	x	14	A	N1-C2-N3	5.50	132.05	129.30
34	a	550	G	N1-C6-O6	-5.50	116.60	119.90
1	A	2633	C	N1-C2-O2	-5.50	115.60	118.90
1	A	2622	U	N1-C2-O2	-5.49	118.96	122.80
1	A	2120	U	N3-C2-O2	-5.49	118.36	122.20
22	Y	67	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	36	C	N3-C2-O2	-5.48	118.06	121.90
34	a	551	G	C5-C6-O6	-5.48	125.31	128.60
1	A	1746	A	O5'-P-OP1	-5.48	100.77	105.70
1	A	2583	A	N1-C6-N6	5.48	121.89	118.60
1	A	1125	C	C2-N1-C1'	5.48	124.82	118.80
1	A	709	G	N1-C6-O6	-5.47	116.62	119.90
1	A	1662	C	N1-C2-O2	-5.47	115.62	118.90
58	y	46	G	C6-N1-C2	-5.47	121.82	125.10
1	A	1758	C	C5-C6-N1	5.46	123.73	121.00
1	A	2554	G	N1-C6-O6	-5.46	116.62	119.90
1	A	598	U	C5-C4-O4	-5.45	122.63	125.90
1	A	1017	A	C5-C6-N6	5.44	128.05	123.70
1	A	2398	U	N3-C4-O4	5.44	123.21	119.40
34	a	361	U	C6-N1-C2	5.44	124.27	121.00
34	a	116	G	O5'-P-OP1	-5.44	100.80	105.70
1	A	2431	C	N3-C4-C5	5.44	124.08	121.90
34	a	1109	U	N3-C4-O4	5.44	123.21	119.40
1	A	1746	A	O5'-P-OP2	5.43	117.22	110.70
1	A	1106	U	N3-C2-O2	-5.42	118.40	122.20
41	h	112	LEU	CA-CB-CG	5.42	127.75	115.30
1	A	1066	A	N3-C4-C5	5.41	130.59	126.80
1	A	701	A	N1-C6-N6	5.41	121.85	118.60
25	1	80	LEU	CA-CB-CG	-5.41	102.86	115.30
1	A	1366	A	N1-C6-N6	5.41	121.85	118.60
1	A	2370	C	C6-N1-C2	-5.41	118.14	120.30
34	a	1445	G	O5'-P-OP2	-5.41	100.83	105.70
1	A	89	A	C8-N9-C4	-5.41	103.64	105.80
1	A	1292	A	N9-C4-C5	-5.41	103.64	105.80
1	A	2617	C	C2-N1-C1'	-5.41	112.85	118.80
1	A	136	G	C5-N7-C8	-5.40	101.60	104.30
27	3	4	LEU	CA-CB-CG	5.39	127.70	115.30
56	w	63	G	C6-C5-N7	-5.39	127.16	130.40
1	A	1154	C	C6-N1-C2	-5.39	118.14	120.30
1	A	1818	C	N1-C2-O2	5.38	122.13	118.90
1	A	989	A	C5-C6-N6	-5.38	119.40	123.70
1	A	1646	G	N1-C6-O6	-5.37	116.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1417	U	N1-C2-O2	5.36	126.56	122.80
50	q	6	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	2120	U	N1-C2-O2	5.35	126.55	122.80
1	A	2591	U	C2-N1-C1'	5.35	124.12	117.70
34	a	797	U	OP2-P-O3'	5.35	116.97	105.20
34	a	891	A	O5'-P-OP2	-5.35	100.89	105.70
34	a	1267	A	N1-C6-N6	5.35	121.81	118.60
1	A	2505	G	C5-C6-O6	5.34	131.81	128.60
57	x	17	C	C6-N1-C2	-5.34	118.16	120.30
1	A	657	A	C8-N9-C4	5.34	107.94	105.80
34	a	28	G	OP2-P-O3'	5.33	116.94	105.20
1	A	989	A	N7-C8-N9	5.33	116.47	113.80
34	a	417	U	C2-N1-C1'	5.33	124.10	117.70
34	a	1203	G	C6-C5-N7	5.33	133.60	130.40
1	A	2456	G	N3-C2-N2	5.33	123.63	119.90
57	x	76	A	N1-C6-N6	5.33	121.80	118.60
1	A	1091	A	C6-C5-N7	-5.33	128.57	132.30
1	A	2801	C	C2-N1-C1'	-5.33	112.94	118.80
1	A	2298	A	N3-C4-N9	-5.33	123.14	127.40
34	a	715	G	O5'-P-OP2	-5.33	100.91	105.70
1	A	1818	C	N3-C2-O2	-5.32	118.17	121.90
1	A	2589	G	N3-C2-N2	-5.32	116.17	119.90
1	A	1612	A	N1-C2-N3	-5.32	126.64	129.30
1	A	2018	G	O5'-P-OP1	5.31	117.08	110.70
1	A	2428	C	C6-N1-C2	-5.31	118.18	120.30
1	A	2505	G	N1-C6-O6	-5.30	116.72	119.90
1	A	1256	G	C8-N9-C4	5.30	108.52	106.40
1	A	2331	A	N9-C4-C5	-5.29	103.68	105.80
1	A	2070	G	O5'-P-OP2	-5.29	100.94	105.70
56	w	75	C	N3-C2-O2	-5.29	118.20	121.90
1	A	2535	G	OP2-P-O3'	5.28	116.83	105.20
34	a	872	G	N1-C6-O6	-5.28	116.73	119.90
1	A	2418	G	C4-N9-C1'	5.28	133.36	126.50
34	a	1301	A	C8-N9-C4	-5.28	103.69	105.80
1	A	542	G	N1-C6-O6	-5.28	116.73	119.90
34	a	891	A	P-O3'-C3'	5.28	126.03	119.70
1	A	88	U	O4'-C1'-N1	5.27	112.42	108.20
34	a	1503	G	N1-C6-O6	-5.27	116.74	119.90
1	A	1955	C	N3-C4-N4	-5.27	114.31	118.00
1	A	794	G	C8-N9-C4	5.26	108.51	106.40
1	A	2831	G	C5-C6-O6	-5.26	125.44	128.60
34	a	877	C	N1-C2-O2	-5.26	115.74	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1768	G	O5'-P-OP1	-5.25	100.97	105.70
1	A	353	A	N9-C4-C5	5.25	107.90	105.80
1	A	242	G	O5'-P-OP2	-5.25	100.98	105.70
1	A	1856	G	N1-C6-O6	-5.25	116.75	119.90
1	A	2891	A	N1-C6-N6	-5.25	115.45	118.60
1	A	2624	U	C5-C6-N1	-5.24	120.08	122.70
34	a	547	A	N9-C4-C5	-5.24	103.70	105.80
56	w	2	C	N3-C4-N4	-5.23	114.34	118.00
57	x	16	C	OP1-P-O3'	5.23	116.71	105.20
1	A	2189	G	N9-C4-C5	-5.22	103.31	105.40
1	A	1425	G	O5'-P-OP2	-5.22	101.00	105.70
1	A	2100	U	N1-C2-O2	-5.22	119.15	122.80
34	a	1441	C	C6-N1-C2	5.22	122.39	120.30
56	w	72	C	N3-C2-O2	-5.22	118.25	121.90
1	A	1196	G	C8-N9-C4	5.21	108.49	106.40
59	z	373	ALA	C-N-CA	5.21	143.87	122.00
1	A	441	A	C2-N3-C4	5.20	113.20	110.60
1	A	598	U	OP1-P-OP2	5.20	127.41	119.60
1	A	1865	G	OP2-P-O3'	5.20	116.64	105.20
34	a	953	A	N7-C8-N9	5.20	116.40	113.80
34	a	1389	U	C5-C6-N1	-5.20	120.10	122.70
58	y	1	G	N3-C4-C5	-5.20	126.00	128.60
34	a	356	A	N1-C6-N6	-5.20	115.48	118.60
1	A	504	A	N1-C6-N6	-5.19	115.48	118.60
1	A	1853	G	N3-C4-N9	-5.19	122.88	126.00
1	A	11	U	N3-C2-O2	-5.19	118.56	122.20
1	A	2114	G	C8-N9-C4	5.19	108.48	106.40
34	a	23	G	N1-C6-O6	5.19	123.02	119.90
34	a	1420	C	OP2-P-O3'	5.19	116.62	105.20
34	a	1496	A	C5-C6-N1	-5.19	115.10	117.70
1	A	2297	A	C5-C6-N1	-5.19	115.11	117.70
1	A	538	A	OP1-P-OP2	5.18	127.38	119.60
1	A	1774	C	N1-C2-O2	5.18	122.01	118.90
34	a	1008	C	C2-N1-C1'	5.18	124.50	118.80
34	a	1482	G	C6-N1-C2	5.18	128.21	125.10
1	A	942	C	C2-N1-C1'	5.17	124.49	118.80
1	A	1017	A	N9-C4-C5	5.17	107.87	105.80
1	A	1814	A	C8-N9-C4	5.16	107.86	105.80
34	a	514	G	OP2-P-O3'	5.16	116.55	105.20
1	A	837	C	C2-N1-C1'	-5.16	113.13	118.80
58	y	25	C	C6-N1-C2	-5.16	118.24	120.30
1	A	597	A	O5'-P-OP1	-5.15	101.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2495	G	C5-C6-O6	-5.15	125.51	128.60
1	A	1761	G	C4-N9-C1'	-5.14	119.82	126.50
34	a	25	U	N3-C4-O4	5.14	123.00	119.40
1	A	1773	C	C6-N1-C1'	5.13	126.96	120.80
34	a	1398	G	O5'-P-OP2	-5.13	101.08	105.70
1	A	1808	U	C2-N3-C4	-5.13	123.92	127.00
1	A	552	A	N3-C4-N9	-5.12	123.30	127.40
1	A	854	G	C8-N9-C4	5.12	108.45	106.40
1	A	553	A	C5-N7-C8	-5.12	101.34	103.90
58	y	19	G	C4-N9-C1'	-5.12	119.84	126.50
1	A	2675	G	N1-C6-O6	-5.12	116.83	119.90
1	A	1185	U	N1-C2-O2	-5.11	119.22	122.80
34	a	671	A	P-O3'-C3'	5.11	125.83	119.70
1	A	2092	A	C8-N9-C4	-5.11	103.76	105.80
1	A	554	G	C5-N7-C8	-5.11	101.75	104.30
1	A	1248	A	C6-C5-N7	-5.10	128.73	132.30
1	A	604	G	C5-C6-O6	5.10	131.66	128.60
1	A	1821	A	O5'-P-OP1	-5.10	101.11	105.70
1	A	2528	C	N3-C4-C5	5.10	123.94	121.90
1	A	554	G	C4-C5-N7	5.10	112.84	110.80
1	A	2621	C	C2-N3-C4	-5.09	117.35	119.90
34	a	324	C	O5'-P-OP1	-5.09	101.12	105.70
1	A	2614	G	N9-C4-C5	5.09	107.44	105.40
34	a	323	A	O4'-C1'-N9	5.09	112.27	108.20
34	a	293	G	C8-N9-C4	5.09	108.44	106.40
34	a	1502	C	C6-N1-C2	5.09	122.33	120.30
19	V	18	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	604	G	N1-C6-O6	-5.08	116.85	119.90
55	v	13	A	C4-C5-N7	5.08	113.24	110.70
1	A	732	G	N3-C2-N2	5.08	123.45	119.90
1	A	1005	C	O5'-P-OP2	-5.08	101.13	105.70
56	w	75	C	N1-C2-O2	5.07	121.94	118.90
1	A	182	G	N9-C4-C5	-5.07	103.37	105.40
34	a	847	G	C5-C6-O6	-5.07	125.56	128.60
1	A	989	A	C8-N9-C4	-5.07	103.77	105.80
1	A	1915	C	N1-C2-O2	5.07	121.94	118.90
1	A	2249	G	N3-C4-C5	-5.07	126.07	128.60
34	a	953	A	C4-C5-N7	5.07	113.23	110.70
1	A	1955	C	C5-C4-N4	5.07	123.75	120.20
1	A	843	C	N1-C2-O2	-5.06	115.86	118.90
1	A	932	C	O5'-P-OP2	-5.06	101.15	105.70
34	a	844	C	N1-C2-O2	-5.06	115.87	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2319	G	C4-C5-N7	5.05	112.82	110.80
1	A	2120	U	C2-N1-C1'	5.05	123.76	117.70
45	l	84	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	951	G	C8-N9-C1'	5.04	133.55	127.00
1	A	1699	G	C4-N9-C1'	5.04	133.05	126.50
1	A	2103	A	O5'-P-OP2	-5.04	101.17	105.70
1	A	1643	C	C2-N1-C1'	5.03	124.33	118.80
1	A	2219	A	O4'-C1'-N9	5.03	112.22	108.20
1	A	592	G	N1-C6-O6	-5.03	116.89	119.90
1	A	1292	A	C5-C6-N6	-5.03	119.68	123.70
1	A	1853	G	N1-C2-N2	5.03	120.72	116.20
1	A	2163	C	C5-C6-N1	5.03	123.51	121.00
1	A	2591	U	C5-C4-O4	-5.02	122.89	125.90
34	a	1006	C	C6-N1-C2	-5.02	118.29	120.30
57	x	25	C	N1-C2-O2	-5.02	115.89	118.90
58	y	14	A	N1-C6-N6	5.01	121.61	118.60
1	A	1761	G	C4-C5-N7	5.01	112.80	110.80

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	2	44	LEU	Peptide
28	4	65	ASP	Peptide
10	K	70	LYS	Peptide
19	V	43	GLU	Peptide
37	d	179	GLU	Peptide
39	f	97	PHE	Peptide
42	i	117	HIS	Peptide
42	i	45	ALA	Peptide
52	s	29	ARG	Peptide
52	s	8	GLY	Peptide
53	t	9	ASN	Peptide
59	z	185	ILE	Peptide
59	z	246	THR	Peptide
59	z	372	THR	Peptide
59	z	396	LEU	Peptide
59	z	419	GLU	Peptide
59	z	480	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61902	0	31210	820	1
2	B	2573	0	1306	29	0
3	C	1024	0	1007	81	0
4	D	2136	0	2218	65	0
5	E	1559	0	1618	46	0
6	F	1584	0	1625	52	0
7	G	1425	0	1443	56	0
8	H	1330	0	1407	47	0
9	J	641	0	309	19	0
10	K	1025	0	1066	64	0
11	N	1117	0	1184	27	0
12	O	933	0	996	30	0
13	P	1135	0	1212	38	0
14	Q	1122	0	1179	23	0
15	R	968	0	1033	12	0
16	S	877	0	938	32	0
17	T	1091	0	1151	33	0
18	U	959	0	1019	26	0
19	V	771	0	830	19	0
20	W	886	0	940	23	1
21	X	750	0	814	19	0
22	Y	806	0	881	17	0
23	Z	784	0	796	18	0
24	0	591	0	607	15	0
25	1	755	0	826	22	0
26	2	588	0	643	15	0
27	3	469	0	518	8	0
28	4	557	0	535	28	0
29	5	459	0	476	13	0
30	6	453	0	473	7	0
31	7	430	0	480	8	0
32	8	511	0	571	16	0
33	9	307	0	335	13	0
34	a	32207	0	16255	0	0
35	b	1850	0	1871	0	0
36	c	1550	0	1539	0	0
37	d	1655	0	1673	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	e	1129	0	1185	0	0
39	f	806	0	793	0	0
40	g	1227	0	1232	0	0
41	h	1088	0	1126	0	0
42	i	983	0	986	0	0
43	j	698	0	637	0	0
44	k	829	0	825	0	0
45	l	930	0	980	0	0
46	m	924	0	960	0	0
47	n	492	0	529	0	0
48	o	728	0	760	0	0
49	p	681	0	697	0	0
50	q	823	0	891	0	0
51	r	555	0	618	0	0
52	s	650	0	655	0	0
53	t	724	0	787	0	0
54	u	199	0	208	0	0
55	v	277	0	140	0	0
56	w	1586	0	819	0	0
57	x	1645	0	839	0	0
58	y	1580	0	801	0	0
59	z	5200	0	5309	0	0
60	0	4	0	0	0	0
60	5	2	0	0	0	0
60	6	2	0	0	0	0
60	7	1	0	0	0	0
60	8	1	0	0	0	0
60	9	1	0	0	0	0
60	A	644	0	0	0	0
60	B	18	0	0	0	0
60	D	6	0	0	0	0
60	E	5	0	0	0	0
60	F	6	0	0	0	0
60	G	2	0	0	0	0
60	H	1	0	0	0	0
60	N	1	0	0	0	0
60	O	2	0	0	0	0
60	P	3	0	0	0	0
60	Q	2	0	0	0	0
60	R	2	0	0	0	0
60	U	1	0	0	0	0
60	V	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	W	1	0	0	0	0
60	X	1	0	0	0	0
60	Z	1	0	0	0	0
60	a	188	0	0	0	0
60	d	1	0	0	0	0
60	e	1	0	0	0	0
60	f	1	0	0	0	0
60	l	1	0	0	0	0
60	m	2	0	0	0	0
60	n	3	0	0	0	0
60	v	2	0	0	0	0
60	x	9	0	0	0	0
60	z	2	0	0	0	0
61	4	1	0	0	0	0
61	5	1	0	0	0	0
61	6	1	0	0	0	0
61	9	1	0	0	0	0
61	Y	1	0	0	0	0
61	n	1	0	0	0	0
62	d	8	0	0	0	0
63	z	32	0	14	0	0
64	0	3	0	0	0	0
64	1	1	0	0	0	0
64	3	1	0	0	0	0
64	7	1	0	0	0	0
64	8	4	0	0	0	0
64	A	715	0	0	37	0
64	B	32	0	0	0	0
64	D	4	0	0	0	0
64	E	6	0	0	1	0
64	F	5	0	0	0	0
64	H	1	0	0	0	0
64	N	1	0	0	0	0
64	O	3	0	0	0	0
64	P	8	0	0	0	0
64	Q	3	0	0	0	0
64	T	2	0	0	0	0
64	U	3	0	0	0	0
64	V	1	0	0	0	0
64	a	165	0	0	0	0
64	l	1	0	0	0	0
64	p	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	v	3	0	0	0	0
64	w	1	0	0	0	0
64	z	1	0	0	0	0
All	All	155465	0	104775	1518	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1518) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:PRO:C	3:C:203:GLY:HA2	1.75	1.06
3:C:199:HIS:O	3:C:201:PRO:HD3	1.57	1.03
1:A:1091:A:N1	9:J:6:ASN:N	2.14	0.95
1:A:679:G:O6	1:A:698:C:N4	2.02	0.92
1:A:1649:C:OP2	64:A:3701:HOH:O	1.90	0.89
1:A:1064:U:HO2'	1:A:1066:A:H2	0.92	0.89
1:A:1105:U:H4'	1:A:1106:U:H5'	1.55	0.89
1:A:1813:A:OP2	64:A:3702:HOH:O	1.91	0.88
1:A:1448:C:H5''	1:A:1517:A:H1'	1.56	0.87
5:E:72:VAL:HA	5:E:73:GLU:HB2	1.53	0.86
3:C:201:PRO:C	3:C:203:GLY:CA	2.44	0.86
8:H:42:ARG:NH1	8:H:53:GLU:OE2	2.09	0.86
1:A:2126:C:H41	1:A:2205:G:H1	1.22	0.85
1:A:1812:C:OP1	64:A:3702:HOH:O	1.94	0.85
1:A:1103:G:N2	10:K:126:MET:SD	2.52	0.83
1:A:817:G:OP1	31:7:10:ARG:NH1	2.12	0.82
8:H:40:GLU:OE2	8:H:60:ARG:NH1	2.10	0.82
1:A:2330:G:H22	16:S:3:ARG:HB2	1.45	0.81
27:3:8:LEU:HD13	27:3:31:LEU:HD23	1.63	0.81
1:A:2803:C:O2	1:A:2815:G:N1	2.14	0.80
11:N:20:GLY:HA2	11:N:61:ARG:HD2	1.63	0.80
1:A:324:G:OP2	22:Y:84:ARG:NH2	2.15	0.80
1:A:1038:G:OP1	18:U:50:ARG:NH2	2.14	0.79
4:D:69:ARG:NH2	4:D:128:GLY:O	2.15	0.79
4:D:274:ARG:HA	4:D:275:LYS:HB2	1.64	0.79
1:A:1759:U:N3	1:A:1775:G:O6	2.14	0.79
1:A:1091:A:OP2	1:A:1091:A:H4'	1.75	0.79
1:A:1828:U:H5'	4:D:259:THR:HG22	1.64	0.79
16:S:58:LEU:HB3	16:S:59:LYS:HB2	1.65	0.79
1:A:1099:A:H62	1:A:1150:U:H3	1.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1758:C:H42	1:A:1776:G:H1	1.31	0.79
1:A:1735:A:H62	1:A:1744:A:H2	1.28	0.78
1:A:2018:G:OP2	64:A:3703:HOH:O	1.99	0.78
25:1:50:ARG:HG2	25:1:59:THR:HG22	1.65	0.78
10:K:13:PRO:HG2	10:K:16:LYS:HB3	1.65	0.78
1:A:136:G:N2	21:X:44:GLU:OE1	2.17	0.78
13:P:100:LEU:HD22	13:P:105:LEU:HD12	1.65	0.78
1:A:1248:A:H2	1:A:1286:A:H62	1.30	0.78
1:A:1116:G:N2	1:A:1124:C:O2	18.16	0.78
8:H:121:ILE:HD11	8:H:140:LYS:HG3	1.66	0.78
1:A:786:U:OP2	64:A:3704:HOH:O	2.01	0.78
1:A:655:A:OP1	13:P:65:ARG:NH1	2.18	0.76
1:A:908:G:OP2	64:A:3705:HOH:O	2.02	0.76
28:4:53:GLU:HG3	28:4:55:ARG:H	1.51	0.76
8:H:54:ARG:HH21	8:H:57:ASP:HB2	1.49	0.76
1:A:2415:C:OP2	64:A:3706:HOH:O	2.03	0.76
1:A:1775:G:H3'	1:A:1776:G:C8	2.21	0.76
1:A:1760:G:H1	1:A:1774:C:N4	1.84	0.76
1:A:238:G:OP2	32:8:13:ARG:NH2	2.19	0.75
3:C:209:LEU:H	3:C:209:LEU:HD13	1.51	0.75
1:A:2866:G:N2	1:A:2869:A:OP2	2.20	0.74
21:X:31:HIS:HD2	21:X:33:LYS:H	1.33	0.74
25:1:76:ARG:HB2	25:1:97:LEU:HD13	1.70	0.73
3:C:201:PRO:O	3:C:203:GLY:HA2	1.87	0.73
20:W:68:ARG:HD3	20:W:111:HIS:CD2	2.23	0.73
1:A:1184:C:O3'	11:N:25:ARG:NH1	2.21	0.73
4:D:180:GLY:HA3	4:D:275:LYS:HG2	1.68	0.73
8:H:137:ASP:HB3	8:H:140:LYS:HG2	1.69	0.73
1:A:679:G:O6	1:A:698:C:N3	2.21	0.73
1:A:2145:G:H5'	3:C:174:PRO:HD3	1.71	0.73
17:T:54:ARG:HA	17:T:59:THR:HB	1.70	0.73
24:0:11:ARG:O	24:0:14:ARG:NH2	2.21	0.73
8:H:46:GLU:OE1	8:H:51:ARG:NH2	2.21	0.73
19:V:40:LEU:HB2	19:V:46:VAL:HG12	1.69	0.73
28:4:45:GLY:O	28:4:47:GLN:N	2.20	0.72
1:A:1813:A:OP1	64:A:3704:HOH:O	2.08	0.72
7:G:80:PHE:O	7:G:82:LEU:N	2.21	0.72
1:A:1402:U:OP1	31:7:23:ARG:NH1	2.22	0.72
16:S:15:ARG:HH11	16:S:25:ARG:HH21	1.35	0.72
20:W:65:LEU:HD12	20:W:68:ARG:HH21	1.54	0.72
1:A:1218:A:H4'	1:A:1219:U:OP1	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1552:A:O2'	1:A:1553:A:O5'	2.07	0.72
10:K:13:PRO:HB3	10:K:52:ILE:HG12	1.71	0.72
1:A:2330:G:N2	16:S:3:ARG:HB2	2.04	0.72
3:C:21:THR:H	3:C:24:GLU:HB2	1.54	0.72
23:Z:77:ASP:HB2	23:Z:84:GLU:HG3	1.72	0.72
1:A:1232:U:H4'	19:V:79:VAL:HG22	1.71	0.71
7:G:18:GLU:OE1	7:G:22:ARG:NH2	2.23	0.71
1:A:955:A:H62	14:Q:12:GLN:HA	1.55	0.71
1:A:1311:G:O5'	20:W:15:ARG:NH2	2.23	0.71
6:F:116:ASP:OD1	6:F:119:ARG:NH2	2.24	0.71
7:G:145:THR:OG1	7:G:146:TYR:N	2.18	0.71
1:A:2648:U:H5''	5:E:82:ARG:HH21	1.55	0.71
1:A:596:C:OP2	64:A:3708:HOH:O	2.09	0.71
1:A:2197:A:OP1	3:C:7:TYR:OH	2.07	0.70
1:A:2155:A:H1'	1:A:2180:G:H21	1.54	0.70
1:A:88:U:O2'	1:A:89:A:O4'	2.09	0.70
4:D:137:PRO:O	4:D:140:THR:HG23	1.90	0.70
2:B:40:U:O4	28:4:1:MET:N	2.24	0.70
1:A:1140:A:N1	1:A:1160:G:N2	51.75	0.70
6:F:185:ASP:HA	6:F:188:ARG:HD3	1.74	0.70
16:S:59:LYS:HE2	16:S:60:GLY:N	2.07	0.69
1:A:2280:A:OP1	64:A:3707:HOH:O	2.09	0.69
3:C:175:VAL:HG22	3:C:176:GLY:H	1.57	0.69
21:X:31:HIS:CD2	21:X:33:LYS:H	2.09	0.69
1:A:624:G:O2'	1:A:701:A:N6	2.25	0.69
15:R:97:VAL:HG22	15:R:114:VAL:HG13	1.73	0.69
1:A:1784:C:OP1	17:T:96:ARG:NH1	2.25	0.69
1:A:2360:G:OP1	64:A:3709:HOH:O	2.11	0.69
2:B:6:C:H2'	2:B:7:G:H5''	1.75	0.69
3:C:163:PHE:HB2	3:C:171:ILE:HD11	1.75	0.69
14:Q:67:ARG:O	14:Q:101:ARG:NH2	2.25	0.69
17:T:55:ASN:H	17:T:59:THR:HG22	1.58	0.69
1:A:1220:G:N2	1:A:1222:C:OP2	2.26	0.69
10:K:102:GLU:HA	10:K:105:LEU:HB2	1.74	0.69
16:S:59:LYS:HE2	16:S:60:GLY:H	1.57	0.69
8:H:127:GLU:OE2	8:H:129:THR:OG1	2.11	0.69
1:A:1150:U:H2'	1:A:1151:G:C8	2.27	0.69
1:A:1765:G:N2	1:A:1767:U:OP2	2.27	0.68
1:A:2493:G:OP1	64:A:3710:HOH:O	2.11	0.68
3:C:171:ILE:O	3:C:172:HIS:ND1	2.27	0.68
3:C:62:VAL:HG13	3:C:63:SER:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:C:OP2	64:A:3711:HOH:O	2.12	0.68
1:A:1739:U:O2'	4:D:14:ARG:NH2	2.26	0.68
1:A:2622:U:C4	29:5:3:LYS:HG2	2.29	0.68
12:O:7:TYR:HE1	12:O:20:MET:HE3	1.57	0.68
10:K:69:THR:OG1	10:K:70:LYS:N	2.24	0.68
1:A:2316:A:H5''	7:G:134:GLY:HA3	1.76	0.68
1:A:679:G:O6	1:A:698:C:C4	2.46	0.68
3:C:179:SER:HA	3:C:180:PHE:O	1.92	0.68
17:T:84:GLN:HG2	17:T:85:LYS:HG2	1.76	0.68
1:A:1898:A:H5'	1:A:1899:G:OP2	1.94	0.67
9:J:26:LEU:HA	9:J:84:GLU:HA	1.74	0.67
1:A:1067:G:N2	1:A:1068:U:O4	2.23	0.67
7:G:161:THR:HG22	7:G:163:ALA:H	1.58	0.67
19:V:34:GLU:OE2	19:V:100:ARG:NH2	2.27	0.67
1:A:1310:A:OP2	64:A:3712:HOH:O	2.12	0.67
1:A:1637:C:H2'	1:A:1638:G:C8	2.29	0.67
1:A:1109:C:HO2'	10:K:89:HIS:HE2	1.35	0.67
3:C:21:THR:HB	3:C:24:GLU:H	1.59	0.67
1:A:1127:U:H3'	1:A:1128:U:H5''	1.76	0.67
1:A:926:G:N2	1:A:943:C:N3	2.43	0.67
7:G:18:GLU:OE2	7:G:21:ARG:NH1	2.27	0.67
1:A:2803:C:H2'	1:A:2804:G:C8	2.30	0.66
1:A:1648:A:OP1	64:A:3701:HOH:O	2.12	0.66
10:K:41:PHE:HZ	10:K:53:VAL:HB	1.61	0.66
2:B:8:U:H5''	16:S:15:ARG:HH12	1.61	0.66
9:J:73:GLY:O	9:J:75:GLN:N	2.27	0.66
20:W:25:ARG:NH2	20:W:74:ALA:O	2.27	0.66
1:A:448:A:OP2	64:A:3715:HOH:O	2.14	0.66
3:C:194:ARG:NH2	3:C:197:GLU:OE1	2.28	0.66
1:A:1768:G:H3'	1:A:1769:A:H8	1.59	0.66
1:A:1775:G:H3'	1:A:1776:G:H8	1.59	0.66
1:A:931:C:H3'	1:A:932:C:H5''	1.78	0.66
1:A:2824:C:H5'	29:5:29:THR:HG21	1.78	0.66
1:A:1091:A:N6	9:J:8:GLU:H	1.94	0.65
1:A:1814:A:OP2	64:A:3704:HOH:O	2.14	0.65
1:A:240:G:P	13:P:50:ARG:HH12	2.19	0.65
1:A:2157:C:N4	1:A:2176:G:H1	1.95	0.65
1:A:1153:U:O2'	1:A:1154:C:O5'	2.09	0.65
1:A:1828:U:OP2	4:D:274:ARG:NH2	2.28	0.65
1:A:850:A:OP2	64:A:3714:HOH:O	2.14	0.65
1:A:2417:U:C2	13:P:72:PRO:HG2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:33:ALA:O	24:0:35:ASN:N	2.29	0.65
29:5:16:ARG:HH11	29:5:16:ARG:HG2	1.62	0.65
6:F:157:VAL:HB	6:F:194:MET:HG2	1.77	0.65
1:A:1423:A:O2'	1:A:1425:G:N7	2.26	0.65
1:A:926:G:H2'	1:A:927:G:C8	2.31	0.64
1:A:1249:U:C2	6:F:171:PRO:HB3	2.32	0.64
1:A:1845:A:OP2	4:D:54:ARG:NH2	2.30	0.64
20:W:79:GLY:HA3	20:W:100:THR:HG22	1.78	0.64
11:N:34:LEU:O	11:N:49:GLY:HA3	1.97	0.64
1:A:1153:U:O2'	1:A:1154:C:H6	1.81	0.64
1:A:2125:G:O6	1:A:2206:C:N4	2.31	0.64
1:A:904:U:OP2	24:0:77:ARG:NH2	2.28	0.64
1:A:1873:C:H5'	4:D:253:GLN:HE22	1.63	0.64
1:A:237:C:O2	32:8:12:LYS:NZ	2.28	0.64
1:A:2204:C:H2'	1:A:2205:G:C8	2.33	0.64
1:A:964:G:N2	1:A:2280:A:OP2	2.31	0.64
1:A:1124:C:H4'	10:K:132:ARG:CZ	2.28	0.64
1:A:732:G:H5''	31:7:11:LYS:HE2	1.79	0.63
1:A:1092:G:OP1	1:A:1092:G:H4'	1.99	0.63
1:A:1810:A:OP1	64:A:3702:HOH:O	2.15	0.63
1:A:2135:A:O2'	1:A:2188:U:O2'	2.07	0.63
1:A:308:C:H42	1:A:379:G:H1	1.46	0.63
1:A:1891:G:H5''	3:C:206:GLY:HA2	1.80	0.63
10:K:23:VAL:HA	10:K:27:LEU:HD13	1.80	0.63
14:Q:16:ARG:HG2	14:Q:18:LYS:HG3	1.81	0.63
1:A:2121:G:H1	1:A:2210:U:H5	1.46	0.63
1:A:33:C:H2'	1:A:34:G:H5'	1.81	0.63
4:D:70:TRP:CE2	4:D:150:LYS:HD2	2.34	0.63
1:A:332:G:N3	1:A:352:G:O2'	2.31	0.63
3:C:182:PRO:C	3:C:184:LYS:H	2.02	0.63
1:A:2456:G:OP1	6:F:74:ARG:NH2	2.32	0.63
1:A:1735:A:N6	1:A:1744:A:H2	1.97	0.62
1:A:677:A:O3'	1:A:678:A:O4'	2.16	0.62
25:1:3:LYS:O	25:1:12:PRO:HD3	2.00	0.62
1:A:1820:C:H2'	1:A:1821:A:C5	2.34	0.62
1:A:554:G:N1	64:A:3719:HOH:O	2.18	0.62
15:R:20:LEU:HD21	15:R:40:LYS:HD2	1.81	0.62
1:A:2330:G:N1	16:S:3:ARG:HA	2.15	0.62
1:A:2762:A:OP2	8:H:62:LYS:NZ	2.28	0.62
15:R:28:LEU:HD12	15:R:48:VAL:HG21	1.80	0.62
20:W:83:LYS:O	20:W:84:ARG:HD3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:U:O2'	1:A:1066:A:H2	1.73	0.62
1:A:1682:C:OP2	64:A:3718:HOH:O	2.15	0.62
1:A:1000:G:OP2	14:Q:14:ARG:NH2	2.33	0.62
1:A:2131:G:O2'	1:A:2141:G:H5'	1.99	0.62
1:A:609:C:OP2	13:P:21:ARG:NH2	2.33	0.62
1:A:926:G:H2'	1:A:927:G:H8	1.64	0.62
10:K:17:ALA:HB1	10:K:38:VAL:HG22	1.80	0.62
19:V:46:VAL:HG13	19:V:52:VAL:HG11	1.80	0.62
1:A:2595:U:H2'	1:A:2596:U:H2'	1.81	0.62
6:F:132:VAL:HA	6:F:138:GLU:HB3	1.82	0.62
4:D:17:THR:O	4:D:211:ARG:NH2	2.32	0.61
17:T:74:ARG:HG2	17:T:74:ARG:HH11	1.64	0.61
1:A:1070:G:C4	1:A:1179:C:H1'	2.35	0.61
1:A:1210:U:H2'	1:A:1211:C:C6	2.35	0.61
1:A:1632:A:H2'	1:A:1633:C:C6	2.35	0.61
1:A:775:G:OP2	4:D:13:ARG:HD3	2.01	0.61
1:A:2430:U:O4	64:A:3713:HOH:O	2.14	0.61
6:F:143:ALA:HB1	6:F:148:LEU:HB2	1.82	0.61
10:K:14:ALA:HB2	10:K:53:VAL:HG23	1.82	0.61
18:U:36:ARG:HD2	18:U:40:PHE:CZ	2.35	0.61
10:K:108:ALA:O	10:K:112:MET:HG2	2.01	0.61
1:A:1150:U:H2'	1:A:1151:G:H8	1.65	0.61
1:A:1288:G:O2'	13:P:7:ARG:NH2	2.33	0.61
1:A:1295:G:N7	13:P:18:ARG:NH2	2.49	0.61
1:A:2148:G:O6	1:A:2182:C:N4	2.33	0.61
1:A:353:A:H2	1:A:1254:A:H2'	1.66	0.60
25:1:85:LEU:HB3	25:1:89:GLU:HG3	1.82	0.60
28:4:14:ILE:HB	28:4:22:ILE:HG13	1.84	0.60
1:A:596:C:N3	5:E:145:LYS:NZ	2.49	0.60
7:G:12:TYR:HA	7:G:16:ARG:HG3	1.81	0.60
7:G:5:VAL:HG23	7:G:8:LYS:HE2	1.82	0.60
25:1:80:LEU:HG	25:1:81:LYS:H	1.66	0.60
8:H:106:THR:HG22	8:H:112:PRO:HB3	1.84	0.60
13:P:88:LEU:HD11	13:P:114:ILE:HD12	1.83	0.60
1:A:1643:C:H5'	21:X:36:LYS:HB2	1.83	0.60
1:A:1873:C:H5'	4:D:253:GLN:NE2	2.16	0.60
5:E:117:MET:O	5:E:118:LYS:HB3	2.02	0.60
8:H:98:LEU:HG	8:H:125:VAL:HG23	1.84	0.60
1:A:235:G:H4'	1:A:412:G:C5	2.36	0.60
25:1:23:LYS:HB3	25:1:29:GLY:HA3	1.82	0.60
1:A:1091:A:N1	9:J:7:VAL:N	2.46	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:U:H2'	1:A:1451:U:C6	2.36	0.60
1:A:1125:C:O2	1:A:1126:U:H6	1.84	0.60
6:F:18:ARG:HH12	6:F:20:LEU:HD23	1.67	0.60
11:N:42:TRP:HA	11:N:48:MET:HE1	1.82	0.60
1:A:1603:C:OP2	1:A:1604:A:O2'	2.09	0.60
1:A:648:C:O2'	1:A:703:U:OP1	2.17	0.60
1:A:732:G:OP1	31:7:11:LYS:NZ	2.29	0.60
1:A:1833:A:O2'	4:D:259:THR:HG21	2.02	0.60
17:T:23:ARG:HG3	17:T:120:ARG:NH1	2.17	0.60
20:W:18:ARG:NH1	20:W:76:VAL:O	2.35	0.60
25:1:72:GLU:OE1	25:1:76:ARG:NH2	2.35	0.59
1:A:2143:U:O2	3:C:172:HIS:NE2	2.36	0.59
1:A:2298:A:H62	1:A:2355:U:H3	1.50	0.59
19:V:72:VAL:HG13	19:V:85:LYS:HB3	1.83	0.59
1:A:713:U:O2	32:8:2:PRO:HD2	2.02	0.59
1:A:2148:G:O2'	1:A:2149:C:H5'	2.03	0.59
1:A:505:A:OP2	22:Y:47:LYS:NZ	2.34	0.59
6:F:53:THR:CG2	6:F:55:GLY:H	2.16	0.59
10:K:76:TYR:HB2	10:K:79:ARG:HH21	1.67	0.59
17:T:122:ASP:OD1	17:T:125:ARG:NH2	2.34	0.59
1:A:1125:C:O2	1:A:1125:C:H2'	2.00	0.59
8:H:76:VAL:O	8:H:80:SER:HB2	2.02	0.59
1:A:69:A:N7	21:X:31:HIS:HE1	2.00	0.59
1:A:938:C:H2'	1:A:939:C:C6	2.37	0.59
10:K:51:ALA:HB3	10:K:72:PRO:HB3	1.84	0.59
1:A:2548:U:H2'	1:A:2549:C:C6	2.38	0.59
20:W:18:ARG:HG3	20:W:76:VAL:HB	1.83	0.59
21:X:41:ASN:O	21:X:45:THR:HG23	2.03	0.59
1:A:1091:A:N6	9:J:5:ARG:H	2.01	0.59
1:A:2449:U:O2'	1:A:2451:C:OP1	2.18	0.59
1:A:330:G:H22	1:A:333:A:H5''	1.67	0.59
1:A:644:G:H5'	1:A:644:G:N3	2.18	0.59
1:A:931:C:H3'	1:A:932:C:C5'	2.32	0.59
13:P:118:GLY:O	13:P:137:LYS:NZ	2.36	0.59
20:W:46:PHE:O	20:W:50:VAL:HG23	2.03	0.59
24:0:33:ALA:O	24:0:61:ALA:HB3	2.02	0.58
1:A:1099:A:N6	1:A:1150:U:H3	1.97	0.58
2:B:66:A:H61	2:B:108:U:H2'	1.68	0.58
14:Q:135:ASP:HB3	14:Q:137:TYR:H	1.66	0.58
1:A:1992:A:OP2	4:D:242:ARG:NH2	2.34	0.58
1:A:696:C:H2'	1:A:697:G:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:ILE:HG23	3:C:172:HIS:H	1.66	0.58
6:F:184:TYR:CE2	6:F:188:ARG:HD2	2.37	0.58
8:H:20:ALA:HB1	8:H:21:PRO:HD2	1.84	0.58
9:J:56:ASN:HA	9:J:83:TYR:HA	1.85	0.58
1:A:1221:A:H3'	1:A:1222:C:C6	2.38	0.58
3:C:212:VAL:HG21	3:C:226:PRO:HG3	1.84	0.58
12:O:2:ILE:HD12	12:O:6:THR:HG21	1.85	0.58
1:A:2135:A:H2'	1:A:2136:G:O4'	2.04	0.58
1:A:2157:C:H42	1:A:2176:G:H1	1.51	0.58
1:A:2431:C:H2'	1:A:2432:G:H5''	1.85	0.58
1:A:2623:C:OP2	29:5:2:ALA:N	2.36	0.58
1:A:2858:U:H4'	1:A:2877:A:C2	2.39	0.58
1:A:794:G:OP1	20:W:88:ARG:NH2	2.27	0.58
2:B:8:U:H5''	16:S:15:ARG:NH1	2.18	0.58
6:F:53:THR:HG22	6:F:55:GLY:H	1.68	0.58
4:D:127:VAL:HA	4:D:193:VAL:HG22	1.84	0.58
6:F:140:LEU:HD21	6:F:170:LEU:HD11	1.85	0.58
10:K:30:HIS:HA	10:K:59:ILE:HD12	1.85	0.58
1:A:1538:C:C4	1:A:2226:G:H1'	2.39	0.58
1:A:2417:U:C6	1:A:2417:U:H5'	2.39	0.58
1:A:678:A:H3'	1:A:678:A:N3	2.18	0.58
3:C:181:PRO:HG2	3:C:184:LYS:HB2	1.84	0.58
3:C:62:VAL:HG22	3:C:63:SER:HA	1.85	0.58
5:E:24:THR:HG23	5:E:184:VAL:HG23	1.85	0.58
10:K:10:LEU:O	10:K:11:GLN:NE2	2.36	0.58
5:E:36:ARG:HH11	5:E:85:ASN:ND2	2.01	0.58
5:E:2:LYS:HB2	5:E:95:ILE:HD12	1.86	0.58
8:H:3:ARG:HG3	8:H:6:ARG:NH2	2.19	0.58
1:A:138:A:H8	1:A:1453:C:HO2'	1.52	0.58
3:C:164:ARG:HB2	3:C:164:ARG:HH21	1.67	0.58
13:P:86:LYS:HB3	13:P:118:GLY:HA3	1.84	0.58
29:5:35:GLU:HG3	29:5:51:TYR:CG	2.39	0.57
1:A:681:G:H2'	1:A:682:G:C8	2.39	0.57
1:A:1091:A:C6	9:J:7:VAL:N	2.62	0.57
1:A:1734:U:O2	1:A:1746:A:H5'	2.04	0.57
1:A:172:C:H2'	1:A:173:U:C6	2.38	0.57
1:A:1897:A:H8	1:A:1897:A:OP2	1.87	0.57
1:A:2339:A:H2'	1:A:2340:G:C8	2.40	0.57
1:A:982:G:H5''	1:A:982:G:H8	1.68	0.57
5:E:71:GLY:HA2	5:E:72:VAL:O	2.04	0.57
1:A:629:U:OP1	6:F:102:PRO:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:VAL:HG13	5:E:122:PHE:HB2	1.85	0.57
19:V:95:LEU:HD13	19:V:97:LYS:HD3	1.86	0.57
5:E:4:ILE:HD11	5:E:29:GLY:HA2	1.86	0.57
8:H:100:GLY:HA3	8:H:102:ALA:N	2.19	0.57
32:8:29:LYS:HE2	32:8:45:GLY:HA2	1.87	0.57
3:C:179:SER:HA	3:C:180:PHE:C	2.24	0.57
13:P:65:ARG:HG3	32:8:25:MET:HG3	1.87	0.57
1:A:605:G:OP2	18:U:10:ARG:HD2	2.05	0.57
1:A:1424:A:H8	1:A:1424:A:O5'	1.87	0.57
1:A:353:A:H2	1:A:1254:A:HO2'	1.52	0.57
1:A:922:C:H2'	1:A:923:U:O4'	2.05	0.57
1:A:1699:G:H3'	15:R:2:ARG:HD3	1.86	0.56
17:T:65:LYS:HE3	17:T:67:SER:HB2	1.86	0.56
1:A:2033:G:OP1	20:W:11:ARG:NH2	2.36	0.56
1:A:2043:U:O2'	1:A:2628:C:H5'	2.05	0.56
1:A:658:C:H2'	1:A:659:C:C6	2.41	0.56
1:A:679:G:C6	1:A:698:C:N3	2.73	0.56
6:F:183:VAL:O	6:F:187:VAL:HG23	2.05	0.56
10:K:73:PRO:O	10:K:76:TYR:N	2.31	0.56
1:A:353:A:H2	1:A:1254:A:C2'	2.18	0.56
1:A:2171:U:H2'	1:A:2172:G:C8	2.41	0.56
10:K:109:LYS:HA	10:K:112:MET:CE	2.35	0.56
10:K:3:LYS:HD3	10:K:29:GLN:HA	1.88	0.56
1:A:2657:C:OP2	1:A:2744:G:O2'	2.23	0.56
1:A:758:G:OP1	4:D:202:LYS:NZ	46.07	0.56
1:A:1126:U:O2	10:K:117:THR:N	2.38	0.56
1:A:186:C:O2	1:A:193:G:N2	20.43	0.56
1:A:2226:G:H5'	1:A:2227:G:N7	2.21	0.56
1:A:2370:C:H2'	1:A:2371:A:O4'	2.06	0.56
13:P:65:ARG:HG3	32:8:25:MET:CG	2.36	0.56
1:A:1313:A:C2	1:A:2034:A:C4	2.94	0.56
1:A:678:A:H5''	1:A:679:G:OP2	2.06	0.56
7:G:44:GLY:O	7:G:47:LYS:HB2	2.06	0.56
1:A:11:U:O2	1:A:11:U:H2'	2.06	0.55
7:G:83:ARG:O	7:G:86:MET:HB2	2.06	0.55
1:A:90:G:H2'	1:A:91:C:C6	2.41	0.55
4:D:242:ARG:N	4:D:242:ARG:HD3	2.20	0.55
12:O:107:ARG:HG3	12:O:112:MET:SD	2.46	0.55
1:A:150:C:H2'	1:A:151:G:H8	1.94	0.55
1:A:2217:C:OP2	64:A:3720:HOH:O	2.18	0.55
1:A:468:A:H1'	1:A:1245:C:O4'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1758:C:N4	1:A:1776:G:H1	2.03	0.55
2:B:2:C:H42	2:B:119:G:H1	1.54	0.55
15:R:44:LEU:HD22	15:R:48:VAL:HG23	1.87	0.55
1:A:794:G:P	20:W:88:ARG:HH21	2.29	0.55
3:C:10:LEU:HD22	3:C:32:LEU:HA	1.89	0.55
1:A:2678:C:H1'	8:H:109:PHE:CD2	2.41	0.55
1:A:1113:G:O6	1:A:1114:A:N6	2.39	0.55
1:A:2575:A:C2	1:A:2658:U:H4'	2.41	0.55
22:Y:67:LEU:HD22	22:Y:71:LYS:HD3	1.88	0.55
7:G:179:PRO:HB2	28:4:42:PHE:HE2	1.70	0.55
1:A:1108:G:O2'	10:K:87:GLY:N	2.40	0.55
10:K:103:GLN:HG2	10:K:106:GLU:OE2	2.07	0.55
1:A:2428:C:OP1	13:P:65:ARG:NH2	2.40	0.55
14:Q:56:ARG:NH1	14:Q:56:ARG:HB2	2.22	0.55
28:4:15:ILE:HD12	28:4:32:TYR:HE1	1.72	0.55
1:A:2197:A:H2'	1:A:2198:C:C6	2.41	0.55
11:N:120:LEU:HD22	11:N:122:VAL:HG23	1.89	0.55
1:A:1067:G:N7	11:N:66:LYS:HE2	2.21	0.55
11:N:108:PRO:O	11:N:113:GLY:HA3	2.06	0.55
1:A:1066:A:C8	1:A:1066:A:H3'	2.42	0.54
1:A:2873:G:OP1	17:T:119:LYS:HD2	2.07	0.54
1:A:1856:G:H4'	4:D:242:ARG:CZ	2.37	0.54
23:Z:27:VAL:HG12	23:Z:85:HIS:CE1	2.42	0.54
1:A:1406:G:OP1	12:O:49:ARG:NH2	111.46	0.54
1:A:237:C:N3	1:A:281:G:N1	60.63	0.54
3:C:39:GLU:HG2	3:C:217:THR:HB	1.89	0.54
9:J:23:SER:HA	9:J:117:LEU:O	2.07	0.54
1:A:1039:C:O2'	1:A:1041:A:OP1	2.16	0.54
4:D:275:LYS:HG3	4:D:276:LYS:H	1.72	0.54
1:A:142:C:O2'	21:X:2:LYS:NZ	2.40	0.54
1:A:2131:G:OP1	1:A:2139:U:N3	2.40	0.54
1:A:2226:G:H5'	1:A:2227:G:C5	2.42	0.54
1:A:527:A:H4'	1:A:528:U:H5''	1.88	0.54
16:S:43:GLU:OE1	16:S:43:GLU:N	4.81	0.54
1:A:552:A:C2	1:A:2064:C:H4'	2.42	0.54
1:A:703:U:H2'	1:A:704:C:C6	2.42	0.54
1:A:859:U:H2'	1:A:860:C:C6	2.42	0.54
7:G:32:PRO:HB3	7:G:163:ALA:HB2	1.89	0.54
9:J:74:LEU:O	9:J:76:GLY:N	2.33	0.54
28:4:46:GLN:C	28:4:48:ARG:H	2.10	0.54
1:A:1774:C:H3'	1:A:1775:G:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2202:G:O2'	1:A:2203:G:OP1	2.24	0.54
1:A:2750:A:OP2	64:A:3721:HOH:O	2.19	0.54
1:A:57:U:H2'	1:A:58:G:C8	5.52	0.54
3:C:6:ARG:NH1	3:C:218:MET:O	2.40	0.54
13:P:62:LEU:O	32:8:13:ARG:HD3	2.08	0.54
1:A:1051:C:C2	1:A:1182:G:N2	2.75	0.54
8:H:3:ARG:HH12	8:H:5:GLY:N	2.05	0.54
10:K:76:TYR:O	10:K:78:ILE:N	2.41	0.54
1:A:1772:C:H42	1:A:1773:C:N4	2.05	0.54
1:A:2226:G:H5'	1:A:2227:G:C6	2.43	0.54
1:A:924:A:H2'	1:A:925:G:C8	4.88	0.54
8:H:21:PRO:O	8:H:23:ARG:NH1	2.41	0.54
1:A:1231:G:H5''	19:V:81:TYR:CE2	2.43	0.54
23:Z:27:VAL:HG22	23:Z:29:TYR:HD2	1.72	0.54
1:A:2450:A:C8	1:A:2450:A:H5'	2.43	0.54
2:B:8:U:O3'	16:S:25:ARG:NH2	2.30	0.54
4:D:27:THR:OG1	4:D:28:GLU:N	2.41	0.54
1:A:2797:C:O2'	5:E:66:HIS:ND1	2.38	0.54
33:9:7:VAL:HG23	33:9:25:VAL:HG23	1.90	0.54
1:A:1064:U:H3	1:A:1187:A:H62	1.56	0.54
1:A:541:C:OP1	29:5:16:ARG:NH2	2.41	0.54
4:D:166:GLN:HE22	4:D:176:ARG:HH12	1.56	0.54
1:A:2638:G:O2'	1:A:2793:A:N1	2.36	0.53
1:A:679:G:N1	1:A:698:C:N3	2.55	0.53
5:E:111:ARG:HG3	5:E:160:TYR:CD1	2.43	0.53
13:P:138:LEU:HD23	13:P:145:PRO:HG3	1.90	0.53
1:A:2318:G:H4'	1:A:2319:G:O5'	2.09	0.53
1:A:2812:G:H2'	1:A:2813:C:O4'	2.08	0.53
3:C:57:ASN:H	3:C:201:PRO:HG2	1.73	0.53
12:O:104:ARG:HH22	17:T:43:GLN:HE22	1.56	0.53
15:R:33:ARG:NH1	15:R:115:GLU:OE2	2.38	0.53
1:A:425:G:OP2	64:A:3722:HOH:O	2.19	0.53
3:C:177:LYS:HB2	3:C:180:PHE:CD1	2.43	0.53
11:N:49:GLY:O	11:N:119:ARG:NH1	2.42	0.53
1:A:1593:C:H2'	1:A:1594:C:C6	2.44	0.53
1:A:2622:U:H6	1:A:2622:U:H5'	1.73	0.53
1:A:792:A:H2'	1:A:2623:C:H5''	1.90	0.53
1:A:238:G:P	32:8:13:ARG:HH22	2.32	0.53
1:A:1521:G:H2'	1:A:1522:C:C6	2.44	0.53
1:A:636:U:O4	1:A:736:G:O2'	77.93	0.53
1:A:1126:U:H1'	10:K:117:THR:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2388:A:H2'	1:A:2389:A:C8	2.44	0.53
1:A:879:U:O2	13:P:55:ARG:NH2	2.41	0.53
1:A:1355:G:OP2	31:7:9:ARG:HD2	2.09	0.53
3:C:41:VAL:HB	3:C:176:GLY:HA3	1.90	0.53
7:G:161:THR:CG2	7:G:163:ALA:H	2.21	0.53
10:K:60:TYR:HD2	10:K:64:SER:HB2	1.73	0.53
10:K:7:VAL:HG22	10:K:9:LYS:HE2	1.90	0.53
1:A:271:U:O2'	1:A:272:G:OP1	2.20	0.53
16:S:28:VAL:HG21	16:S:98:VAL:HG13	1.90	0.53
28:4:15:ILE:HD12	28:4:32:TYR:CE1	2.44	0.53
28:4:58:ARG:O	28:4:58:ARG:HG3	2.08	0.53
33:9:32:HIS:O	33:9:34:GLN:HG3	2.09	0.53
33:9:23:VAL:H	33:9:36:GLN:NE2	2.07	0.53
1:A:1514:C:H2'	1:A:1515:A:C8	2.44	0.53
1:A:2601:A:H5''	4:D:239:ARG:HE	1.74	0.53
4:D:134:ARG:NH1	4:D:188:GLU:OE2	2.40	0.53
8:H:52:VAL:HG23	8:H:65:HIS:CD2	2.43	0.53
13:P:47:ASP:OD2	13:P:50:ARG:NH2	2.40	0.53
22:Y:102:CYS:SG	22:Y:103:GLY:N	2.82	0.53
1:A:1839:A:H2'	1:A:1840:A:C8	2.45	0.53
6:F:136:THR:HA	6:F:166:ALA:O	2.09	0.53
7:G:82:LEU:HD23	7:G:88:ILE:HG21	1.91	0.53
17:T:51:ARG:HG3	17:T:98:LYS:HD2	1.90	0.53
26:2:17:SER:OG	26:2:20:GLU:OE1	2.25	0.52
7:G:17:PRO:HA	7:G:20:ILE:HD12	1.90	0.52
8:H:91:GLY:O	8:H:93:GLY:N	2.42	0.52
9:J:70:GLU:O	9:J:72:ASP:N	2.42	0.52
11:N:42:TRP:CD1	11:N:48:MET:HE1	2.44	0.52
12:O:17:ARG:HH11	12:O:17:ARG:HG3	4.63	0.52
16:S:35:ILE:C	16:S:36:TYR:HD1	2.12	0.52
1:A:206:A:C2	1:A:223:U:H4'	2.45	0.52
4:D:71:ASP:CB	4:D:103:ARG:HH22	2.21	0.52
13:P:101:VAL:HG23	13:P:106:LEU:HD12	1.90	0.52
24:0:23:VAL:HB	24:0:38:VAL:HG22	1.90	0.52
1:A:492:G:OP1	31:7:33:ARG:NH1	2.42	0.52
1:A:2196:C:H1'	3:C:217:THR:O	2.09	0.52
17:T:35:LYS:HD3	17:T:36:GLU:N	2.24	0.52
17:T:74:ARG:NH1	17:T:74:ARG:HG2	2.24	0.52
28:4:40:HIS:HB3	28:4:43:TYR:HD2	1.74	0.52
1:A:1105:U:C4'	1:A:1106:U:H5'	2.35	0.52
3:C:192:PHE:HD2	3:C:193:ILE:HD12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:9:ILE:HD13	6:F:123:LEU:HD23	1.92	0.52
7:G:18:GLU:HG2	7:G:175:LEU:HD21	1.90	0.52
15:R:104:ARG:HD2	15:R:109:ALA:HB3	1.90	0.52
22:Y:97:ARG:HD3	22:Y:107:ASP:O	2.09	0.52
1:A:1906:A:H2'	1:A:1907:C:O4'	2.10	0.52
1:A:2801:C:H1'	1:A:2900:A:C2	2.44	0.52
6:F:103:LYS:HA	6:F:106:ARG:HG3	1.90	0.52
1:A:1091:A:C6	9:J:5:ARG:N	2.71	0.52
1:A:1474:G:H2'	1:A:1475:C:C6	2.45	0.52
1:A:1512:G:H2'	1:A:1593:C:H41	1.75	0.52
1:A:2338:A:H2'	1:A:2339:A:C8	2.43	0.52
3:C:182:PRO:O	3:C:184:LYS:N	2.43	0.52
10:K:27:LEU:HD12	10:K:27:LEU:H	1.74	0.52
7:G:18:GLU:HA	7:G:21:ARG:HH11	1.75	0.52
10:K:101:TRP:NE1	10:K:139:VAL:O	2.42	0.52
1:A:1097:C:H42	1:A:1152:G:H1	1.58	0.52
1:A:1220:G:H1'	1:A:1221:A:O5'	2.10	0.52
1:A:1775:G:H5'	1:A:1776:G:OP2	2.10	0.52
1:A:820:A:N3	1:A:820:A:H2'	2.25	0.52
1:A:116:A:H4'	1:A:117:U:OP1	2.09	0.52
1:A:2483:G:H2'	1:A:2486:C:H42	1.74	0.52
1:A:2859:A:OP2	1:A:2875:U:H5	1.91	0.52
6:F:11:VAL:HB	6:F:18:ARG:HB3	1.92	0.52
6:F:192:LEU:HD13	6:F:194:MET:HE2	1.91	0.52
29:5:16:ARG:HG2	29:5:16:ARG:NH1	2.25	0.52
1:A:1711:A:H4'	12:O:67:LYS:HB2	1.91	0.52
1:A:1894:U:OP1	1:A:2421:G:O2'	2.20	0.52
1:A:504:A:N3	1:A:506:G:H5"	2.25	0.52
4:D:38:LYS:HE3	4:D:39:LYS:O	2.10	0.52
1:A:2045:G:H2'	1:A:2046:C:H6	1.75	0.51
1:A:2494:C:N3	14:Q:124:LYS:NZ	2.58	0.51
6:F:29:ASN:H	6:F:112:MET:CE	2.23	0.51
32:8:32:LEU:O	32:8:36:LYS:HE3	2.10	0.51
1:A:19:C:OP1	18:U:22:LYS:NZ	2.29	0.51
1:A:2181:G:N2	1:A:2182:C:O2	2.43	0.51
1:A:2609:A:OP1	64:A:3723:HOH:O	2.19	0.51
5:E:72:VAL:CA	5:E:73:GLU:HB2	2.35	0.51
19:V:28:GLU:O	19:V:61:VAL:HG21	2.10	0.51
1:A:1214:G:H2'	1:A:1215:G:O4'	2.10	0.51
4:D:108:PRO:HB3	4:D:143:HIS:CE1	2.45	0.51
8:H:56:SER:HB3	8:H:61:HIS:ND1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:100:THR:O	10:K:104:VAL:HG12	2.10	0.51
16:S:25:ARG:HD3	16:S:42:ASP:OD1	2.10	0.51
17:T:27:THR:HB	17:T:89:VAL:HG22	1.93	0.51
33:9:23:VAL:H	33:9:36:GLN:HE21	1.56	0.51
1:A:1008:C:H2'	1:A:1010:G:C8	7.45	0.51
1:A:1218:A:H1'	1:A:1219:U:H5''	1.91	0.51
1:A:214:G:H21	1:A:216:A:H62	1.57	0.51
1:A:293:C:H2'	1:A:294:C:H6	1.76	0.51
1:A:678:A:N3	1:A:678:A:C2'	2.73	0.51
3:C:189:ILE:HD11	3:C:214:VAL:HG21	1.92	0.51
9:J:71:LEU:O	9:J:73:GLY:N	2.43	0.51
10:K:109:LYS:HA	10:K:112:MET:HE3	1.91	0.51
11:N:73:THR:OG1	11:N:82:LEU:HD11	2.11	0.51
1:A:558:U:H5'	18:U:42:ALA:HB1	1.93	0.51
1:A:1066:A:H8	1:A:1066:A:H3'	1.75	0.51
1:A:2045:G:H2'	1:A:2046:C:C6	2.45	0.51
1:A:670:A:H2'	1:A:671:G:O4'	2.10	0.51
1:A:573:G:O2'	1:A:1264:A:N3	2.37	0.51
1:A:1616:A:H2'	1:A:1617:A:C8	2.44	0.51
1:A:1775:G:H2'	1:A:1775:G:N3	2.26	0.51
1:A:2157:C:H3'	1:A:2158:C:C6	2.46	0.51
1:A:35:G:N3	1:A:475:G:O2'	2.44	0.51
3:C:66:HIS:HE2	3:C:184:LYS:HD2	1.75	0.51
4:D:148:GLU:HB2	4:D:151:LYS:HD2	1.92	0.51
5:E:9:VAL:HG13	5:E:25:VAL:O	2.11	0.51
8:H:154:PRO:HB3	8:H:163:TYR:CZ	2.46	0.51
10:K:57:ILE:HG12	10:K:67:PHE:HB3	1.93	0.51
22:Y:92:ASN:N	22:Y:93:GLY:HA2	2.25	0.51
1:A:79:G:HO2'	1:A:318:G:HO2'	1.57	0.51
5:E:127:ASP:OD2	64:E:401:HOH:O	2.19	0.51
7:G:113:ARG:O	7:G:140:ILE:HD11	2.11	0.51
1:A:539:A:H2	1:A:1305:G:N3	2.09	0.51
3:C:56:GLN:HA	3:C:201:PRO:CB	2.41	0.51
6:F:124:LEU:HB3	6:F:193:VAL:HG22	1.92	0.51
22:Y:11:ASP:OD1	22:Y:97:ARG:NH2	2.39	0.51
1:A:115:A:C8	1:A:116:A:C8	2.99	0.51
1:A:2845:U:H2'	1:A:2846:G:C8	2.46	0.51
1:A:353:A:H2	1:A:1254:A:O2'	1.92	0.51
1:A:598:U:H2'	1:A:599:G:C8	2.46	0.51
1:A:885:U:H2'	1:A:886:C:C6	2.46	0.51
1:A:2573:U:O2'	12:O:23:ARG:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:15:ARG:O	16:S:19:LYS:HG2	2.11	0.51
1:A:1097:C:H2'	1:A:1098:C:H6	3.31	0.50
1:A:216:A:H2'	1:A:218:U:O4'	2.10	0.50
1:A:932:C:OP1	1:A:932:C:H4'	2.10	0.50
5:E:179:GLU:HB3	5:E:181:LEU:HD22	1.93	0.50
8:H:3:ARG:NH1	8:H:6:ARG:H	2.08	0.50
24:0:23:VAL:HA	24:0:38:VAL:HA	1.93	0.50
1:A:1198:C:H2'	1:A:1199:G:O4'	2.10	0.50
1:A:1216:G:N7	1:A:1217:G:C6	2.79	0.50
1:A:506:G:C4	1:A:531:A:C2	3.00	0.50
3:C:62:VAL:CG1	3:C:63:SER:HA	2.40	0.50
6:F:24:LEU:HB3	6:F:115:ALA:HB2	1.94	0.50
23:Z:19:ARG:NH1	23:Z:84:GLU:O	2.42	0.50
1:A:1635:U:H2'	1:A:1636:G:C8	2.47	0.50
1:A:480:C:N3	1:A:498:G:H5'	2.26	0.50
3:C:177:LYS:O	3:C:179:SER:N	2.44	0.50
4:D:274:ARG:CA	4:D:275:LYS:HB2	2.37	0.50
5:E:24:THR:HG22	5:E:186:GLY:O	2.11	0.50
7:G:49:ASP:OD1	7:G:49:ASP:N	2.43	0.50
20:W:37:ARG:HB3	20:W:37:ARG:HH11	1.77	0.50
26:2:66:GLU:HA	26:2:69:ARG:NH1	2.27	0.50
1:A:1416:G:HO2'	1:A:1417:U:H5	1.60	0.50
1:A:2205:G:H8	1:A:2205:G:OP2	1.95	0.50
1:A:745:A:H2'	1:A:746:G:O4'	2.12	0.50
1:A:2250:G:P	4:D:244:ARG:HH12	2.34	0.50
13:P:97:PRO:HD3	13:P:126:VAL:O	2.11	0.50
1:A:1223:C:H2'	1:A:1224:C:C6	2.47	0.50
1:A:1774:C:C5	1:A:1775:G:C8	3.00	0.50
1:A:924:A:N1	1:A:944:A:H2	2.09	0.50
1:A:1612:A:OP1	4:D:211:ARG:NH1	2.43	0.50
11:N:56:ASN:N	11:N:125:GLY:O	2.42	0.50
13:P:88:LEU:HD22	13:P:95:VAL:HG11	1.93	0.50
1:A:171:C:H2'	1:A:172:C:C6	3.69	0.50
1:A:1824:U:H2'	1:A:1825:C:C6	2.46	0.50
1:A:2820:G:H5'	5:E:60:ASN:HD22	1.76	0.50
3:C:175:VAL:HG22	3:C:176:GLY:N	2.26	0.50
10:K:131:ALA:O	10:K:135:GLY:N	2.43	0.50
10:K:14:ALA:H	10:K:53:VAL:H	1.59	0.50
16:S:61:ASN:O	16:S:65:VAL:HG23	2.12	0.50
24:0:50:ASN:HB3	24:0:63:VAL:HG22	1.92	0.50
32:8:8:LYS:O	32:8:12:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:A:H2'	1:A:77:G:H8	1.76	0.50
12:O:64:ARG:HB3	12:O:79:PHE:CG	2.47	0.50
28:4:46:GLN:CD	28:4:48:ARG:HE	2.15	0.50
4:D:10:THR:OG1	4:D:13:ARG:HG2	2.12	0.50
5:E:119:ARG:HG2	5:E:160:TYR:HB2	1.93	0.50
6:F:17:ARG:NH1	6:F:17:ARG:HB3	2.27	0.50
12:O:34:THR:OG1	12:O:35:VAL:N	2.44	0.50
1:A:1732:C:H2'	1:A:1733:G:O4'	2.12	0.50
1:A:552:A:C2	1:A:2063:A:H2'	2.46	0.50
1:A:2166:C:OP2	1:A:2167:C:N4	2.43	0.50
1:A:2888:C:OP2	64:A:3724:HOH:O	2.19	0.50
1:A:31:C:O2'	1:A:32:U:H5'	2.11	0.50
10:K:37:PHE:O	10:K:41:PHE:HB3	2.12	0.50
1:A:1633:C:H2'	1:A:1634:C:C6	2.47	0.49
1:A:1667:G:OP2	64:A:3725:HOH:O	2.20	0.49
1:A:271:U:O2'	1:A:272:G:P	2.70	0.49
7:G:46:ALA:O	7:G:51:ARG:HG3	2.11	0.49
1:A:2758:U:OP1	8:H:85:LYS:NZ	2.46	0.49
1:A:2189:G:H5''	1:A:2189:G:H8	1.77	0.49
1:A:2696:G:H5'	12:O:68:GLU:OE1	2.12	0.49
1:A:1545:G:O2'	4:D:100:GLY:O	2.28	0.49
10:K:52:ILE:HB	10:K:73:PRO:HG3	1.94	0.49
10:K:88:ALA:O	10:K:90:LYS:N	2.37	0.49
1:A:1115:A:H5'	1:A:1117:C:OP2	2.12	0.49
1:A:1132:G:C6	1:A:1148:A:C2	3.01	0.49
1:A:1824:U:H2'	1:A:1825:C:H6	1.76	0.49
1:A:2811:A:H1'	1:A:2903:U:H1'	1.93	0.49
1:A:333:A:O2'	1:A:335:G:N7	2.32	0.49
7:G:7:LEU:HB2	7:G:104:GLU:HB2	1.94	0.49
18:U:58:ARG:HA	18:U:61:TRP:CE3	2.47	0.49
23:Z:45:ASP:O	23:Z:49:ARG:HG3	2.12	0.49
1:A:1091:A:C5	9:J:8:GLU:N	2.80	0.49
1:A:1100:G:H2'	1:A:1101:G:O4'	2.13	0.49
1:A:1548:U:H2'	1:A:1549:C:C6	2.48	0.49
1:A:2155:A:H5''	1:A:2156:A:OP2	2.12	0.49
1:A:2186:G:H2'	1:A:2187:G:C8	2.47	0.49
1:A:2044:G:H5'	1:A:2628:C:H4'	1.92	0.49
1:A:264:U:H2'	1:A:265:C:C6	2.47	0.49
1:A:88:U:O2'	1:A:89:A:C8	2.59	0.49
2:B:63:G:H2'	2:B:64:C:C6	2.48	0.49
3:C:161:ILE:HD12	3:C:174:PRO:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:ARG:CZ	4:D:88:ARG:HB3	2.42	0.49
8:H:21:PRO:HG2	8:H:23:ARG:HH12	1.77	0.49
1:A:2568:G:H2'	1:A:2569:C:C6	2.48	0.49
4:D:16:MET:HE1	4:D:208:LYS:HD3	1.95	0.49
4:D:76:PRO:O	4:D:98:VAL:HG23	2.11	0.49
9:J:118:THR:O	9:J:120:LYS:N	2.40	0.49
10:K:32:ALA:HB1	10:K:65:PHE:CD1	2.47	0.49
12:O:111:PHE:O	12:O:115:VAL:HG23	2.13	0.49
15:R:37:THR:OG1	15:R:40:LYS:HB2	2.13	0.49
17:T:56:GLY:O	17:T:59:THR:HG23	2.13	0.49
18:U:19:LYS:O	18:U:22:LYS:HG3	2.13	0.49
7:G:108:ASN:ND2	28:4:22:ILE:HG21	2.27	0.49
1:A:98:G:O2'	26:2:7:ARG:NH2	2.46	0.49
1:A:1121:C:H2'	1:A:1122:A:H8	1.78	0.49
10:K:65:PHE:H	10:K:65:PHE:HD2	1.59	0.49
13:P:121:LYS:HB2	13:P:123:LEU:HG	1.94	0.49
23:Z:8:TYR:HB2	23:Z:38:TYR:CE2	2.47	0.49
26:2:10:LEU:HB3	26:2:14:ARG:NH1	2.28	0.49
1:A:1101:G:H5''	1:A:1102:A:O4'	2.12	0.49
1:A:2817:U:H5''	1:A:2899:G:O6	2.13	0.49
1:A:925:G:H1	1:A:943:C:H42	1.59	0.49
6:F:17:ARG:CZ	6:F:17:ARG:HB3	2.43	0.49
1:A:1124:C:O3'	10:K:132:ARG:NH2	2.45	0.49
1:A:1228:G:H5'	27:3:29:ARG:NH1	2.27	0.49
1:A:173:U:H4'	1:A:206:A:H4'	1.94	0.49
1:A:2698:U:H2'	1:A:2699:U:O4'	2.13	0.49
1:A:76:A:H2'	1:A:77:G:C8	2.48	0.49
3:C:56:GLN:HA	3:C:201:PRO:HB2	1.95	0.49
13:P:1:MET:SD	13:P:1:MET:N	4.50	0.49
14:Q:56:ARG:HH11	14:Q:56:ARG:HB2	1.76	0.49
25:1:62:VAL:HG22	25:1:63:ALA:O	2.13	0.49
1:A:2212:G:O2'	1:A:2213:G:H8	1.96	0.49
1:A:678:A:H2'	1:A:678:A:N3	2.28	0.49
1:A:963:A:N3	2:B:80:U:O2'	2.39	0.49
1:A:1643:C:O3'	21:X:35:THR:HG22	2.13	0.49
1:A:1245:C:H2'	1:A:1246:C:C6	2.97	0.48
1:A:1826:U:H2'	1:A:1827:C:C6	2.48	0.48
1:A:2412:U:OP1	30:6:18:ARG:NH2	2.42	0.48
1:A:64:C:H2'	1:A:65:U:C6	2.48	0.48
2:B:12:C:H2'	24:0:73:GLY:HA3	1.95	0.48
3:C:21:THR:HG22	3:C:23:ASP:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:104:ARG:HH22	17:T:43:GLN:NE2	2.11	0.48
27:3:3:ARG:HH11	27:3:60:GLU:HB3	1.77	0.48
1:A:1121:C:H2'	1:A:1122:A:C8	2.48	0.48
1:A:1116:G:O2'	1:A:1134:G:OP2	2.27	0.48
1:A:1138:G:H21	1:A:1143:A:H62	1.61	0.48
1:A:1268:G:N2	1:A:1271:A:OP2	2.38	0.48
1:A:1097:C:H2'	1:A:1098:C:C6	4.03	0.48
1:A:2172:G:H2'	1:A:2173:G:H8	1.78	0.48
1:A:2297:A:H4'	1:A:2298:A:O4'	2.13	0.48
1:A:346:G:C8	6:F:171:PRO:HG3	2.48	0.48
1:A:947:C:H2'	1:A:948:C:H6	1.79	0.48
3:C:48:GLY:HA2	3:C:210:ARG:HH11	1.79	0.48
5:E:12:THR:HG22	5:E:13:ARG:H	1.78	0.48
1:A:1404:A:H61	1:A:1417:U:H3	1.62	0.48
1:A:1896:C:H2'	1:A:1897:A:O4'	2.13	0.48
3:C:47:LEU:HD11	3:C:171:ILE:HB	1.95	0.48
7:G:15:VAL:HG22	7:G:175:LEU:HB3	1.94	0.48
8:H:41:MET:CE	8:H:54:ARG:HB3	2.44	0.48
14:Q:110:THR:HG23	14:Q:113:GLN:OE1	2.14	0.48
17:T:26:ASP:OD1	17:T:91:ARG:HA	2.12	0.48
1:A:398:G:P	25:1:69:LYS:HZ1	2.36	0.48
28:4:18:CYS:SG	28:4:19:GLY:N	2.86	0.48
28:4:63:TYR:CD1	28:4:63:TYR:N	2.80	0.48
13:P:63:PRO:HG2	32:8:25:MET:HB2	1.96	0.48
1:A:1153:U:HO2'	1:A:1154:C:C5'	2.23	0.48
1:A:1920:G:H2'	1:A:1920:G:N3	2.29	0.48
1:A:2659:C:H2'	1:A:2660:U:C6	2.49	0.48
1:A:2802:A:H2'	1:A:2802:A:N3	2.28	0.48
1:A:941:A:H4'	1:A:941:A:OP1	2.14	0.48
10:K:131:ALA:HB1	10:K:136:VAL:O	2.14	0.48
10:K:35:MET:HA	10:K:38:VAL:HG23	1.95	0.48
16:S:36:TYR:N	16:S:36:TYR:CD1	2.82	0.48
1:A:1200:A:OP1	18:U:55:ARG:HD3	2.13	0.48
1:A:179:A:H2'	1:A:180:C:C6	2.49	0.48
1:A:1887:G:C6	1:A:1888:G:C6	3.02	0.48
6:F:29:ASN:H	6:F:112:MET:HE3	1.78	0.48
1:A:1106:U:O2	10:K:11:GLN:HG2	2.14	0.48
13:P:89:ALA:HA	13:P:121:LYS:HD2	1.95	0.48
25:1:80:LEU:HG	25:1:81:LYS:N	2.29	0.48
27:3:46:ASN:O	27:3:50:VAL:HG22	2.14	0.48
1:A:1300:U:O5'	1:A:1301:G:H5''	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:C:H2'	1:A:161:G:H8	1.78	0.48
1:A:2661:U:H2'	1:A:2662:C:C6	2.49	0.48
1:A:39:C:C5	1:A:39:C:N1	2.78	0.48
3:C:43:VAL:O	3:C:172:HIS:HA	2.14	0.48
10:K:14:ALA:HB2	10:K:41:PHE:CZ	2.48	0.48
28:4:59:PHE:N	28:4:60:GLN:HB3	2.29	0.48
1:A:1265:C:H2'	1:A:1266:C:C6	2.49	0.48
1:A:1766:A:O2'	1:A:1767:U:H2'	2.13	0.48
1:A:1953:A:H2'	1:A:1954:G:O4'	2.14	0.48
1:A:2702:C:O3'	1:A:2880:C:H4'	2.14	0.48
1:A:946:A:H2'	1:A:947:C:O4'	2.14	0.48
3:C:164:ARG:CB	3:C:164:ARG:HH21	2.26	0.48
7:G:96:ARG:O	7:G:99:MET:HB3	2.13	0.48
10:K:18:THR:HA	10:K:35:MET:HE1	1.96	0.48
16:S:34:HIS:CB	16:S:36:TYR:HE1	2.27	0.48
18:U:85:LYS:HB3	18:U:85:LYS:HE2	1.60	0.48
1:A:323:A:H3'	22:Y:84:ARG:NH2	2.28	0.48
1:A:1127:U:H3'	1:A:1128:U:C5'	2.41	0.48
1:A:2658:U:H2'	1:A:2659:C:C6	2.49	0.48
1:A:312:A:H2'	1:A:313:G:O4'	2.13	0.48
7:G:179:PRO:HG3	28:4:43:TYR:OH	2.13	0.48
25:1:3:LYS:HD2	25:1:61:ARG:HH12	1.78	0.47
27:3:23:LEU:HD13	27:3:50:VAL:HG11	1.95	0.47
6:F:197:ASP:O	6:F:200:GLU:HB2	2.14	0.47
1:A:1073:A:H61	1:A:1170:G:H2'	1.79	0.47
1:A:29:G:H2'	1:A:30:C:C6	2.49	0.47
5:E:47:VAL:O	5:E:80:GLU:HA	2.15	0.47
12:O:98:VAL:HG22	12:O:118:ALA:HA	1.96	0.47
1:A:2754:C:OP1	33:9:35:ARG:HD3	2.14	0.47
1:A:1109:C:H2'	1:A:1110:U:O4'	2.14	0.47
1:A:1153:U:O2'	1:A:1154:C:C6	2.66	0.47
1:A:2157:C:H3'	1:A:2158:C:C5	2.49	0.47
1:A:216:A:H3'	1:A:217:A:C5'	2.43	0.47
18:U:34:LYS:HD2	18:U:34:LYS:HA	1.52	0.47
23:Z:40:ASP:HB3	23:Z:43:GLU:HB2	1.95	0.47
29:5:8:LYS:O	29:5:9:LYS:HD2	2.14	0.47
30:6:9:LEU:HD13	30:6:51:GLU:HG3	1.97	0.47
1:A:1073:A:N6	1:A:1170:G:H2'	2.28	0.47
1:A:1335:C:H2'	1:A:1336:C:H6	1.79	0.47
1:A:1659:A:C2	20:W:93:ALA:HB2	2.50	0.47
1:A:341:C:OP2	17:T:39:ARG:NH2	164.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:G:H2'	1:A:516:A:C8	2.50	0.47
1:A:1265:C:H2'	1:A:1266:C:H6	1.79	0.47
1:A:2129:C:O2'	1:A:2130:U:H5'	2.14	0.47
1:A:2294:C:C2	1:A:2400:G:C2	3.02	0.47
6:F:34:TRP:CE3	6:F:35:GLU:HG2	2.49	0.47
8:H:3:ARG:HH22	8:H:5:GLY:H	1.63	0.47
10:K:99:ILE:HG23	10:K:103:GLN:HB3	1.96	0.47
25:1:54:ALA:HB1	25:1:83:GLU:HG3	1.96	0.47
28:4:48:ARG:HA	28:4:48:ARG:CZ	2.44	0.47
1:A:1431:C:H2'	1:A:1432:C:C6	2.49	0.47
1:A:2134:U:O5'	1:A:2134:U:H6	1.98	0.47
1:A:2249:G:N3	1:A:2249:G:H2'	2.28	0.47
1:A:839:A:OP2	1:A:2093:G:H5'	2.15	0.47
3:C:186:ALA:HA	3:C:189:ILE:HG22	1.96	0.47
10:K:76:TYR:HB2	10:K:79:ARG:NH2	2.27	0.47
5:E:9:VAL:HB	17:T:3:ARG:HG2	1.96	0.47
11:N:4:TYR:CD2	18:U:100:VAL:HG11	2.50	0.47
1:A:1042:G:OP1	18:U:92:ARG:HG2	2.15	0.47
1:A:1217:G:H2'	1:A:1217:G:OP2	2.15	0.47
1:A:1344:G:H5'	1:A:1346:A:O4'	2.14	0.47
1:A:860:C:H2'	1:A:861:C:H6	1.79	0.47
12:O:26:LYS:O	12:O:30:ALA:HB2	2.14	0.47
18:U:28:ARG:NH1	18:U:38:THR:OG1	2.46	0.47
1:A:2801:C:H1'	1:A:2900:A:H2	1.79	0.47
1:A:722:A:H2	1:A:2090:G:N3	2.13	0.47
1:A:786:U:H2'	1:A:787:G:C8	2.49	0.47
1:A:982:G:H5''	1:A:982:G:C8	2.50	0.47
3:C:26:ALA:HB1	3:C:182:PRO:HA	1.96	0.47
7:G:16:ARG:NH1	7:G:31:VAL:HG22	2.30	0.47
9:J:118:THR:N	9:J:121:ASP:O	2.45	0.47
13:P:44:GLY:CA	13:P:45:LEU:HB2	2.45	0.47
17:T:29:ARG:HD3	17:T:44:ASP:OD1	2.15	0.47
33:9:7:VAL:HG13	33:9:36:GLN:HG3	1.97	0.47
1:A:1128:U:H2'	1:A:1130:A:OP2	2.14	0.47
1:A:1402:U:H2'	1:A:1403:G:O4'	2.15	0.47
1:A:64:C:H2'	1:A:65:U:H6	1.79	0.47
11:N:19:GLU:H	11:N:21:LYS:HG2	1.79	0.47
16:S:11:LYS:HD3	16:S:15:ARG:NH2	2.30	0.47
21:X:50:LYS:O	21:X:84:ALA:N	2.48	0.47
21:X:53:LYS:HB3	21:X:82:GLN:HB3	1.95	0.47
1:A:508:A:O4'	22:Y:48:ALA:HB1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2290:G:O6	24:0:14:ARG:HD2	2.15	0.47
1:A:1039:C:OP1	18:U:53:ARG:NH2	2.48	0.47
1:A:173:U:H2'	1:A:174:G:C8	2.50	0.47
1:A:2376:G:O6	32:8:39:LYS:HE3	2.14	0.47
1:A:235:G:H4'	1:A:412:G:C6	2.49	0.47
1:A:719:C:H5''	6:F:81:PRO:HD2	1.97	0.47
2:B:31:C:H4'	7:G:29:TRP:CZ2	2.50	0.47
10:K:121:GLU:HB3	10:K:125:ARG:HH21	1.80	0.47
18:U:104:GLN:HG3	18:U:104:GLN:H	1.36	0.47
25:1:8:SER:HB3	25:1:66:HIS:CD2	2.50	0.47
1:A:1126:U:H2'	1:A:1127:U:H5'	1.97	0.47
1:A:1416:G:O2'	1:A:1417:U:H5	1.98	0.47
1:A:2282:G:OP1	24:0:18:ALA:HB1	2.16	0.47
1:A:2803:C:H5	1:A:2901:G:O2'	1.98	0.47
1:A:696:C:H2'	1:A:697:G:H8	1.80	0.47
2:B:60:C:H2'	2:B:61:G:H8	1.80	0.47
4:D:132:PRO:HG3	4:D:190:TYR:CE1	2.50	0.47
7:G:49:ASP:O	7:G:51:ARG:N	2.47	0.47
12:O:4:PRO:O	12:O:5:GLN:HB2	2.15	0.47
18:U:108:GLU:O	18:U:112:ARG:HG2	2.15	0.47
22:Y:90:LEU:HD21	22:Y:96:ILE:HG12	1.97	0.47
1:A:1295:G:OP2	13:P:21:ARG:NH1	2.45	0.46
1:A:1594:C:H2'	1:A:1595:C:H6	1.80	0.46
1:A:1638:G:H2'	1:A:1639:G:C8	2.50	0.46
1:A:172:C:H2'	1:A:173:U:H6	1.80	0.46
1:A:201:A:H2'	1:A:202:G:O4'	2.15	0.46
1:A:2143:U:H1'	3:C:166:ASP:HB3	1.96	0.46
1:A:2709:U:H2'	1:A:2710:C:C6	2.50	0.46
1:A:2900:A:H3'	1:A:2901:G:C8	2.50	0.46
2:B:3:C:H2'	2:B:4:C:C6	2.50	0.46
3:C:55:ASP:OD1	3:C:55:ASP:N	2.28	0.46
4:D:112:GLN:OE1	4:D:112:GLN:HA	2.15	0.46
5:E:143:ASN:HD22	5:E:147:PRO:HD2	1.80	0.46
21:X:34:ALA:O	21:X:77:LYS:NZ	2.46	0.46
1:A:1097:C:O2'	1:A:1098:C:OP1	2.24	0.46
1:A:1127:U:H5''	1:A:1128:U:OP2	2.15	0.46
1:A:1223:C:H2'	1:A:1224:C:H6	1.80	0.46
1:A:1828:U:OP2	4:D:273:ARG:NH2	2.47	0.46
1:A:2723:U:OP1	1:A:2726:G:H4'	2.15	0.46
1:A:301:A:H2'	1:A:302:C:C6	2.51	0.46
1:A:554:G:C5	1:A:2043:U:H5''	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:C:N3	1:A:697:G:O6	2.48	0.46
20:W:29:LEU:O	20:W:33:ARG:HG3	2.16	0.46
28:4:61:ARG:HG3	28:4:62:ARG:H	1.79	0.46
1:A:1446:G:H2'	1:A:1447:C:O4'	2.14	0.46
1:A:2800:C:O2'	1:A:2818:A:N3	2.39	0.46
7:G:140:ILE:HA	7:G:140:ILE:HD12	1.75	0.46
10:K:36:GLU:HG3	10:K:67:PHE:HZ	1.80	0.46
1:A:1659:A:N1	20:W:93:ALA:HB2	2.30	0.46
23:Z:13:GLU:N	23:Z:13:GLU:OE1	2.31	0.46
23:Z:23:LYS:HB3	23:Z:38:TYR:HD1	1.78	0.46
24:0:27:GLU:CG	24:0:68:GLU:HA	2.45	0.46
1:A:1093:A:OP2	1:A:1155:G:N2	2.47	0.46
1:A:1628:C:O2'	1:A:1631:A:N3	2.42	0.46
1:A:1652:C:H4'	1:A:1653:A:O5'	2.15	0.46
1:A:2054:A:O2'	1:A:2056:G:OP2	2.28	0.46
4:D:146:GLU:HB2	4:D:189:CYS:HB3	1.97	0.46
4:D:79:VAL:HG21	4:D:111:LEU:HD21	1.97	0.46
1:A:2323:U:H5'	7:G:88:ILE:HD11	1.97	0.46
11:N:94:HIS:HB3	11:N:97:ARG:HD3	1.98	0.46
14:Q:55:VAL:O	14:Q:58:PHE:N	2.45	0.46
1:A:1228:G:H5'	27:3:29:ARG:HH11	1.80	0.46
1:A:138:A:C8	1:A:1453:C:O2'	2.69	0.46
1:A:2244:U:H2'	1:A:2245:G:C8	2.50	0.46
1:A:517:G:H2'	1:A:518:G:O4'	2.15	0.46
1:A:926:G:H8	1:A:926:G:OP2	1.99	0.46
8:H:83:TYR:CE2	8:H:138:LYS:HB2	2.51	0.46
1:A:2651:G:OP1	11:N:97:ARG:NH2	2.49	0.46
28:4:63:TYR:N	28:4:64:GLY:HA2	2.30	0.46
1:A:1633:C:H2'	1:A:1634:C:H6	1.80	0.46
2:B:63:G:H2'	2:B:64:C:H6	1.80	0.46
3:C:193:ILE:O	3:C:197:GLU:HB2	2.15	0.46
8:H:155:SER:HB3	8:H:158:HIS:O	2.16	0.46
1:A:2428:C:P	13:P:65:ARG:HH21	2.39	0.46
29:5:16:ARG:HD2	29:5:20:ARG:NH1	2.31	0.46
1:A:2297:A:N1	30:6:24:GLU:O	2.49	0.46
33:9:14:CYS:HA	33:9:27:CYS:HB2	1.97	0.46
1:A:150:C:H2'	1:A:151:G:C8	2.59	0.46
1:A:2247:C:H2'	1:A:2248:G:O4'	2.15	0.46
1:A:277:G:OP1	25:1:76:ARG:HB3	2.16	0.46
1:A:307:U:H2'	1:A:308:C:C6	2.49	0.46
7:G:126:ASP:HB3	7:G:128:ARG:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:15:ARG:HH11	16:S:25:ARG:NH2	2.09	0.46
25:1:86:SER:OG	25:1:89:GLU:HG2	2.16	0.46
1:A:138:A:H8	1:A:1453:C:O2'	1.97	0.46
1:A:1399:A:H2'	1:A:1400:G:O4'	2.16	0.46
1:A:267:G:C2'	1:A:268:G:H5'	2.45	0.46
1:A:2874:U:C4	1:A:2875:U:C4	3.03	0.46
1:A:549:U:H5'	1:A:578:G:OP1	2.16	0.46
1:A:894:G:H2'	1:A:895:A:C8	2.51	0.46
14:Q:12:GLN:HG2	14:Q:73:PRO:HD2	1.98	0.46
19:V:50:PRO:HG2	19:V:51:VAL:HG12	1.97	0.46
30:6:37:ARG:O	30:6:38:LYS:HD2	2.16	0.46
1:A:1461:G:N2	1:A:1628:C:O2	2.48	0.46
1:A:1524:G:N2	1:A:1561:U:C2	2.84	0.46
1:A:1758:C:N3	1:A:1776:G:N2	2.53	0.46
1:A:1774:C:H5'	1:A:1775:G:OP2	2.16	0.46
1:A:2221:C:H5''	1:A:2221:C:C6	2.50	0.46
2:B:91:C:OP2	14:Q:16:ARG:NH1	2.47	0.46
7:G:126:ASP:HB2	7:G:130:ASN:H	1.81	0.46
20:W:51:LEU:HD23	20:W:105:VAL:HG11	1.98	0.46
25:1:19:GLN:HB2	25:1:35:THR:HG22	1.98	0.46
1:A:2220:A:H5'	25:1:50:ARG:HH21	1.81	0.46
1:A:159:G:C2	1:A:160:C:C2	3.04	0.46
1:A:2713:U:H4'	1:A:2714:C:OP1	2.16	0.46
1:A:550:A:OP1	64:A:3726:HOH:O	2.21	0.46
1:A:1829:G:O2'	4:D:181:GLU:OE2	2.28	0.46
1:A:1857:C:OP2	4:D:222:ARG:NH1	2.48	0.46
12:O:17:ARG:HH21	12:O:47:ILE:HD13	1.81	0.46
1:A:865:A:C4	1:A:1233:A:C2	3.05	0.45
1:A:2832:A:OP1	5:E:159:HIS:NE2	2.48	0.45
8:H:163:TYR:CE2	8:H:169:VAL:HG22	2.51	0.45
10:K:57:ILE:HA	10:K:66:THR:O	2.15	0.45
11:N:34:LEU:HD12	11:N:34:LEU:HA	1.75	0.45
32:8:29:LYS:HE2	32:8:45:GLY:CA	2.45	0.45
1:A:1096:G:H5''	1:A:1097:C:OP2	2.16	0.45
1:A:25:G:H1'	1:A:538:A:N6	2.32	0.45
10:K:28:GLY:O	10:K:30:HIS:N	2.49	0.45
21:X:60:ARG:NH1	31:7:47:ARG:HH22	2.13	0.45
27:3:3:ARG:NH1	27:3:60:GLU:OE2	2.48	0.45
28:4:55:ARG:C	28:4:57:GLU:H	2.20	0.45
1:A:1602:C:H2'	1:A:1603:C:C6	2.51	0.45
1:A:2172:G:H2'	1:A:2173:G:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2186:G:H8	1:A:2186:G:O5'	1.98	0.45
1:A:2235:G:H4'	1:A:2237:C:C2	2.51	0.45
1:A:2375:C:H2'	1:A:2376:G:O4'	2.17	0.45
1:A:610:U:H1'	6:F:90:PHE:CG	2.52	0.45
3:C:43:VAL:HG21	3:C:189:ILE:HG13	1.97	0.45
3:C:209:LEU:CD1	3:C:209:LEU:H	2.25	0.45
5:E:15:PHE:CE1	5:E:20:ALA:HB2	2.51	0.45
8:H:24:VAL:HG13	8:H:37:VAL:HG21	1.97	0.45
16:S:3:ARG:HH11	16:S:3:ARG:HG2	1.80	0.45
19:V:25:LEU:HD12	19:V:25:LEU:HA	1.84	0.45
26:2:15:LYS:HE3	26:2:15:LYS:HB2	1.64	0.45
1:A:1835:U:O2	4:D:50:THR:HB	2.16	0.45
1:A:238:G:C6	1:A:239:A:C6	3.04	0.45
1:A:37:A:H2'	1:A:38:C:C6	2.52	0.45
3:C:68:LEU:HD23	3:C:161:ILE:HG22	1.97	0.45
4:D:173:VAL:C	4:D:174:ILE:HD13	2.37	0.45
17:T:78:LEU:O	17:T:78:LEU:HD13	2.17	0.45
1:A:904:U:P	24:0:77:ARG:HH22	2.40	0.45
1:A:1076:G:H21	33:9:36:GLN:HE22	1.65	0.45
1:A:1216:G:H5'	1:A:1217:G:OP2	2.16	0.45
1:A:1531:A:H2'	1:A:1532:G:C8	2.52	0.45
3:C:186:ALA:O	3:C:189:ILE:HG22	2.16	0.45
1:A:2198:C:H5''	3:C:213:TYR:CD2	2.51	0.45
5:E:175:VAL:HG22	5:E:177:PRO:HD3	1.98	0.45
5:E:7:VAL:HG12	5:E:51:PHE:CE1	2.52	0.45
15:R:55:ALA:HB2	15:R:79:LEU:HD13	1.98	0.45
1:A:1232:U:C4'	19:V:79:VAL:HG22	2.44	0.45
22:Y:56:PRO:C	22:Y:58:GLY:H	2.20	0.45
23:Z:40:ASP:OD1	23:Z:42:VAL:HG13	2.15	0.45
1:A:901:G:O2'	24:0:27:GLU:OE2	2.29	0.45
1:A:1120:C:H5'	1:A:1121:C:OP2	2.17	0.45
1:A:2765:A:O2'	33:9:15:LYS:HE3	2.16	0.45
3:C:200:LYS:HD3	3:C:204:ALA:H	1.81	0.45
8:H:3:ARG:HH12	8:H:6:ARG:H	1.65	0.45
1:A:1066:A:H62	1:A:1185:U:H3	1.64	0.45
1:A:1763:G:C6	1:A:1764:U:C5	3.05	0.45
1:A:2039:G:OP1	29:5:9:LYS:HE3	2.16	0.45
1:A:2114:G:C6	1:A:2236:A:C8	3.05	0.45
1:A:1501:G:O2'	1:A:2862:C:OP1	2.26	0.45
1:A:427:A:H2'	1:A:428:A:O4'	2.49	0.45
2:B:66:A:N6	2:B:108:U:H2'	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:VAL:HG22	3:C:63:SER:O	2.17	0.45
7:G:27:ASN:O	7:G:30:GLU:HG2	2.17	0.45
13:P:55:ARG:HD2	13:P:55:ARG:HA	4.42	0.45
20:W:79:GLY:CA	20:W:100:THR:HG22	2.47	0.45
1:A:1202:G:O2'	27:3:31:LEU:HD12	2.16	0.45
1:A:2077:G:OP2	64:A:3729:HOH:O	2.21	0.45
1:A:228:G:H1'	1:A:258:A:N1	40.11	0.45
1:A:935:C:H1'	1:A:936:A:H1'	1.99	0.45
1:A:940:U:O2	1:A:940:U:H2'	2.15	0.45
1:A:926:G:N2	1:A:943:C:C4	2.85	0.45
4:D:166:GLN:HE22	4:D:176:ARG:NH1	2.14	0.45
6:F:65:TRP:CZ2	6:F:75:HIS:HD2	2.34	0.45
12:O:98:VAL:CG2	12:O:118:ALA:HA	2.47	0.45
1:A:1444:C:OP1	21:X:25:LYS:NZ	2.49	0.45
23:Z:45:ASP:OD1	23:Z:49:ARG:NH1	2.47	0.45
1:A:1337:U:H2'	1:A:1338:C:C6	2.51	0.45
1:A:159:G:H2'	1:A:160:C:C6	2.51	0.45
1:A:867:A:H2'	1:A:990:G:H5''	1.98	0.45
1:A:1614:G:H5''	4:D:61:LEU:HD22	1.98	0.45
5:E:143:ASN:HD22	5:E:147:PRO:CD	2.30	0.45
7:G:3:LEU:HD12	7:G:3:LEU:H	1.82	0.45
7:G:47:LYS:HB3	7:G:49:ASP:OD1	2.16	0.45
19:V:29:PRO:HA	19:V:61:VAL:HG23	1.99	0.45
23:Z:74:VAL:HG13	23:Z:86:VAL:HG22	1.97	0.45
1:A:1463:G:O2'	1:A:1626:A:N6	2.48	0.45
1:A:2824:C:O2	29:5:43:HIS:HE1	1.99	0.45
1:A:679:G:N3	1:A:679:G:H2'	2.32	0.45
1:A:6:G:H2'	1:A:7:A:C8	2.52	0.45
3:C:62:VAL:CG2	3:C:63:SER:HA	2.47	0.45
7:G:18:GLU:HA	7:G:21:ARG:HD3	1.99	0.45
12:O:24:VAL:HB	12:O:33:ALA:HB2	1.99	0.45
16:S:65:VAL:O	16:S:69:VAL:HG12	2.16	0.45
23:Z:52:SER:OG	23:Z:53:ILE:N	2.49	0.45
1:A:1070:G:H3'	1:A:1071:U:H5'	1.99	0.44
1:A:1097:C:C2'	1:A:1098:C:H5'	2.48	0.44
1:A:1594:C:H2'	1:A:1595:C:C6	2.51	0.44
8:H:11:VAL:HG13	8:H:15:VAL:HG22	1.98	0.44
30:6:19:ARG:HD2	30:6:19:ARG:N	2.32	0.44
1:A:2026:A:H5''	64:A:3771:HOH:O	2.17	0.44
1:A:2544:A:H2'	1:A:2545:A:O4'	2.18	0.44
1:A:916:A:C2	1:A:953:C:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:3:ARG:HB3	8:H:3:ARG:HH11	1.81	0.44
8:H:7:LEU:HD12	8:H:8:PRO:HD2	1.99	0.44
11:N:131:GLN:CD	11:N:131:GLN:H	2.18	0.44
16:S:59:LYS:HB3	16:S:60:GLY:H	1.67	0.44
24:O:27:GLU:HG2	24:O:68:GLU:HA	1.99	0.44
1:A:1143:A:H2'	1:A:1144:G:H5'	1.99	0.44
1:A:2155:A:O2'	1:A:2181:G:H1'	2.18	0.44
1:A:2208:G:H2'	1:A:2209:C:O4'	2.16	0.44
1:A:2855:G:H2'	1:A:2856:U:C6	2.52	0.44
1:A:703:U:H2'	1:A:704:C:H6	1.81	0.44
5:E:181:LEU:HA	5:E:181:LEU:HD12	1.81	0.44
7:G:16:ARG:HB2	7:G:17:PRO:HD3	2.00	0.44
1:A:2261:G:OP1	14:Q:85:LYS:NZ	2.51	0.44
1:A:1832:A:N1	1:A:1852:G:H1'	2.33	0.44
1:A:2783:C:H2'	1:A:2784:C:C6	2.52	0.44
1:A:469:C:H4'	6:F:49:ALA:HB2	2.00	0.44
1:A:928:G:H1	1:A:939:C:H42	1.65	0.44
1:A:988:G:H2'	1:A:988:G:N3	2.79	0.44
3:C:24:GLU:O	3:C:27:HIS:HB2	2.18	0.44
3:C:62:VAL:HG13	3:C:63:SER:CA	2.44	0.44
3:C:67:GLY:C	3:C:175:VAL:HG11	2.37	0.44
7:G:145:THR:HG23	7:G:148:MET:SD	2.57	0.44
11:N:55:VAL:HG13	11:N:126:PRO:HA	1.98	0.44
1:A:1011:C:H2'	1:A:1012:G:C8	3.40	0.44
1:A:2166:C:H3'	1:A:2167:C:N1	2.33	0.44
1:A:2862:C:H2'	1:A:2863:G:C8	2.53	0.44
1:A:810:A:H5'	4:D:210:GLY:CA	2.48	0.44
3:C:201:PRO:O	3:C:203:GLY:CA	2.59	0.44
1:A:775:G:OP1	4:D:12:SER:HB2	2.18	0.44
6:F:184:TYR:CD2	6:F:188:ARG:HD2	2.52	0.44
26:2:66:GLU:HA	26:2:69:ARG:HH11	1.82	0.44
1:A:105:U:OP1	1:A:316:U:O2'	2.34	0.44
1:A:1097:C:H2'	1:A:1098:C:H5'	2.00	0.44
1:A:1404:A:N1	1:A:1417:U:O4	2.50	0.44
1:A:459:C:C4	1:A:460:U:O4	2.70	0.44
1:A:682:G:H8	1:A:682:G:O5'	2.00	0.44
1:A:907:A:C2	1:A:962:A:C4	3.05	0.44
3:C:64:LEU:HA	3:C:65:PRO:O	2.17	0.44
5:E:7:VAL:HG12	5:E:51:PHE:HE1	1.82	0.44
6:F:120:GLU:H	6:F:120:GLU:HG3	1.67	0.44
17:T:106:SER:O	17:T:110:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2141:G:O2'	1:A:2142:G:H5'	2.17	0.44
1:A:2752:A:C6	1:A:2776:A:C8	3.06	0.44
1:A:671:G:H2'	1:A:672:G:O4'	2.18	0.44
3:C:192:PHE:CD2	3:C:193:ILE:HD12	2.53	0.44
8:H:152:ARG:HD3	8:H:152:ARG:HA	1.75	0.44
1:A:1302:C:H2'	1:A:1303:C:C6	2.53	0.44
1:A:1803:A:C5	1:A:1859:A:H1'	2.53	0.44
1:A:2346:A:C8	1:A:2348:G:C5	3.05	0.44
1:A:2783:C:H2'	1:A:2784:C:H6	1.82	0.44
1:A:715:G:H5'	64:A:3870:HOH:O	2.17	0.44
3:C:44:HIS:HA	3:C:172:HIS:HB3	2.00	0.44
9:J:71:LEU:C	9:J:73:GLY:H	2.21	0.44
10:K:103:GLN:HA	10:K:106:GLU:OE1	2.18	0.44
1:A:341:C:H3'	17:T:41:ARG:CZ	160.93	0.44
18:U:94:ASN:HB3	19:V:4:ILE:HD13	2.00	0.44
22:Y:13:VAL:HB	22:Y:72:VAL:HG13	2.00	0.44
32:8:16:ILE:HD12	32:8:59:LYS:HG2	1.99	0.44
33:9:11:CYS:O	33:9:14:CYS:HB2	2.18	0.44
1:A:1132:G:N2	1:A:1148:A:H1'	2.32	0.44
1:A:1910:A:N1	1:A:2245:G:H1'	2.33	0.44
1:A:1991:A:OP2	64:A:3727:HOH:O	2.21	0.44
1:A:2155:A:H1'	1:A:2180:G:N2	2.29	0.44
1:A:989:A:C4	1:A:2459:A:C2	3.06	0.44
2:B:20:C:H2'	2:B:21:G:O4'	2.18	0.44
3:C:182:PRO:C	3:C:184:LYS:N	2.69	0.44
3:C:62:VAL:CB	3:C:63:SER:HA	2.48	0.44
1:A:1844:G:H4'	4:D:51:VAL:HG21	1.99	0.44
5:E:117:MET:O	5:E:118:LYS:CB	2.65	0.44
5:E:54:GLN:OE1	5:E:55:ASN:N	2.51	0.44
6:F:12:LEU:HD12	6:F:12:LEU:HA	1.71	0.44
7:G:61:ALA:O	7:G:65:GLY:N	2.41	0.44
1:A:7:A:H5'	11:N:51:PHE:CE2	2.53	0.44
26:2:38:GLN:HB3	26:2:44:LEU:HB2	2.00	0.43
1:A:2181:G:H5'	1:A:2182:C:OP2	2.18	0.43
1:A:185:A:N6	1:A:2441:A:H2'	2.32	0.43
4:D:71:ASP:HB3	4:D:103:ARG:HH22	1.83	0.43
7:G:173:LEU:HB3	7:G:178:PHE:CG	2.53	0.43
12:O:7:TYR:CE1	12:O:20:MET:HB2	2.53	0.43
19:V:52:VAL:O	19:V:52:VAL:HG23	2.18	0.43
1:A:1210:U:H2'	1:A:1211:C:H6	1.81	0.43
1:A:1446:G:H4'	1:A:1569:G:H4'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1884:A:H2'	1:A:1885:G:O4'	2.18	0.43
1:A:2113:U:H4'	1:A:2114:G:O5'	2.19	0.43
1:A:2189:G:H3'	1:A:2190:A:H5''	2.00	0.43
1:A:699:A:H2'	1:A:700:A:O4'	2.18	0.43
1:A:989:A:H2	64:A:4351:HOH:O	2.01	0.43
4:D:242:ARG:HG2	4:D:246:PRO:HG3	2.00	0.43
4:D:5:LYS:HE3	4:D:17:THR:HG22	1.99	0.43
12:O:73:ASP:OD1	12:O:75:SER:OG	2.35	0.43
1:A:1043:C:P	18:U:92:ARG:HH22	2.41	0.43
1:A:1092:G:N2	1:A:1156:A:N6	2.65	0.43
1:A:1760:G:H2'	1:A:1761:G:O4'	2.18	0.43
1:A:2046:C:H2'	1:A:2047:C:C6	2.53	0.43
1:A:224:C:H2'	1:A:225:C:H6	1.83	0.43
1:A:2588:A:H5''	1:A:2589:G:H5'	2.00	0.43
1:A:2693:U:O2	5:E:22:PRO:HB3	2.18	0.43
1:A:366:C:C2	1:A:388:G:N2	73.11	0.43
1:A:681:G:C6	1:A:682:G:C6	3.06	0.43
2:B:30:C:O2'	2:B:57:A:N1	2.39	0.43
1:A:2153:U:C4	3:C:5:LYS:HG3	2.53	0.43
5:E:52:LEU:HA	5:E:52:LEU:HD12	1.85	0.43
6:F:126:VAL:O	6:F:196:LEU:N	2.51	0.43
7:G:36:LYS:C	7:G:99:MET:HE3	2.39	0.43
8:H:117:PRO:HB3	8:H:123:PHE:CE2	2.54	0.43
8:H:164:TYR:HB2	8:H:167:GLU:HB2	1.99	0.43
18:U:97:ASP:OD2	18:U:101:ARG:HD2	2.18	0.43
26:2:45:SER:O	26:2:46:GLN:HB2	2.17	0.43
31:7:10:ARG:HG2	31:7:14:LYS:HD3	2.00	0.43
1:A:1209:G:H2'	1:A:1210:U:C6	2.52	0.43
1:A:2678:C:H1'	8:H:109:PHE:HD2	1.81	0.43
1:A:269:C:O2'	1:A:271:U:OP2	2.37	0.43
1:A:293:C:H2'	1:A:294:C:C6	2.54	0.43
1:A:509:C:H2'	1:A:510:C:C6	2.53	0.43
1:A:666:G:H21	1:A:670:A:H2	1.62	0.43
7:G:16:ARG:HH22	7:G:28:VAL:HB	1.82	0.43
16:S:80:LEU:HD12	16:S:80:LEU:HA	1.78	0.43
28:4:62:ARG:HB3	28:4:63:TYR:H	1.60	0.43
1:A:1016:G:H8	1:A:1016:G:O5'	2.02	0.43
1:A:1404:A:C6	1:A:1417:U:O4	2.72	0.43
1:A:1768:G:H3'	1:A:1769:A:C8	2.46	0.43
1:A:1778:G:N2	1:A:1779:A:C4	2.86	0.43
1:A:793:U:O2	1:A:2035:A:H1'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2226:G:H5'	1:A:2227:G:O6	2.19	0.43
1:A:2507:C:O2'	1:A:2508:A:H5'	2.18	0.43
4:D:26:LYS:NZ	4:D:30:GLU:OE1	2.51	0.43
4:D:3:VAL:HG13	4:D:17:THR:HB	2.00	0.43
6:F:153:SER:OG	6:F:190:GLU:HG3	2.18	0.43
6:F:184:TYR:O	6:F:188:ARG:HG3	2.19	0.43
6:F:31:HIS:NE2	6:F:35:GLU:OE2	2.52	0.43
12:O:29:ASN:OD1	12:O:29:ASN:N	2.50	0.43
1:A:358:C:H4'	22:Y:73:ARG:HD3	2.00	0.43
1:A:1026:A:OP1	64:A:3730:HOH:O	2.22	0.43
1:A:1468:G:OP1	1:A:1537:G:O2'	2.36	0.43
1:A:1587:G:OP2	1:A:1588:A:O2'	2.28	0.43
1:A:1593:C:H2'	1:A:1594:C:H6	1.84	0.43
2:B:29:A:H2'	2:B:30:C:C6	2.54	0.43
1:A:810:A:H5'	4:D:210:GLY:HA2	1.99	0.43
6:F:64:ILE:HG21	6:F:78:ILE:HG23	2.00	0.43
7:G:150:ASP:CG	7:G:153:ARG:HH12	2.21	0.43
7:G:32:PRO:HB2	7:G:172:LEU:HD22	2.00	0.43
10:K:127:ILE:HG12	10:K:127:ILE:H	1.67	0.43
12:O:77:ILE:HG13	17:T:74:ARG:HG3	2.00	0.43
19:V:1:MET:HB3	19:V:99:ILE:HD12	2.00	0.43
26:2:70:GLN:HE21	26:2:70:GLN:C	2.22	0.43
28:4:59:PHE:H	28:4:59:PHE:HD1	1.67	0.43
1:A:1218:A:H1'	1:A:1219:U:C5'	2.48	0.43
1:A:2602:C:H2'	1:A:2603:G:C8	2.53	0.43
1:A:283:G:C2	1:A:284:U:O4	2.70	0.43
1:A:503:A:C6	1:A:505:A:C6	3.07	0.43
1:A:771:G:C6	1:A:772:G:N1	2.86	0.43
1:A:908:G:H2'	1:A:909:A:O4'	2.18	0.43
2:B:3:C:H2'	2:B:4:C:H6	1.83	0.43
2:B:96:U:H2'	2:B:97:G:C8	2.54	0.43
7:G:150:ASP:OD2	7:G:153:ARG:NH1	2.51	0.43
11:N:12:ARG:HD3	11:N:14:VAL:HG23	2.00	0.43
13:P:115:LEU:HA	13:P:131:SER:HB3	2.01	0.43
18:U:27:LEU:HB3	18:U:31:SER:HB3	2.01	0.43
19:V:61:VAL:HG23	19:V:61:VAL:O	2.18	0.43
28:4:59:PHE:N	28:4:59:PHE:CD1	2.87	0.43
1:A:1066:A:C3'	1:A:1066:A:C8	3.02	0.43
1:A:1144:G:O2'	1:A:1145:C:H5'	2.19	0.43
1:A:1283:G:O2'	1:A:1284:G:H5'	2.19	0.43
1:A:1765:G:H5'	1:A:1766:A:H5''	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:C:H2'	1:A:225:C:C6	2.53	0.43
1:A:31:C:C2'	1:A:32:U:H5'	2.48	0.43
1:A:928:G:H22	1:A:939:C:N4	2.17	0.43
6:F:32:LEU:O	6:F:36:VAL:HG23	2.19	0.43
7:G:143:GLU:H	7:G:143:GLU:CD	2.22	0.43
8:H:111:HIS:H	8:H:111:HIS:CD2	2.36	0.43
10:K:18:THR:O	10:K:20:ALA:N	2.51	0.43
16:S:59:LYS:HB3	16:S:65:VAL:HG22	2.00	0.43
16:S:23:ARG:NH1	16:S:85:VAL:O	2.47	0.43
1:A:1008:C:H6	1:A:1010:G:N7	8.89	0.43
1:A:1092:G:H2'	1:A:1155:G:N2	2.33	0.43
1:A:800:C:O2'	1:A:1317:A:N1	2.47	0.43
1:A:1335:C:H2'	1:A:1336:C:C6	2.54	0.43
1:A:1369:G:H2'	1:A:1370:G:H8	7.94	0.43
1:A:138:A:H2'	1:A:138:A:N3	3.94	0.43
1:A:140:C:H2'	1:A:141:G:O4'	2.19	0.43
1:A:2700:U:O2	1:A:2700:U:H2'	2.17	0.43
1:A:2736:C:OP1	5:E:118:LYS:NZ	2.51	0.43
1:A:641:G:H2'	1:A:642:C:O4'	2.19	0.43
5:E:67:PHE:CE1	5:E:75:VAL:HG22	2.54	0.43
10:K:77:LEU:O	10:K:78:ILE:HB	2.18	0.43
1:A:955:A:C5	14:Q:13:GLN:HG3	2.54	0.43
19:V:31:ALA:O	19:V:61:VAL:HG22	2.19	0.43
19:V:52:VAL:HG23	19:V:55:ALA:HB3	2.01	0.43
1:A:1216:G:H3'	1:A:1217:G:C8	2.54	0.43
1:A:1404:A:N6	1:A:1417:U:H3	2.16	0.43
1:A:2107:U:H2'	1:A:2108:G:C8	2.53	0.43
1:A:2256:U:H5''	1:A:2257:G:H5'	2.01	0.43
1:A:2558:U:H2'	1:A:2559:G:C8	2.53	0.43
1:A:353:A:HO2'	1:A:354:A:H8	1.61	0.43
1:A:360:C:H2'	1:A:361:G:O4'	2.19	0.43
1:A:12:A:N1	1:A:549:U:H2'	2.34	0.43
4:D:145:VAL:HB	4:D:155:LEU:HB2	1.99	0.43
4:D:34:VAL:HA	4:D:62:TYR:O	2.19	0.43
7:G:39:ILE:HD11	7:G:102:PHE:CZ	2.54	0.43
8:H:24:VAL:HG11	8:H:43:VAL:HG11	2.01	0.43
10:K:9:LYS:HB2	10:K:9:LYS:HE3	1.78	0.43
1:A:2330:G:H1	16:S:3:ARG:HA	1.83	0.43
25:1:82:LEU:HA	25:1:85:LEU:CD2	2.49	0.42
28:4:9:LEU:HD12	28:4:9:LEU:HA	1.88	0.42
1:A:1008:C:H2'	1:A:1008:C:H6	3.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:G:C6	1:A:1114:A:C6	3.07	0.42
1:A:1635:U:H2'	1:A:1636:G:H8	1.82	0.42
1:A:1711:A:H2'	1:A:1712:G:O4'	2.19	0.42
1:A:173:U:H2'	1:A:174:G:H8	1.82	0.42
1:A:2085:C:H2'	1:A:2086:C:C6	2.54	0.42
1:A:2190:A:C8	1:A:2190:A:OP1	2.72	0.42
1:A:830:A:C6	4:D:229:VAL:HG11	2.53	0.42
6:F:136:THR:HG22	6:F:140:LEU:HD23	2.00	0.42
8:H:32:GLU:N	8:H:32:GLU:OE1	2.52	0.42
10:K:125:ARG:HG3	10:K:125:ARG:H	1.62	0.42
1:A:1761:G:O6	1:A:1773:C:N3	2.52	0.42
1:A:2126:C:H2'	1:A:2127:G:H5''	2.00	0.42
1:A:2903:U:H2'	1:A:2904:C:C6	2.54	0.42
1:A:669:C:H6	1:A:669:C:H3'	1.84	0.42
7:G:106:LEU:HA	7:G:110:ALA:HB3	2.02	0.42
12:O:120:GLU:OE2	17:T:67:SER:OG	2.30	0.42
14:Q:39:PRO:HA	14:Q:97:VAL:O	2.19	0.42
21:X:12:VAL:HG22	21:X:29:TRP:CE2	2.55	0.42
22:Y:86:ARG:NH1	22:Y:100:ALA:HA	2.35	0.42
22:Y:9:LYS:HA	22:Y:10:GLY:HA2	1.71	0.42
1:A:242:G:O6	32:8:5:LYS:HD3	2.19	0.42
1:A:1093:A:OP2	1:A:1154:C:N4	2.53	0.42
1:A:1185:U:OP1	11:N:25:ARG:NH1	2.53	0.42
1:A:828:A:H5'	1:A:829:A:N7	2.34	0.42
2:B:41:U:H5	7:G:70:VAL:O	2.02	0.42
17:T:50:ILE:HB	17:T:99:LEU:HB2	2.01	0.42
21:X:43:VAL:HG13	21:X:47:PHE:HD1	1.83	0.42
26:2:1:MET:HB2	26:2:52:ASP:OD1	2.19	0.42
1:A:1251:C:H2'	1:A:1252:C:H6	1.85	0.42
1:A:1424:A:H4'	1:A:1425:G:OP2	2.19	0.42
1:A:2143:U:O2	3:C:172:HIS:CE1	2.73	0.42
1:A:240:G:OP2	13:P:50:ARG:NH1	2.52	0.42
3:C:68:LEU:HD12	3:C:70:LYS:HB3	2.02	0.42
5:E:101:ARG:CZ	5:E:171:GLU:HB2	2.50	0.42
20:W:37:ARG:NH1	20:W:37:ARG:HB3	2.34	0.42
21:X:34:ALA:HA	21:X:38:GLU:OE1	2.18	0.42
30:6:11:LEU:HB2	30:6:21:TYR:HB2	2.01	0.42
1:A:2488:C:O2	33:9:4:ARG:NH2	2.47	0.42
1:A:935:C:H1'	1:A:936:A:C1'	2.50	0.42
3:C:190:ARG:O	3:C:194:ARG:HG2	2.19	0.42
7:G:173:LEU:HD13	7:G:178:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:131:GLN:N	11:N:131:GLN:OE1	2.52	0.42
12:O:101:PRO:HG3	17:T:67:SER:HB3	2.01	0.42
16:S:34:HIS:HB2	16:S:36:TYR:HE1	1.83	0.42
28:4:61:ARG:HG3	28:4:62:ARG:N	2.35	0.42
30:6:21:TYR:CD2	30:6:38:LYS:HG2	2.54	0.42
1:A:1344:G:H5''	1:A:1345:U:OP1	2.20	0.42
1:A:1670:C:H2'	1:A:1671:G:O4'	2.20	0.42
1:A:1883:A:H2'	1:A:1884:A:C8	2.54	0.42
2:B:93:G:H2'	2:B:94:C:C6	2.54	0.42
7:G:77:ILE:HD12	7:G:82:LEU:HD11	2.02	0.42
10:K:89:HIS:C	10:K:91:PRO:HD3	2.40	0.42
10:K:97:GLY:C	10:K:136:VAL:HG23	2.40	0.42
17:T:45:PHE:HE2	17:T:63:VAL:HB	1.85	0.42
1:A:1054:A:O4'	18:U:59:ARG:HG2	2.20	0.42
25:1:57:GLU:H	25:1:57:GLU:CD	2.22	0.42
1:A:183:A:H5''	13:P:46:LYS:HZ1	1.84	0.42
1:A:2132:C:OP2	1:A:2166:C:N4	2.48	0.42
1:A:2505:G:O2'	14:Q:80:GLU:HA	2.19	0.42
1:A:483:G:O2'	1:A:494:G:O6	2.25	0.42
1:A:769:G:H2'	1:A:770:U:O4'	2.18	0.42
1:A:914:U:C4	1:A:915:G:N7	2.88	0.42
5:E:59:VAL:CG1	5:E:64:LYS:HG3	2.50	0.42
6:F:133:ASN:N	6:F:138:GLU:OE1	2.44	0.42
7:G:41:GLN:HG2	7:G:154:GLY:O	2.20	0.42
1:A:1091:A:C6	9:J:6:ASN:N	2.83	0.42
10:K:76:TYR:CE2	10:K:77:LEU:HD23	2.55	0.42
16:S:51:ALA:HB3	16:S:73:LEU:HB2	2.00	0.42
1:A:1185:U:H4'	1:A:1187:A:O4'	2.20	0.42
1:A:2049:U:H2'	1:A:2050:G:O4'	2.19	0.42
1:A:2129:C:C2'	1:A:2130:U:H5'	2.49	0.42
1:A:2137:G:H2'	1:A:2138:A:N7	2.35	0.42
1:A:2254:U:H2'	1:A:2255:U:C6	2.55	0.42
1:A:2432:G:C5'	1:A:2432:G:H8	2.33	0.42
1:A:2641:G:O4'	1:A:2902:G:H1'	2.19	0.42
1:A:557:G:H5'	18:U:24:TYR:CE2	2.55	0.42
1:A:1185:U:P	11:N:25:ARG:HH12	2.42	0.42
26:2:28:LYS:HG3	26:2:53:LEU:HD21	2.01	0.42
29:5:16:ARG:NH1	29:5:17:ASP:OD1	2.52	0.42
15:R:33:ARG:NH2	29:5:57:VAL:O	2.42	0.42
1:A:150:C:C2	1:A:151:G:C8	3.64	0.42
1:A:1358:U:H2'	1:A:1655:A:C2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1820:C:H5''	1:A:1821:A:OP1	2.20	0.42
1:A:2226:G:HO2'	1:A:2227:G:P	2.40	0.42
1:A:2622:U:H3'	1:A:2622:U:OP2	2.20	0.42
1:A:504:A:H4'	1:A:505:A:OP1	2.20	0.42
1:A:660:G:H4'	1:A:662:G:O3'	2.20	0.42
3:C:29:VAL:C	3:C:31:GLU:H	2.23	0.42
1:A:1850:U:C2	4:D:202:LYS:HD2	2.54	0.42
8:H:144:VAL:O	8:H:148:ILE:HG12	2.19	0.42
1:A:1185:U:H6	11:N:63:THR:OG1	2.03	0.42
17:T:51:ARG:HG3	17:T:98:LYS:CD	2.50	0.42
23:Z:14:LYS:HE2	23:Z:14:LYS:HB2	1.88	0.42
33:9:4:ARG:O	33:9:36:GLN:HA	2.20	0.42
1:A:1162:G:H2'	1:A:1163:C:C6	2.54	0.42
1:A:137:G:H3'	1:A:138:A:H8	9.24	0.42
20:W:32:ALA:CB	20:W:51:LEU:HD11	2.49	0.42
14:Q:139:GLU:OE2	23:Z:54:HIS:HE1	2.03	0.42
25:1:10:LYS:NZ	25:1:65:SER:OG	2.51	0.41
1:A:1685:U:O2'	1:A:1686:C:H5'	2.19	0.41
1:A:2118:C:H2'	1:A:2119:U:O4'	2.19	0.41
1:A:955:A:N1	1:A:2288:G:H1'	2.35	0.41
1:A:2333:A:H2'	1:A:2334:G:O4'	2.20	0.41
1:A:2878:G:H2'	1:A:2879:C:O4'	2.20	0.41
1:A:435:C:O2'	1:A:436:G:H5'	2.20	0.41
1:A:480:C:H3'	1:A:481:C:H5''	2.02	0.41
1:A:998:G:H5''	14:Q:13:GLN:HB3	2.01	0.41
6:F:9:ILE:HD12	6:F:22:ALA:HB2	2.02	0.41
10:K:71:THR:HA	10:K:72:PRO:HD2	1.90	0.41
21:X:54:VAL:HG22	21:X:81:VAL:HG12	2.02	0.41
22:Y:9:LYS:HD2	22:Y:28:LYS:O	2.20	0.41
1:A:1090:A:H5''	1:A:1091:A:O5'	2.20	0.41
1:A:195:A:H2'	1:A:196:C:O4'	2.19	0.41
1:A:394:C:H2'	1:A:395:C:O4'	2.20	0.41
1:A:770:U:H2'	1:A:771:G:O4'	2.19	0.41
1:A:89:A:H2'	1:A:90:G:O4'	2.19	0.41
3:C:163:PHE:N	3:C:163:PHE:CD1	2.88	0.41
5:E:50:GLY:HA2	5:E:77:ILE:O	2.19	0.41
12:O:98:VAL:HG13	12:O:117:LEU:HB3	2.02	0.41
24:O:33:ALA:C	24:O:35:ASN:H	2.23	0.41
1:A:74:C:OP1	26:2:55:ARG:HD3	2.20	0.41
26:2:64:LEU:HD11	26:2:68:ARG:NH2	2.35	0.41
1:A:1774:C:H6	1:A:1774:C:H5''	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2148:G:C6	1:A:2183:G:C2	3.08	0.41
1:A:947:C:H2'	1:A:948:C:C6	2.55	0.41
3:C:10:LEU:HD21	3:C:34:THR:OG1	2.20	0.41
5:E:108:SER:O	5:E:162:ALA:HA	2.19	0.41
12:O:91:LEU:HB3	12:O:111:PHE:CE1	2.55	0.41
13:P:148:LEU:N	13:P:148:LEU:HD23	2.34	0.41
13:P:98:GLU:HA	13:P:101:VAL:HB	2.01	0.41
26:2:52:ASP:O	26:2:56:GLN:HG3	2.21	0.41
1:A:1381:A:H2'	1:A:1382:G:C8	2.55	0.41
1:A:1525:G:H5'	1:A:1604:A:C2	2.55	0.41
1:A:1786:G:H4'	1:A:1788:G:O4'	2.20	0.41
1:A:2198:C:H2'	1:A:2199:C:O4'	2.20	0.41
1:A:2594:G:H2'	1:A:2595:U:O4'	2.21	0.41
1:A:319:C:OP2	22:Y:4:LYS:NZ	2.46	0.41
1:A:628:U:H4'	1:A:704:C:H4'	2.03	0.41
1:A:88:U:O2'	1:A:89:A:H8	2.02	0.41
3:C:189:ILE:HD11	3:C:214:VAL:CG2	2.50	0.41
6:F:179:GLU:H	6:F:179:GLU:CD	2.23	0.41
7:G:37:VAL:HG23	7:G:99:MET:HE3	2.02	0.41
8:H:41:MET:HE3	8:H:54:ARG:HB3	2.02	0.41
8:H:41:MET:HE2	8:H:65:HIS:HA	2.02	0.41
12:O:23:ARG:HG3	12:O:24:VAL:N	2.34	0.41
1:A:1552:A:O2'	1:A:1553:A:H8	2.03	0.41
1:A:1945:C:H2'	1:A:1946:C:O4'	2.21	0.41
1:A:728:G:N2	1:A:842:C:C2	2.88	0.41
1:A:998:G:N3	1:A:2285:A:C2	2.89	0.41
2:B:14:U:O2	2:B:108:U:H4'	2.20	0.41
2:B:9:G:OP1	16:S:19:LYS:NZ	2.52	0.41
1:A:2198:C:H5''	3:C:213:TYR:CG	2.55	0.41
3:C:68:LEU:O	3:C:175:VAL:HG21	2.20	0.41
3:C:8:ARG:HA	3:C:11:LEU:HB3	2.02	0.41
4:D:102:LYS:C	4:D:103:ARG:HG2	2.40	0.41
6:F:74:ARG:H	6:F:74:ARG:HG3	1.48	0.41
13:P:130:PHE:HB3	13:P:135:LEU:HG	2.03	0.41
14:Q:7:MET:HE1	14:Q:93:TYR:HE2	1.86	0.41
17:T:37:GLY:HA2	17:T:38:ASN:HA	1.63	0.41
18:U:90:VAL:CG1	18:U:95:LEU:HD13	2.51	0.41
1:A:1389:G:H4'	1:A:1429:A:C5	2.56	0.41
1:A:1531:A:H2'	1:A:1532:G:H8	1.85	0.41
1:A:1621:C:H2'	1:A:1622:U:C6	2.55	0.41
1:A:1904:G:H8	1:A:1904:G:O5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2166:C:H3'	1:A:2167:C:C6	2.55	0.41
1:A:2563:U:C2	1:A:2565:U:H5'	2.55	0.41
1:A:2759:G:O6	1:A:2767:C:H5''	2.20	0.41
1:A:2901:G:O5'	1:A:2901:G:H8	2.04	0.41
1:A:388:G:H2'	1:A:389:G:O4'	2.19	0.41
1:A:552:A:N1	1:A:2063:A:H2'	2.35	0.41
1:A:857:U:H2'	13:P:21:ARG:HA	2.01	0.41
4:D:85:ASP:OD2	4:D:88:ARG:HD2	2.21	0.41
8:H:98:LEU:HD23	8:H:98:LEU:HA	1.86	0.41
10:K:12:LEU:H	10:K:54:PRO:HA	1.86	0.41
1:A:2558:U:O2	12:O:23:ARG:NH2	2.53	0.41
15:R:70:LEU:O	15:R:72:ASP:N	2.49	0.41
20:W:24:ILE:HA	20:W:27:LYS:HG3	2.01	0.41
1:A:1113:G:N2	1:A:1140:A:O2'	2.53	0.41
1:A:601:G:C2	1:A:1307:A:C4	3.08	0.41
1:A:1457:A:H61	1:A:1635:U:H3	1.68	0.41
1:A:1467:G:H1'	1:A:1541:A:N1	2.34	0.41
1:A:2120:U:H2'	1:A:2120:U:O2	2.20	0.41
1:A:2152:G:H5''	1:A:2154:G:O4'	2.20	0.41
1:A:2473:U:H2'	1:A:2474:C:C6	2.56	0.41
1:A:2649:G:P	5:E:82:ARG:HH22	2.44	0.41
5:E:195:LEU:HD12	5:E:196:VAL:N	2.36	0.41
20:W:29:LEU:HD21	20:W:33:ARG:NH2	2.35	0.41
1:A:1217:G:H1'	1:A:1218:A:H5'	2.03	0.41
1:A:1489:G:H2'	1:A:1491:C:C5	2.56	0.41
1:A:1631:A:OP2	1:A:1631:A:H8	2.04	0.41
1:A:2159:C:N4	1:A:2174:G:N2	2.69	0.41
1:A:33:C:H2'	1:A:34:G:C5'	2.49	0.41
1:A:464:G:H2'	1:A:465:G:H8	1.86	0.41
14:Q:12:GLN:HB2	14:Q:12:GLN:HE21	1.53	0.41
1:A:2039:G:O2'	18:U:34:LYS:HE3	2.21	0.41
23:Z:70:LEU:HA	23:Z:70:LEU:HD23	1.75	0.41
1:A:422:G:H1'	25:1:42:GLN:HB3	2.02	0.41
1:A:1043:C:P	18:U:92:ARG:NH2	2.93	0.41
1:A:1128:U:O2'	1:A:1130:A:N7	2.49	0.41
1:A:2146:G:OP1	3:C:40:THR:OG1	2.34	0.41
1:A:2189:G:N1	1:A:2191:A:H3'	2.36	0.41
1:A:271:U:HO2'	1:A:272:G:P	2.38	0.41
1:A:2845:U:C4	1:A:2892:A:N6	2.89	0.41
1:A:401:C:H2'	1:A:402:C:C6	2.56	0.41
1:A:464:G:H2'	1:A:465:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:G:H2'	1:A:516:A:H8	1.86	0.41
1:A:609:C:N4	13:P:31:ALA:HB3	2.36	0.41
11:N:42:TRP:HD1	11:N:48:MET:HE1	1.86	0.41
16:S:78:LEU:HD12	16:S:108:GLY:O	2.20	0.41
20:W:17:VAL:HG13	20:W:76:VAL:HG21	2.02	0.41
26:2:32:LEU:HD23	26:2:32:LEU:HA	1.86	0.41
1:A:1213:G:H2'	1:A:1214:G:O4'	2.21	0.41
1:A:1597:C:H2'	1:A:1598:G:O4'	2.20	0.41
1:A:1784:C:H2'	1:A:1785:A:O4'	2.21	0.41
5:E:36:ARG:HH11	5:E:85:ASN:HD22	1.68	0.41
6:F:135:LYS:HB2	6:F:138:GLU:CD	2.40	0.41
6:F:137:LYS:HA	6:F:140:LEU:HB2	2.02	0.41
1:A:345:A:OP2	6:F:169:ASN:HB2	2.21	0.41
6:F:178:PRO:HB3	6:F:198:ALA:HB1	2.03	0.41
7:G:146:TYR:C	7:G:148:MET:H	2.25	0.41
14:Q:30:GLY:O	14:Q:134:ARG:HD3	2.21	0.41
15:R:48:VAL:O	15:R:51:LEU:N	2.54	0.41
17:T:74:ARG:HH11	17:T:74:ARG:CG	2.33	0.41
19:V:30:GLY:H	19:V:61:VAL:HG23	1.86	0.41
28:4:49:PHE:HB3	28:4:50:VAL:H	1.65	0.41
1:A:1011:C:H2'	1:A:1012:G:H8	2.81	0.41
1:A:1132:G:C6	1:A:1134:G:C2	3.08	0.41
1:A:2648:U:C4	1:A:2649:G:C6	3.09	0.41
1:A:491:A:N3	1:A:729:C:H1'	2.36	0.41
1:A:898:G:H2'	1:A:899:G:C8	2.55	0.41
2:B:89:G:C6	2:B:90:A:C6	3.09	0.41
1:A:810:A:OP1	4:D:208:LYS:HE3	2.21	0.41
10:K:14:ALA:CB	10:K:53:VAL:HG23	2.49	0.41
16:S:36:TYR:N	16:S:36:TYR:HD1	2.19	0.41
17:T:119:LYS:O	17:T:123:GLN:HG3	2.21	0.41
17:T:16:ARG:HG3	17:T:18:ASP:OD2	2.20	0.41
1:A:1130:A:H1'	1:A:1150:U:H1'	2.03	0.40
1:A:1847:G:H2'	1:A:1848:U:H5'	2.02	0.40
1:A:2147:A:C6	1:A:2184:C:H4'	2.56	0.40
1:A:2139:U:O4	1:A:2170:G:H1'	2.20	0.40
1:A:858:C:H1'	1:A:1295:G:C2	2.56	0.40
2:B:73:A:C4	2:B:105:A:C2	3.08	0.40
4:D:147:LEU:HD13	4:D:155:LEU:HD11	2.02	0.40
10:K:99:ILE:HG12	10:K:136:VAL:CG2	2.50	0.40
13:P:85:LEU:HG	13:P:116:GLY:HA2	2.03	0.40
1:A:2283:U:H5''	1:A:2284:A:OP1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2052:A:C6	1:A:2509:C:H1'	2.57	0.40
1:A:2706:C:H2'	1:A:2707:U:H6	1.85	0.40
1:A:2858:U:N3	1:A:2876:G:O4'	2.52	0.40
1:A:26:G:N2	1:A:536:G:H1'	2.36	0.40
2:B:44:G:OP2	28:4:1:MET:N	2.33	0.40
6:F:22:ALA:O	6:F:23:ASP:HB3	2.21	0.40
1:A:1091:A:H61	9:J:5:ARG:C	2.25	0.40
25:1:83:GLU:HA	25:1:84:GLY:HA2	1.55	0.40
1:A:2430:U:OP1	32:8:41:ILE:HD12	2.21	0.40
1:A:137:G:C4	1:A:138:A:C8	8.35	0.40
1:A:182:G:H2'	1:A:183:A:O4'	2.21	0.40
1:A:2363:A:H8	1:A:2363:A:O5'	2.04	0.40
1:A:251:C:H2'	1:A:252:C:O4'	2.21	0.40
1:A:274:C:H2'	1:A:275:C:C6	2.56	0.40
1:A:330:G:H21	1:A:353:A:H62	1.68	0.40
1:A:353:A:O2'	1:A:354:A:C8	2.72	0.40
1:A:635:G:O2'	1:A:639:A:N1	2.40	0.40
1:A:830:A:H3'	64:A:4065:HOH:O	2.20	0.40
1:A:839:A:H1'	64:A:4127:HOH:O	2.21	0.40
2:B:42:C:O2	7:G:93:THR:N	2.48	0.40
3:C:68:LEU:HA	3:C:175:VAL:HG21	2.02	0.40
8:H:101:ARG:H	8:H:101:ARG:HG3	1.41	0.40
10:K:56:GLU:O	10:K:67:PHE:HA	2.22	0.40
18:U:92:ARG:HA	18:U:95:LEU:HB2	2.01	0.40
28:4:14:ILE:HB	28:4:22:ILE:CG1	2.50	0.40
33:9:3:VAL:HA	33:9:35:ARG:O	2.21	0.40
1:A:111:U:O2'	21:X:33:LYS:NZ	2.48	0.40
1:A:1463:G:H8	1:A:1463:G:O5'	2.05	0.40
1:A:409:U:H2'	1:A:411:C:H5	1.86	0.40
1:A:531:A:H4'	1:A:532:G:O5'	4.54	0.40
1:A:875:A:N7	1:A:2258:A:O2'	2.51	0.40
1:A:941:A:H2'	1:A:941:A:N3	2.36	0.40
4:D:141:VAL:HG23	4:D:162:SER:HB2	2.03	0.40
5:E:115:GLY:O	5:E:119:ARG:HB2	2.21	0.40
5:E:8:LYS:HD3	5:E:191:PRO:O	2.20	0.40
6:F:56:GLU:OE2	6:F:93:LYS:NZ	2.47	0.40
8:H:54:ARG:NH2	8:H:57:ASP:HB2	2.27	0.40
11:N:96:GLU:O	11:N:100:GLU:HG3	2.21	0.40
14:Q:68:ILE:HG22	14:Q:101:ARG:HE	1.87	0.40
14:Q:114:ALA:O	14:Q:118:LEU:HG	2.22	0.40
23:Z:14:LYS:HB3	23:Z:17:ALA:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:24:LEU:HD21	23:Z:86:VAL:HG23	2.03	0.40
1:A:1385:U:OP1	21:X:16:LYS:NZ	2.49	0.40
1:A:1958:A:C8	1:A:1960:U:H2'	2.56	0.40
1:A:2641:G:H2'	1:A:2642:G:C8	2.55	0.40
1:A:514:G:P	1:A:514:G:H3'	3.99	0.40
1:A:587:C:H2'	1:A:588:U:O4'	2.22	0.40
1:A:830:A:C8	1:A:838:G:C5	3.10	0.40
5:E:94:GLU:H	5:E:94:GLU:HG2	1.59	0.40
7:G:43:LEU:HB3	7:G:44:GLY:H	1.66	0.40
11:N:30:ILE:HG22	11:N:34:LEU:HD22	2.01	0.40
12:O:2:ILE:HB	12:O:33:ALA:HB3	2.04	0.40
13:P:95:VAL:HA	13:P:99:LEU:HD23	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1519:G:N2	20:W:111:HIS:O[4_557]	2.15	0.05

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	130/228 (57%)	94 (72%)	25 (19%)	11 (8%)	1	1
4	D	273/276 (99%)	255 (93%)	15 (6%)	3 (1%)	14	30
5	E	202/206 (98%)	188 (93%)	11 (5%)	3 (2%)	10	21
6	F	201/210 (96%)	184 (92%)	12 (6%)	5 (2%)	5	9
7	G	179/182 (98%)	162 (90%)	10 (6%)	7 (4%)	3	4
8	H	172/180 (96%)	148 (86%)	17 (10%)	7 (4%)	3	3
9	J	128/173 (74%)	76 (59%)	22 (17%)	30 (23%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	137/147 (93%)	85 (62%)	31 (23%)	21 (15%)	0	0
11	N	138/140 (99%)	129 (94%)	5 (4%)	4 (3%)	4	7
12	O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	39
13	P	147/150 (98%)	129 (88%)	16 (11%)	2 (1%)	11	22
14	Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	43
15	R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
16	S	108/112 (96%)	96 (89%)	10 (9%)	2 (2%)	8	15
17	T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	19	39
18	U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
19	V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	7	14
20	W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
21	X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	30
22	Y	105/110 (96%)	89 (85%)	12 (11%)	4 (4%)	3	4
23	Z	92/206 (45%)	84 (91%)	8 (9%)	0	100	100
24	0	72/85 (85%)	67 (93%)	3 (4%)	2 (3%)	5	7
25	1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	4	6
26	2	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	10	21
27	3	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	4	67/71 (94%)	45 (67%)	15 (22%)	7 (10%)	0	0
29	5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
31	7	47/49 (96%)	44 (94%)	1 (2%)	2 (4%)	2	3
32	8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
33	9	35/37 (95%)	35 (100%)	0	0	100	100
35	b	229/256 (90%)	192 (84%)	23 (10%)	14 (6%)	1	1
36	c	204/239 (85%)	177 (87%)	20 (10%)	7 (3%)	3	5
37	d	206/209 (99%)	187 (91%)	16 (8%)	3 (2%)	10	21
38	e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	7	13
39	f	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	4	6
40	g	153/156 (98%)	135 (88%)	13 (8%)	5 (3%)	4	6
41	h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	i	125/128 (98%)	113 (90%)	5 (4%)	7 (6%)	2	2
43	j	94/105 (90%)	79 (84%)	6 (6%)	9 (10%)	0	0
44	k	112/129 (87%)	107 (96%)	4 (4%)	1 (1%)	17	35
45	l	120/132 (91%)	112 (93%)	7 (6%)	1 (1%)	19	39
46	m	117/126 (93%)	102 (87%)	9 (8%)	6 (5%)	2	2
47	n	58/61 (95%)	57 (98%)	0	1 (2%)	9	18
48	o	86/89 (97%)	78 (91%)	5 (6%)	3 (4%)	3	5
49	p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	12	24
50	q	97/105 (92%)	86 (89%)	8 (8%)	3 (3%)	4	6
51	r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
52	s	81/93 (87%)	72 (89%)	4 (5%)	5 (6%)	1	1
53	t	94/106 (89%)	84 (89%)	4 (4%)	6 (6%)	1	1
54	u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
59	z	669/679 (98%)	568 (85%)	62 (9%)	39 (6%)	1	1
All	All	6534/7143 (92%)	5800 (89%)	497 (8%)	237 (4%)	3	4

All (237) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	65	PRO
3	C	172	HIS
3	C	224	ILE
4	D	275	LYS
6	F	130	ALA
6	F	165	ARG
7	G	47	LYS
7	G	50	ALA
7	G	81	LYS
8	H	126	PRO
9	J	71	LEU
9	J	74	LEU
9	J	77	PRO
9	J	80	VAL
9	J	104	ILE
9	J	105	PRO
9	J	107	VAL
9	J	128	LEU

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Mol	Chain	Res	Type
10	K	13	PRO
10	K	38	VAL
10	K	39	LYS
10	K	78	ILE
10	K	89	HIS
10	K	93	ARG
10	K	96	VAL
13	P	45	LEU
17	T	127	ALA
19	V	100	ARG
21	X	94	GLY
24	0	33	ALA
28	4	49	PHE
28	4	55	ARG
35	b	8	LYS
35	b	37	ASN
35	b	131	PRO
36	c	47	LEU
36	c	61	ALA
39	f	62	TRP
43	j	29	ARG
43	j	55	LYS
43	j	79	ARG
46	m	85	GLY
47	n	3	ARG
48	o	88	ARG
49	p	67	THR
50	q	14	LYS
52	s	14	HIS
52	s	30	LEU
53	t	95	ALA
53	t	99	LEU
53	t	100	ILE
59	z	98	ALA
59	z	235	LYS
59	z	373	ALA
59	z	390	VAL
59	z	444	ALA
59	z	459	ILE
3	C	66	HIS
3	C	179	SER
3	C	183	GLU

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Mol	Chain	Res	Type
4	D	125	ILE
5	E	118	LYS
6	F	22	ALA
7	G	52	ILE
7	G	126	ASP
7	G	147	ASP
8	H	47	GLU
8	H	92	ILE
9	J	75	GLN
9	J	91	LYS
9	J	93	LEU
9	J	123	GLU
9	J	125	LEU
9	J	132	ASP
10	K	29	GLN
10	K	77	LEU
10	K	91	PRO
12	O	5	GLN
14	Q	60	ARG
16	S	59	LYS
19	V	42	GLY
22	Y	2	ARG
22	Y	6	HIS
24	0	34	GLY
26	2	46	GLN
28	4	46	GLN
28	4	60	GLN
31	7	45	ALA
31	7	46	VAL
35	b	17	PHE
35	b	122	PHE
35	b	135	GLN
35	b	236	TYR
36	c	46	GLU
37	d	5	ILE
37	d	36	ARG
38	e	85	GLY
39	f	38	GLU
40	g	83	ALA
42	i	88	TYR
42	i	118	LYS
43	j	34	VAL

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Mol	Chain	Res	Type
44	k	105	VAL
46	m	7	VAL
46	m	49	THR
50	q	68	ARG
52	s	26	GLY
59	z	-35	GLY
59	z	-34	LEU
59	z	64	VAL
59	z	97	LEU
59	z	268	ILE
59	z	272	HIS
59	z	384	SER
59	z	389	GLU
59	z	400	THR
59	z	417	PRO
59	z	542	GLY
59	z	564	GLY
3	C	178	ALA
4	D	3	VAL
8	H	122	THR
9	J	22	GLY
9	J	33	PRO
9	J	56	ASN
9	J	69	PRO
9	J	84	GLU
9	J	101	PRO
10	K	11	GLN
10	K	14	ALA
10	K	31	GLY
10	K	50	ASP
10	K	54	PRO
10	K	113	PRO
11	N	7	LYS
22	Y	5	MET
25	1	3	LYS
28	4	56	VAL
28	4	62	ARG
35	b	16	HIS
35	b	21	ARG
36	c	81	GLY
36	c	108	ASN
36	c	206	GLU

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Mol	Chain	Res	Type
37	d	166	LYS
39	f	61	LEU
40	g	7	ALA
40	g	84	ASN
42	i	119	ALA
43	j	30	SER
45	l	19	ARG
59	z	288	PRO
59	z	292	PRO
59	z	326	ASN
59	z	382	LEU
59	z	418	GLU
59	z	461	TYR
3	C	159	GLY
3	C	210	ARG
5	E	52	LEU
6	F	23	ASP
8	H	3	ARG
9	J	72	ASP
10	K	16	LYS
10	K	81	ALA
10	K	114	ASP
11	N	88	GLU
16	S	84	GLN
22	Y	54	LYS
25	l	79	GLY
35	b	13	ALA
35	b	15	VAL
35	b	121	LEU
35	b	232	PRO
40	g	55	GLY
40	g	80	VAL
42	i	24	GLY
42	i	105	ASP
43	j	32	ALA
46	m	40	ASN
48	o	24	SER
52	s	29	ARG
59	z	43	GLU
59	z	294	PHE
59	z	445	GLN
59	z	460	LEU

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Mol	Chain	Res	Type
59	z	503	ALA
3	C	220	PRO
5	E	72	VAL
6	F	7	TYR
9	J	5	ARG
9	J	31	GLY
9	J	120	LYS
10	K	4	VAL
10	K	88	ALA
11	N	2	LYS
11	N	19	GLU
25	l	83	GLU
35	b	52	GLU
36	c	66	VAL
38	e	8	GLU
38	e	69	VAL
42	i	12	GLU
46	m	86	CYS
50	q	49	GLU
52	s	25	LYS
59	z	194	ALA
59	z	310	SER
59	z	325	LEU
59	z	421	VAL
59	z	472	ARG
59	z	553	ALA
3	C	180	PHE
7	G	145	THR
8	H	99	VAL
9	J	20	ALA
9	J	114	GLY
43	j	77	PRO
43	j	78	ASN
53	t	10	LEU
53	t	97	ALA
59	z	81	ILE
59	z	267	ALA
43	j	75	ILE
46	m	6	GLY
48	o	87	ILE
59	z	274	VAL
53	t	47	GLY

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Mol	Chain	Res	Type
8	H	100	GLY
9	J	53	VAL
9	J	86	PRO
9	J	85	ASP
28	4	19	GLY
42	i	74	ILE
59	z	186	PRO
9	J	73	GLY
13	P	72	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	X	77/78 (99%)	69 (90%)	8 (10%)	7	13
22	Y	85/91 (93%)	75 (88%)	10 (12%)	5	9
23	Z	84/179 (47%)	73 (87%)	11 (13%)	4	7
24	0	59/67 (88%)	55 (93%)	4 (7%)	16	32
25	1	80/83 (96%)	69 (86%)	11 (14%)	3	6
26	2	65/67 (97%)	54 (83%)	11 (17%)	2	3
27	3	51/52 (98%)	44 (86%)	7 (14%)	3	6
28	4	60/63 (95%)	45 (75%)	15 (25%)	0	1
29	5	51/52 (98%)	45 (88%)	6 (12%)	5	9
30	6	51/52 (98%)	47 (92%)	4 (8%)	12	25
31	7	42/42 (100%)	34 (81%)	8 (19%)	1	2
32	8	53/55 (96%)	48 (91%)	5 (9%)	8	17
33	9	34/34 (100%)	29 (85%)	5 (15%)	3	5
35	b	193/220 (88%)	150 (78%)	43 (22%)	1	1
36	c	142/188 (76%)	130 (92%)	12 (8%)	10	21
37	d	169/181 (93%)	143 (85%)	26 (15%)	2	4
38	e	113/123 (92%)	95 (84%)	18 (16%)	2	4
39	f	83/90 (92%)	69 (83%)	14 (17%)	2	3
40	g	118/127 (93%)	99 (84%)	19 (16%)	2	4
41	h	114/119 (96%)	99 (87%)	15 (13%)	4	7
42	i	90/99 (91%)	76 (84%)	14 (16%)	2	4
43	j	65/92 (71%)	53 (82%)	12 (18%)	1	2
44	k	82/99 (83%)	74 (90%)	8 (10%)	8	15
45	l	97/109 (89%)	85 (88%)	12 (12%)	4	8
46	m	89/101 (88%)	76 (85%)	13 (15%)	3	5
47	n	49/50 (98%)	41 (84%)	8 (16%)	2	3
48	o	78/80 (98%)	71 (91%)	7 (9%)	9	18
49	p	69/74 (93%)	59 (86%)	10 (14%)	3	5
50	q	94/97 (97%)	81 (86%)	13 (14%)	3	6
51	r	59/77 (77%)	50 (85%)	9 (15%)	2	4
52	s	68/80 (85%)	58 (85%)	10 (15%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	t	69/82 (84%)	61 (88%)	8 (12%)	5	10
54	u	18/22 (82%)	16 (89%)	2 (11%)	6	11
59	z	542/560 (97%)	436 (80%)	106 (20%)	1	2
All	All	5236/5760 (91%)	4433 (85%)	803 (15%)	2	4

All (803) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	HIS
3	C	5	LYS
3	C	8	ARG
3	C	11	LEU
3	C	23	ASP
3	C	39	GLU
3	C	42	GLU
3	C	46	LYS
3	C	49	ILE
3	C	55	ASP
3	C	61	THR
3	C	68	LEU
3	C	162	GLU
3	C	163	PHE
3	C	164	ARG
3	C	168	THR
3	C	184	LYS
3	C	185	LEU
3	C	209	LEU
3	C	210	ARG
3	C	211	SER
3	C	216	THR
3	C	222	VAL
3	C	224	ILE
4	D	5	LYS
4	D	18	VAL
4	D	27	THR
4	D	37	LEU
4	D	38	LYS
4	D	61	LEU
4	D	71	ASP
4	D	88	ARG
4	D	94	LEU

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Mol	Chain	Res	Type
4	D	103	ARG
4	D	111	LEU
4	D	112	GLN
4	D	116	GLN
4	D	122	ASP
4	D	140	THR
4	D	141	VAL
4	D	142	VAL
4	D	150	LYS
4	D	183	ARG
4	D	200	ASP
4	D	202	LYS
4	D	211	ARG
4	D	221	VAL
4	D	229	VAL
4	D	242	ARG
4	D	257	LEU
4	D	259	THR
4	D	260	ARG
4	D	274	ARG
5	E	7	VAL
5	E	9	VAL
5	E	21	VAL
5	E	24	THR
5	E	33	VAL
5	E	34	VAL
5	E	41	LYS
5	E	47	VAL
5	E	49	LEU
5	E	52	LEU
5	E	78	LEU
5	E	82	ARG
5	E	85	ASN
5	E	89	ASP
5	E	94	GLU
5	E	116	VAL
5	E	119	ARG
5	E	140	SER
5	E	144	ARG
5	E	149	ARG
5	E	152	LYS
5	E	154	LYS

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Mol	Chain	Res	Type
5	E	163	GLU
5	E	175	VAL
5	E	181	LEU
5	E	196	VAL
6	F	20	LEU
6	F	24	LEU
6	F	28	ILE
6	F	33	LEU
6	F	38	ARG
6	F	53	THR
6	F	74	ARG
6	F	88	VAL
6	F	106	ARG
6	F	120	GLU
6	F	124	LEU
6	F	125	LEU
6	F	135	LYS
6	F	162	LEU
6	F	164	ARG
6	F	165	ARG
6	F	168	ARG
6	F	170	LEU
6	F	175	THR
6	F	176	LEU
6	F	191	ARG
6	F	192	LEU
6	F	195	ASP
6	F	201	VAL
6	F	206	ILE
7	G	3	LEU
7	G	5	VAL
7	G	7	LEU
7	G	26	GLN
7	G	33	ARG
7	G	34	LEU
7	G	43	LEU
7	G	49	ASP
7	G	51	ARG
7	G	75	LYS
7	G	78	SER
7	G	80	PHE
7	G	82	LEU

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Mol	Chain	Res	Type
7	G	86	MET
7	G	91	ARG
7	G	115	ARG
7	G	133	LEU
7	G	139	LEU
7	G	140	ILE
7	G	145	THR
7	G	146	TYR
7	G	148	MET
7	G	149	VAL
7	G	159	VAL
7	G	164	GLU
7	G	175	LEU
7	G	181	ARG
8	H	3	ARG
8	H	23	ARG
8	H	32	GLU
8	H	43	VAL
8	H	57	ASP
8	H	69	ARG
8	H	71	LEU
8	H	80	SER
8	H	92	ILE
8	H	99	VAL
8	H	101	ARG
8	H	104	GLU
8	H	105	LEU
8	H	114	VAL
8	H	116	GLU
8	H	160	LYS
10	K	2	LYS
10	K	4	VAL
10	K	5	VAL
10	K	7	VAL
10	K	11	GLN
10	K	18	THR
10	K	30	HIS
10	K	47	ASN
10	K	48	MET
10	K	50	ASP
10	K	53	VAL
10	K	58	THR

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Mol	Chain	Res	Type
10	K	64	SER
10	K	65	PHE
10	K	66	THR
10	K	69	THR
10	K	75	SER
10	K	80	LYS
10	K	86	LYS
10	K	93	ARG
10	K	94	GLU
10	K	95	LYS
10	K	102	GLU
10	K	103	GLN
10	K	105	LEU
10	K	107	ILE
10	K	112	MET
10	K	115	LEU
10	K	117	THR
10	K	118	THR
10	K	132	ARG
10	K	134	MET
10	K	138	VAL
11	N	1	MET
11	N	5	VAL
11	N	9	VAL
11	N	10	GLU
11	N	12	ARG
11	N	14	VAL
11	N	28	THR
11	N	33	LEU
11	N	34	LEU
11	N	48	MET
11	N	55	VAL
11	N	62	VAL
11	N	67	LEU
11	N	87	LEU
11	N	90	MET
11	N	97	ARG
11	N	99	LEU
11	N	120	LEU
11	N	131	GLN
11	N	133	GLN
11	N	139	GLU

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Mol	Chain	Res	Type
11	N	140	VAL
12	O	8	LEU
12	O	10	VAL
12	O	23	ARG
12	O	24	VAL
12	O	63	VAL
12	O	69	ILE
12	O	94	ARG
12	O	98	VAL
12	O	116	SER
13	P	1	MET
13	P	45	LEU
13	P	55	ARG
13	P	65	ARG
13	P	98	GLU
13	P	102	ARG
13	P	115	LEU
13	P	117	GLU
13	P	125	VAL
13	P	131	SER
13	P	137	LYS
13	P	148	LEU
14	Q	3	MET
14	Q	5	ARG
14	Q	16	ARG
14	Q	45	GLN
14	Q	56	ARG
14	Q	57	HIS
14	Q	60	ARG
14	Q	63	LYS
14	Q	75	THR
14	Q	81	VAL
14	Q	82	ARG
14	Q	85	LYS
14	Q	109	VAL
14	Q	110	THR
14	Q	111	GLU
14	Q	130	LYS
14	Q	135	ASP
15	R	6	SER
15	R	18	LEU
15	R	28	LEU

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Mol	Chain	Res	Type
15	R	29	LEU
15	R	33	ARG
15	R	36	THR
15	R	40	LYS
15	R	44	LEU
15	R	54	LEU
15	R	60	LEU
15	R	65	LEU
15	R	79	LEU
15	R	89	ASP
15	R	91	GLN
15	R	100	LEU
15	R	111	LEU
15	R	114	VAL
16	S	3	ARG
16	S	15	ARG
16	S	20	ARG
16	S	36	TYR
16	S	43	GLU
16	S	48	LEU
16	S	49	VAL
16	S	69	VAL
16	S	73	LEU
16	S	78	LEU
17	T	6	LEU
17	T	13	ARG
17	T	16	ARG
17	T	23	ARG
17	T	39	ARG
17	T	41	ARG
17	T	49	VAL
17	T	50	ILE
17	T	59	THR
17	T	64	ARG
17	T	74	ARG
17	T	96	ARG
17	T	108	ARG
17	T	118	ARG
17	T	125	ARG
18	U	18	LEU
18	U	31	SER
18	U	34	LYS

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Mol	Chain	Res	Type
18	U	36	ARG
18	U	52	ARG
18	U	59	ARG
18	U	74	LEU
18	U	83	LEU
18	U	85	LYS
18	U	92	ARG
18	U	95	LEU
18	U	104	GLN
18	U	108	GLU
19	V	25	LEU
19	V	43	GLU
19	V	46	VAL
19	V	51	VAL
19	V	57	VAL
19	V	58	VAL
19	V	62	LEU
19	V	66	ARG
19	V	71	LEU
19	V	72	VAL
19	V	79	VAL
19	V	80	GLN
19	V	95	LEU
20	W	6	ILE
20	W	11	ARG
20	W	19	LEU
20	W	23	LEU
20	W	37	ARG
20	W	51	LEU
20	W	63	ASP
20	W	92	ARG
20	W	100	THR
20	W	107	LEU
20	W	111	HIS
21	X	23	GLU
21	X	35	THR
21	X	51	VAL
21	X	57	LEU
21	X	65	ARG
21	X	72	LYS
21	X	80	ILE
21	X	95	LEU

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Mol	Chain	Res	Type
22	Y	7	VAL
22	Y	23	ARG
22	Y	43	ASN
22	Y	61	ILE
22	Y	67	LEU
22	Y	72	VAL
22	Y	85	VAL
22	Y	90	LEU
22	Y	99	CYS
22	Y	106	LEU
23	Z	5	LEU
23	Z	18	LEU
23	Z	31	ARG
23	Z	37	VAL
23	Z	41	LEU
23	Z	42	VAL
23	Z	50	GLN
23	Z	72	ARG
23	Z	78	LYS
23	Z	91	LEU
23	Z	93	ASP
24	0	20	ARG
24	0	23	VAL
24	0	27	GLU
24	0	74	ARG
25	1	13	ILE
25	1	14	VAL
25	1	21	ARG
25	1	35	THR
25	1	40	ARG
25	1	51	VAL
25	1	52	ARG
25	1	69	LYS
25	1	71	TYR
25	1	80	LEU
25	1	95	LEU
26	2	1	MET
26	2	20	GLU
26	2	22	GLU
26	2	27	GLU
26	2	30	ARG
26	2	32	LEU

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Mol	Chain	Res	Type
26	2	34	GLU
26	2	40	SER
26	2	53	LEU
26	2	68	ARG
26	2	70	GLN
27	3	3	ARG
27	3	4	LEU
27	3	8	LEU
27	3	18	ASP
27	3	23	LEU
27	3	40	THR
27	3	54	VAL
28	4	9	LEU
28	4	22	ILE
28	4	34	GLU
28	4	35	VAL
28	4	49	PHE
28	4	50	VAL
28	4	52	THR
28	4	58	ARG
28	4	59	PHE
28	4	60	GLN
28	4	61	ARG
28	4	62	ARG
28	4	63	TYR
28	4	67	TYR
28	4	68	ARG
29	5	9	LYS
29	5	16	ARG
29	5	29	THR
29	5	40	LYS
29	5	48	GLU
29	5	56	LYS
30	6	6	ARG
30	6	17	LYS
30	6	24	GLU
30	6	27	LYS
31	7	1	MET
31	7	14	LYS
31	7	23	ARG
31	7	32	LYS
31	7	43	THR

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Mol	Chain	Res	Type
31	7	46	VAL
31	7	47	ARG
31	7	49	ARG
32	8	14	VAL
32	8	23	VAL
32	8	26	LYS
32	8	31	HIS
32	8	32	LEU
33	9	7	VAL
33	9	12	ASP
33	9	22	ARG
33	9	35	ARG
33	9	36	GLN
35	b	8	LYS
35	b	9	GLU
35	b	10	LEU
35	b	11	LEU
35	b	12	GLU
35	b	15	VAL
35	b	17	PHE
35	b	21	ARG
35	b	24	TRP
35	b	37	ASN
35	b	45	GLN
35	b	48	MET
35	b	56	ARG
35	b	76	GLN
35	b	79	ASP
35	b	80	ILE
35	b	93	VAL
35	b	97	TRP
35	b	118	LEU
35	b	119	GLU
35	b	122	PHE
35	b	124	SER
35	b	127	ILE
35	b	128	GLU
35	b	135	GLN
35	b	136	VAL
35	b	138	LEU
35	b	142	LEU
35	b	144	ARG

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Mol	Chain	Res	Type
35	b	145	LEU
35	b	146	GLN
35	b	155	LEU
35	b	156	LYS
35	b	178	ARG
35	b	179	LYS
35	b	185	ILE
35	b	187	LEU
35	b	196	LEU
35	b	208	ILE
35	b	212	GLN
35	b	217	ARG
35	b	221	LEU
35	b	223	ILE
36	c	3	ASN
36	c	47	LEU
36	c	52	LEU
36	c	70	VAL
36	c	104	GLN
36	c	165	THR
36	c	178	LEU
36	c	190	ARG
36	c	191	THR
36	c	192	THR
36	c	195	VAL
36	c	196	LEU
37	d	5	ILE
37	d	9	CYS
37	d	15	GLU
37	d	18	LYS
37	d	21	LEU
37	d	28	SER
37	d	58	LEU
37	d	76	ARG
37	d	107	ARG
37	d	108	LEU
37	d	132	ARG
37	d	135	LEU
37	d	137	SER
37	d	141	ARG
37	d	150	GLU
37	d	156	GLU

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Mol	Chain	Res	Type
37	d	158	ILE
37	d	162	LEU
37	d	163	GLU
37	d	168	ARG
37	d	170	VAL
37	d	173	TRP
37	d	174	LEU
37	d	188	LEU
37	d	194	LEU
37	d	201	GLN
38	e	20	GLN
38	e	31	LEU
38	e	34	VAL
38	e	37	ARG
38	e	38	GLN
38	e	41	VAL
38	e	47	LYS
38	e	57	LYS
38	e	69	VAL
38	e	71	LEU
38	e	80	ILE
38	e	91	LEU
38	e	112	LEU
38	e	116	THR
38	e	121	LYS
38	e	123	LEU
38	e	151	LEU
38	e	152	ARG
39	f	9	VAL
39	f	14	LEU
39	f	15	ASP
39	f	21	LEU
39	f	32	ASN
39	f	54	LYS
39	f	61	LEU
39	f	69	GLU
39	f	73	ASN
39	f	74	ASP
39	f	83	ASP
39	f	87	ARG
39	f	94	GLN
39	f	98	LEU

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Mol	Chain	Res	Type
40	g	12	LEU
40	g	15	ASP
40	g	22	LEU
40	g	32	ARG
40	g	37	ASN
40	g	51	GLN
40	g	59	LEU
40	g	64	GLN
40	g	72	ARG
40	g	75	VAL
40	g	104	LEU
40	g	113	GLU
40	g	115	ARG
40	g	131	LYS
40	g	137	LYS
40	g	138	LYS
40	g	140	ASP
40	g	144	MET
40	g	155	ARG
41	h	2	LEU
41	h	23	SER
41	h	29	SER
41	h	50	ARG
41	h	52	ASP
41	h	63	LEU
41	h	78	GLN
41	h	84	ARG
41	h	85	ARG
41	h	91	ARG
41	h	99	GLU
41	h	112	LEU
41	h	116	LYS
41	h	122	ARG
41	h	133	LEU
42	i	27	THR
42	i	38	GLN
42	i	41	VAL
42	i	47	LEU
42	i	48	GLU
42	i	56	LEU
42	i	58	HIS
42	i	64	THR

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Mol	Chain	Res	Type
42	i	65	VAL
42	i	75	ASP
42	i	83	ARG
42	i	108	VAL
42	i	121	ARG
42	i	124	GLN
43	j	15	THR
43	j	16	LEU
43	j	30	SER
43	j	35	SER
43	j	43	ARG
43	j	46	ARG
43	j	70	ARG
43	j	72	VAL
43	j	89	ASP
43	j	92	THR
43	j	96	ILE
43	j	100	THR
44	k	48	ILE
44	k	54	ARG
44	k	70	LYS
44	k	83	ILE
44	k	93	GLN
44	k	99	GLN
44	k	104	GLN
44	k	109	VAL
45	l	18	VAL
45	l	27	LEU
45	l	33	ARG
45	l	41	ARG
45	l	52	LEU
45	l	53	ARG
45	l	60	LEU
45	l	67	THR
45	l	83	VAL
45	l	84	LEU
45	l	86	ARG
45	l	89	ARG
46	m	9	ILE
46	m	11	ARG
46	m	15	VAL
46	m	34	LEU

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Mol	Chain	Res	Type
46	m	40	ASN
46	m	49	THR
46	m	70	LEU
46	m	73	GLU
46	m	80	ARG
46	m	88	ARG
46	m	102	ARG
46	m	116	THR
46	m	120	LYS
47	n	3	ARG
47	n	6	LEU
47	n	7	ILE
47	n	8	GLU
47	n	18	VAL
47	n	33	VAL
47	n	41	ARG
47	n	50	LYS
48	o	24	SER
48	o	26	GLU
48	o	39	LEU
48	o	66	LEU
48	o	67	LEU
48	o	82	ILE
48	o	83	GLU
49	p	3	LYS
49	p	5	ARG
49	p	19	ILE
49	p	21	VAL
49	p	25	ARG
49	p	27	LYS
49	p	45	THR
49	p	60	LEU
49	p	62	VAL
49	p	79	VAL
50	q	4	LYS
50	q	6	LEU
50	q	9	VAL
50	q	11	VAL
50	q	13	ASP
50	q	52	LYS
50	q	63	ARG
50	q	68	ARG

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Mol	Chain	Res	Type
50	q	70	ARG
50	q	72	ARG
50	q	74	LEU
50	q	78	GLU
50	q	96	GLU
51	r	21	LYS
51	r	31	LEU
51	r	32	ARG
51	r	35	ARG
51	r	42	ARG
51	r	49	LYS
51	r	58	LEU
51	r	84	LYS
51	r	87	ARG
52	s	5	LEU
52	s	14	HIS
52	s	15	LEU
52	s	28	LYS
52	s	37	ARG
52	s	45	VAL
52	s	48	THR
52	s	65	ASN
52	s	67	VAL
52	s	71	LEU
53	t	9	ASN
53	t	10	LEU
53	t	24	LEU
53	t	43	LEU
53	t	51	GLU
53	t	62	LEU
53	t	80	ARG
53	t	84	LEU
54	u	7	ARG
54	u	12	LYS
59	z	-68	MET
59	z	-60	LEU
59	z	-54	VAL
59	z	-34	LEU
59	z	-25	LEU
59	z	-24	LYS
59	z	-22	LEU
59	z	-12	ARG

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Mol	Chain	Res	Type
59	z	-11	LEU
59	z	-7	LYS
59	z	2	ILE
59	z	5	ASN
59	z	10	ARG
59	z	15	ILE
59	z	28	ARG
59	z	32	LEU
59	z	40	GLU
59	z	43	GLU
59	z	46	LEU
59	z	50	GLU
59	z	54	GLU
59	z	67	THR
59	z	75	GLU
59	z	80	LEU
59	z	88	ASP
59	z	101	GLU
59	z	105	LEU
59	z	113	VAL
59	z	126	GLU
59	z	131	ILE
59	z	140	LEU
59	z	142	ASN
59	z	150	LEU
59	z	175	GLU
59	z	181	ILE
59	z	184	ARG
59	z	204	VAL
59	z	208	TYR
59	z	209	GLN
59	z	212	ILE
59	z	216	ARG
59	z	229	ARG
59	z	241	LYS
59	z	245	PHE
59	z	248	GLN
59	z	250	LEU
59	z	251	VAL
59	z	268	ILE
59	z	269	ARG
59	z	274	VAL

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Mol	Chain	Res	Type
59	z	280	ILE
59	z	282	LEU
59	z	298	LYS
59	z	309	ASP
59	z	312	ASP
59	z	316	LEU
59	z	317	ARG
59	z	322	LYS
59	z	325	LEU
59	z	326	ASN
59	z	336	SER
59	z	338	THR
59	z	345	ARG
59	z	355	GLU
59	z	360	ARG
59	z	362	GLU
59	z	369	LEU
59	z	370	ILE
59	z	382	LEU
59	z	384	SER
59	z	387	GLU
59	z	401	ARG
59	z	402	ILE
59	z	405	ILE
59	z	413	THR
59	z	418	GLU
59	z	419	GLU
59	z	424	LEU
59	z	434	ARG
59	z	438	MET
59	z	441	LEU
59	z	445	GLN
59	z	447	ARG
59	z	450	LEU
59	z	461	TYR
59	z	467	LEU
59	z	468	LYS
59	z	471	SER
59	z	476	SER
59	z	480	GLU
59	z	481	GLN
59	z	490	VAL

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Mol	Chain	Res	Type
59	z	495	LEU
59	z	512	LYS
59	z	516	MET
59	z	518	ARG
59	z	521	VAL
59	z	541	ILE
59	z	545	ILE
59	z	546	ILE
59	z	548	ARG
59	z	550	THR
59	z	572	LYS
59	z	576	LYS
59	z	592	VAL
59	z	595	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	115	GLN
4	D	166	GLN
4	D	253	GLN
5	E	85	ASN
6	F	8	GLN
6	F	69	HIS
6	F	169	ASN
7	G	26	GLN
7	G	40	ASN
7	G	108	ASN
8	H	139	GLN
11	N	8	GLN
14	Q	12	GLN
17	T	43	GLN
17	T	123	GLN
18	U	72	HIS
21	X	31	HIS
21	X	82	GLN
23	Z	50	GLN
23	Z	54	HIS
23	Z	65	GLN
24	0	17	GLN
24	0	35	ASN
25	1	19	GLN

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Mol	Chain	Res	Type
25	1	56	GLN
26	2	70	GLN
28	4	20	ASN
28	4	60	GLN
33	9	36	GLN
35	b	16	HIS
35	b	45	GLN
35	b	94	ASN
35	b	113	HIS
35	b	212	GLN
36	c	6	HIS
36	c	37	GLN
36	c	104	GLN
36	c	108	ASN
36	c	118	GLN
36	c	162	GLN
36	c	176	HIS
36	c	181	ASN
37	d	77	ASN
37	d	123	HIS
37	d	125	HIS
37	d	201	GLN
38	e	73	ASN
38	e	141	GLN
39	f	73	ASN
39	f	100	ASN
40	g	28	ASN
40	g	68	ASN
40	g	148	ASN
42	i	89	ASN
42	i	124	GLN
43	j	56	HIS
44	k	38	ASN
44	k	93	GLN
45	l	99	HIS
46	m	40	ASN
48	o	28	GLN
50	q	16	GLN
52	s	14	HIS
52	s	57	HIS
52	s	65	ASN
52	s	83	HIS

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Mol	Chain	Res	Type
53	t	16	HIS
53	t	75	ASN
59	z	127	HIS
59	z	183	GLN
59	z	248	GLN
59	z	275	GLN
59	z	326	ASN
59	z	426	GLN
59	z	429	GLN
59	z	538	GLN
59	z	577	GLN

### 5.3.3 RNA ⓘ

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

All (789) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	10	G
1	A	14	G
1	A	34	G
1	A	44	C
1	A	58	G
1	A	69	A
1	A	72	A
1	A	73	G
1	A	82	A
1	A	86	G
1	A	88	U
1	A	89	A
1	A	93	G

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Mol	Chain	Res	Type
1	A	115	A
1	A	116	A
1	A	117	U
1	A	136	G
1	A	138	A
1	A	161	G
1	A	162	C
1	A	169	A
1	A	184	A
1	A	187	A
1	A	188	U
1	A	193	G
1	A	202	G
1	A	203	G
1	A	204	A
1	A	209	A
1	A	210	A
1	A	217	A
1	A	221	A
1	A	236	G
1	A	253	A
1	A	268	G
1	A	270	U
1	A	271	U
1	A	272	G
1	A	277	G
1	A	286	G
1	A	287	U
1	A	288	G
1	A	295	U
1	A	298	G
1	A	302	C
1	A	306	A
1	A	334	A
1	A	350	G
1	A	352	G
1	A	353	A
1	A	356	G
1	A	375	G
1	A	376	G
1	A	386	G
1	A	412	G

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Mol	Chain	Res	Type
1	A	422	G
1	A	431	U
1	A	437	G
1	A	438	A
1	A	469	C
1	A	473	U
1	A	479	A
1	A	480	C
1	A	481	C
1	A	482	A
1	A	504	A
1	A	506	G
1	A	528	U
1	A	529	A
1	A	530	G
1	A	532	G
1	A	533	C
1	A	555	C
1	A	556	A
1	A	557	G
1	A	568	G
1	A	569	C
1	A	585	G
1	A	595	G
1	A	597	A
1	A	608	A
1	A	615	G
1	A	625	A
1	A	626	G
1	A	629	U
1	A	638	G
1	A	640	G
1	A	651	A
1	A	661	A
1	A	665	C
1	A	669	C
1	A	670	A
1	A	678	A
1	A	679	G
1	A	680	C
1	A	681	G
1	A	696	C

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Mol	Chain	Res	Type
1	A	697	G
1	A	698	C
1	A	702	G
1	A	732	G
1	A	763	G
1	A	776	C
1	A	798	A
1	A	799	C
1	A	811	G
1	A	821	G
1	A	822	G
1	A	828	A
1	A	830	A
1	A	831	G
1	A	838	G
1	A	851	G
1	A	858	C
1	A	865	A
1	A	873	U
1	A	874	U
1	A	876	G
1	A	905	G
1	A	912	A
1	A	915	G
1	A	921	G
1	A	924	A
1	A	926	G
1	A	931	C
1	A	932	C
1	A	933	A
1	A	934	C
1	A	935	C
1	A	936	A
1	A	937	G
1	A	938	C
1	A	940	U
1	A	941	A
1	A	942	C
1	A	943	C
1	A	944	A
1	A	945	A
1	A	946	A

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Mol	Chain	Res	Type
1	A	955	A
1	A	962	A
1	A	976	G
1	A	985	A
1	A	989	A
1	A	990	G
1	A	1005	C
1	A	1018	G
1	A	1019	C
1	A	1028	A
1	A	1041	A
1	A	1050	C
1	A	1057	U
1	A	1058	C
1	A	1060	G
1	A	1067	G
1	A	1078	U
1	A	1084	G
1	A	1090	A
1	A	1091	A
1	A	1092	G
1	A	1093	A
1	A	1096	G
1	A	1097	C
1	A	1098	C
1	A	1099	A
1	A	1103	G
1	A	1106	U
1	A	1107	G
1	A	1111	U
1	A	1114	A
1	A	1115	A
1	A	1117	C
1	A	1118	A
1	A	1120	C
1	A	1121	C
1	A	1125	C
1	A	1127	U
1	A	1128	U
1	A	1131	A
1	A	1132	G
1	A	1133	A

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Mol	Chain	Res	Type
1	A	1135	U
1	A	1136	G
1	A	1142	U
1	A	1145	C
1	A	1154	C
1	A	1156	A
1	A	1157	G
1	A	1173	A
1	A	1174	A
1	A	1175	U
1	A	1179	C
1	A	1180	G
1	A	1185	U
1	A	1186	U
1	A	1187	A
1	A	1194	G
1	A	1216	G
1	A	1217	G
1	A	1218	A
1	A	1219	U
1	A	1220	G
1	A	1221	A
1	A	1222	C
1	A	1254	A
1	A	1255	U
1	A	1264	A
1	A	1265	C
1	A	1281	G
1	A	1284	G
1	A	1289	G
1	A	1293	G
1	A	1295	G
1	A	1298	A
1	A	1301	G
1	A	1302	C
1	A	1316	G
1	A	1317	A
1	A	1318	U
1	A	1345	U
1	A	1346	A
1	A	1350	C
1	A	1404	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1410	A
1	A	1417	U
1	A	1425	G
1	A	1430	G
1	A	1461	G
1	A	1462	C
1	A	1465	U
1	A	1466	G
1	A	1473	C
1	A	1482	C
1	A	1490	A
1	A	1501	G
1	A	1506	A
1	A	1507	G
1	A	1513	C
1	A	1517	A
1	A	1528	G
1	A	1529	G
1	A	1539	A
1	A	1553	A
1	A	1554	C
1	A	1555	A
1	A	1557	G
1	A	1578	C
1	A	1588	A
1	A	1589	C
1	A	1600	A
1	A	1604	A
1	A	1606	G
1	A	1612	A
1	A	1615	A
1	A	1624	U
1	A	1626	A
1	A	1627	G
1	A	1630	C
1	A	1631	A
1	A	1653	A
1	A	1654	A
1	A	1655	A
1	A	1662	C
1	A	1694	C
1	A	1700	A

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Mol	Chain	Res	Type
1	A	1720	G
1	A	1742	G
1	A	1746	A
1	A	1761	G
1	A	1765	G
1	A	1766	A
1	A	1767	U
1	A	1768	G
1	A	1769	A
1	A	1770	G
1	A	1773	C
1	A	1774	C
1	A	1775	G
1	A	1776	G
1	A	1777	G
1	A	1778	G
1	A	1788	G
1	A	1793	G
1	A	1794	G
1	A	1799	G
1	A	1803	A
1	A	1821	A
1	A	1830	C
1	A	1831	G
1	A	1846	G
1	A	1869	G
1	A	1877	A
1	A	1897	A
1	A	1898	A
1	A	1899	G
1	A	1921	A
1	A	1927	G
1	A	1950	G
1	A	1951	G
1	A	1958	A
1	A	1959	A
1	A	1962	C
1	A	1976	U
1	A	1981	A
1	A	1984	U
1	A	1988	C
1	A	1991	A

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Mol	Chain	Res	Type
1	A	1992	A
1	A	1993	A
1	A	2013	G
1	A	2014	U
1	A	2018	G
1	A	2041	A
1	A	2044	G
1	A	2052	A
1	A	2053	G
1	A	2054	A
1	A	2064	C
1	A	2076	C
1	A	2077	G
1	A	2081	A
1	A	2082	G
1	A	2083	A
1	A	2090	G
1	A	2120	U
1	A	2123	U
1	A	2124	C
1	A	2125	G
1	A	2126	C
1	A	2127	G
1	A	2128	C
1	A	2130	U
1	A	2134	U
1	A	2137	G
1	A	2140	A
1	A	2141	G
1	A	2142	G
1	A	2147	A
1	A	2149	C
1	A	2152	G
1	A	2153	U
1	A	2155	A
1	A	2156	A
1	A	2157	C
1	A	2159	C
1	A	2160	C
1	A	2161	C
1	A	2164	C
1	A	2165	U

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Mol	Chain	Res	Type
1	A	2167	C
1	A	2168	G
1	A	2177	G
1	A	2178	G
1	A	2179	A
1	A	2180	G
1	A	2181	G
1	A	2182	C
1	A	2186	G
1	A	2187	G
1	A	2188	U
1	A	2189	G
1	A	2190	A
1	A	2193	U
1	A	2199	C
1	A	2200	C
1	A	2203	G
1	A	2205	G
1	A	2206	C
1	A	2208	G
1	A	2211	G
1	A	2213	G
1	A	2214	G
1	A	2219	A
1	A	2220	A
1	A	2221	C
1	A	2226	G
1	A	2227	G
1	A	2228	A
1	A	2230	G
1	A	2236	A
1	A	2249	G
1	A	2250	G
1	A	2284	A
1	A	2286	C
1	A	2294	C
1	A	2298	A
1	A	2316	A
1	A	2318	G
1	A	2319	G
1	A	2330	G
1	A	2331	A

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Mol	Chain	Res	Type
1	A	2332	G
1	A	2333	A
1	A	2336	G
1	A	2338	A
1	A	2345	G
1	A	2347	A
1	A	2354	C
1	A	2358	C
1	A	2365	G
1	A	2372	A
1	A	2394	G
1	A	2396	C
1	A	2399	A
1	A	2404	A
1	A	2417	U
1	A	2425	G
1	A	2432	G
1	A	2433	A
1	A	2435	C
1	A	2436	A
1	A	2440	G
1	A	2441	A
1	A	2446	A
1	A	2450	A
1	A	2452	C
1	A	2459	A
1	A	2487	A
1	A	2513	G
1	A	2516	G
1	A	2517	U
1	A	2529	A
1	A	2540	G
1	A	2565	U
1	A	2577	A
1	A	2578	G
1	A	2584	C
1	A	2589	G
1	A	2596	U
1	A	2613	A
1	A	2620	U
1	A	2622	U
1	A	2623	C

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Mol	Chain	Res	Type
1	A	2632	A
1	A	2641	G
1	A	2643	A
1	A	2654	G
1	A	2665	A
1	A	2674	G
1	A	2675	G
1	A	2694	C
1	A	2700	U
1	A	2702	C
1	A	2724	A
1	A	2725	A
1	A	2726	G
1	A	2738	U
1	A	2745	A
1	A	2769	A
1	A	2777	A
1	A	2778	G
1	A	2790	A
1	A	2802	A
1	A	2803	C
1	A	2812	G
1	A	2816	G
1	A	2829	A
1	A	2830	A
1	A	2844	A
1	A	2848	G
1	A	2881	G
1	A	2891	A
1	A	2902	G
2	B	2	C
2	B	7	G
2	B	31	C
2	B	35	U
2	B	45	A
2	B	56	G
2	B	65	C
2	B	66	A
2	B	67	G
2	B	72	G
2	B	73	A
2	B	85	G

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Mol	Chain	Res	Type
2	B	110	G
2	B	120	A
34	a	7	G
34	a	8	G
34	a	10	G
34	a	23	G
34	a	32	G
34	a	33	A
34	a	40	G
34	a	49	C
34	a	52	A
34	a	62	G
34	a	72	C
34	a	73	C
34	a	74	G
34	a	76	G
34	a	78	G
34	a	87	C
34	a	88	C
34	a	89	G
34	a	91	G
34	a	92	G
34	a	93	U
34	a	95	A
34	a	114	A
34	a	115	C
34	a	126	C
34	a	137	G
34	a	138	A
34	a	139	G
34	a	152	G
34	a	154	G
34	a	155	A
34	a	158	C
34	a	177	U
34	a	204	A
34	a	209	U
34	a	210	U
34	a	211	U
34	a	212	G
34	a	216	G
34	a	243	G

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Mol	Chain	Res	Type
34	a	247	G
34	a	262	G
34	a	263	C
34	a	282	G
34	a	285	G
34	a	314	G
34	a	317	A
34	a	324	C
34	a	328	G
34	a	338	C
34	a	339	U
34	a	340	A
34	a	341	C
34	a	342	G
34	a	343	G
34	a	348	C
34	a	349	A
34	a	350	G
34	a	352	A
34	a	363	U
34	a	368	C
34	a	380	G
34	a	394	C
34	a	402	G
34	a	407	A
34	a	408	A
34	a	409	G
34	a	410	A
34	a	420	G
34	a	425	U
34	a	426	A
34	a	433	U
34	a	441	G
34	a	447	A
34	a	451	C
34	a	455	A
34	a	456	C
34	a	457	G
34	a	470	G
34	a	481	A
34	a	482	U
34	a	489	G

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Mol	Chain	Res	Type
34	a	493	A
34	a	494	A
34	a	495	C
34	a	502	C
34	a	508	G
34	a	511	G
34	a	514	G
34	a	515	U
34	a	516	A
34	a	531	A
34	a	543	A
34	a	545	U
34	a	556	A
34	a	557	A
34	a	558	A
34	a	560	G
34	a	561	G
34	a	591	A
34	a	614	G
34	a	615	G
34	a	616	A
34	a	621	G
34	a	634	G
34	a	637	A
34	a	649	A
34	a	650	G
34	a	671	A
34	a	672	G
34	a	679	A
34	a	707	U
34	a	715	G
34	a	718	G
34	a	733	C
34	a	739	G
34	a	761	A
34	a	777	U
34	a	778	A
34	a	799	A
34	a	801	C
34	a	803	A
34	a	812	A
34	a	823	U

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Mol	Chain	Res	Type
34	a	824	C
34	a	825	U
34	a	826	C
34	a	837	A
34	a	852	G
34	a	880	G
34	a	892	A
34	a	904	G
34	a	905	G
34	a	912	C
34	a	913	A
34	a	920	G
34	a	938	U
34	a	939	U
34	a	944	G
34	a	946	A
34	a	947	A
34	a	949	G
34	a	953	A
34	a	954	G
34	a	955	A
34	a	971	G
34	a	978	U
34	a	985	C
34	a	986	C
34	a	988	G
34	a	989	G
34	a	996	G
34	a	1002	G
34	a	1003	G
34	a	1004	U
34	a	1005	G
34	a	1006	C
34	a	1007	C
34	a	1008	C
34	a	1009	C
34	a	1010	G
34	a	1014	G
34	a	1016	G
34	a	1017	G
34	a	1019	G
34	a	1020	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	1027	A
34	a	1037	C
34	a	1049	C
34	a	1068	U
34	a	1071	G
34	a	1077	G
34	a	1078	U
34	a	1084	A
34	a	1107	G
34	a	1108	U
34	a	1109	U
34	a	1110	G
34	a	1112	C
34	a	1113	A
34	a	1114	G
34	a	1116	G
34	a	1120	C
34	a	1122	G
34	a	1123	C
34	a	1128	C
34	a	1129	A
34	a	1135	A
34	a	1140	A
34	a	1141	C
34	a	1142	U
34	a	1143	G
34	a	1164	G
34	a	1178	U
34	a	1179	G
34	a	1195	A
34	a	1209	A
34	a	1218	A
34	a	1220	A
34	a	1222	U
34	a	1239	U
34	a	1240	G
34	a	1252	C
34	a	1260	U
34	a	1262	A
34	a	1267	A
34	a	1268	A
34	a	1269	A

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Mol	Chain	Res	Type
34	a	1272	G
34	a	1281	A
34	a	1282	G
34	a	1283	U
34	a	1284	U
34	a	1287	G
34	a	1302	C
34	a	1304	C
34	a	1320	G
34	a	1328	A
34	a	1329	G
34	a	1347	U
34	a	1353	G
34	a	1360	A
34	a	1377	A
34	a	1380	C
34	a	1381	A
34	a	1402	G
34	a	1423	C
34	a	1425	G
34	a	1431	U
34	a	1432	A
34	a	1433	C
34	a	1434	G
34	a	1447	G
34	a	1470	A
34	a	1471	A
34	a	1472	G
34	a	1481	A
34	a	1484	U
34	a	1495	G
34	a	1498	G
34	a	1507	G
34	a	1508	G
34	a	1509	A
55	v	24	A
56	w	6	G
56	w	8	4SU
56	w	9	A
56	w	13	C
56	w	15	G
56	w	19	G

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Mol	Chain	Res	Type
56	w	20	U
56	w	21	A
56	w	26	A
56	w	44	G
56	w	45	U
56	w	46	7MG
56	w	47	U
56	w	48	C
56	w	49	C
56	w	55	PSU
56	w	56	C
56	w	58	A
56	w	59	U
56	w	60	U
56	w	61	C
56	w	63	G
56	w	64	A
56	w	71	G
56	w	74	C
56	w	76	A
57	x	2	G
57	x	9	G
57	x	14	A
57	x	16	C
57	x	17	C
57	x	17(A)	U
57	x	18	G
57	x	19	G
57	x	31	G
57	x	47	U
57	x	48	C
57	x	61	C
57	x	76	A
58	y	2	C
58	y	5	G
58	y	7	A
58	y	8	4SU
58	y	9	A
58	y	13	C
58	y	19	G
58	y	20	U
58	y	21	A

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Mol	Chain	Res	Type
58	y	22	G
58	y	25	C
58	y	26	A
58	y	29	G
58	y	30	G
58	y	32	PSU
58	y	33	U
58	y	35	A
58	y	41	C
58	y	43	C
58	y	44	G
58	y	45	U
58	y	46	G
58	y	47	U
58	y	48	C
58	y	56	C
58	y	59	U
58	y	60	U
58	y	66	U

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	33	C
1	A	88	U
1	A	184	A
1	A	270	U
1	A	271	U
1	A	301	A
1	A	385	U
1	A	514	G
1	A	669	C
1	A	677	A
1	A	731	A
1	A	792	A
1	A	798	A
1	A	810	A
1	A	1008	C
1	A	1018	G
1	A	1037	C
1	A	1097	C
1	A	1120	C

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Mol	Chain	Res	Type
1	A	1132	G
1	A	1153	U
1	A	1218	A
1	A	1220	G
1	A	1238	A
1	A	1254	A
1	A	1424	A
1	A	1465	U
1	A	1653	A
1	A	1699	G
1	A	2013	G
1	A	2123	U
1	A	2166	C
1	A	2202	G
1	A	2212	G
1	A	2329	G
1	A	2417	U
1	A	2432	G
1	A	2433	A
1	A	2450	A
1	A	2622	U
1	A	2768	U
1	A	2901	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
56	PSU	w	39	56	17,21,22	1.64	2 (11%)	20,30,33	3.20	7 (35%)
56	PSU	w	32	56	17,21,22	1.61	3 (17%)	20,30,33	3.22	6 (30%)
58	PSU	y	32	58	17,21,22	1.46	2 (11%)	20,30,33	3.13	5 (25%)
57	5MU	x	54	60,57	15,22,23	0.95	1 (6%)	16,32,35	1.89	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	MIA	y	37	58,34	18,24,32	1.26	2 (11%)	18,35,47	1.25	2 (11%)
57	4SU	x	8	57	14,21,22	1.28	2 (14%)	15,30,33	3.84	2 (13%)
58	5MU	y	54	58	15,22,23	1.12	1 (6%)	16,32,35	2.03	2 (12%)
56	4SU	w	8	56	14,21,22	1.34	2 (14%)	15,30,33	1.62	2 (13%)
56	5MU	w	54	56	15,22,23	1.05	1 (6%)	16,32,35	2.16	1 (6%)
58	4SU	y	8	58	14,21,22	3.42	4 (28%)	15,30,33	1.43	2 (13%)
56	7MG	w	46	56	22,26,27	1.84	4 (18%)	28,39,42	2.74	10 (35%)
56	MIA	w	37	56	24,29,32	2.20	3 (12%)	25,41,47	2.83	10 (40%)
57	5MC	x	32	57	15,22,23	1.34	1 (6%)	19,32,35	1.29	3 (15%)
58	PSU	y	39	58	17,21,22	1.62	3 (17%)	20,30,33	3.30	7 (35%)
56	PSU	w	55	56	17,21,22	1.43	2 (11%)	20,30,33	3.20	6 (30%)
57	PSU	x	55	57	17,21,22	1.71	4 (23%)	20,30,33	3.20	6 (30%)
58	PSU	y	55	58	17,21,22	1.45	3 (17%)	20,30,33	3.09	7 (35%)

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
56	PSU	w	39	56	-	0/7/25/26	0/2/2/2
56	PSU	w	32	56	-	0/7/25/26	0/2/2/2
58	PSU	y	32	58	-	3/7/25/26	0/2/2/2
57	5MU	x	54	60,57	-	0/5/25/26	0/2/2/2
58	MIA	y	37	58,34	-	2/3/25/34	0/3/3/3
57	4SU	x	8	57	-	0/5/25/26	0/2/2/2
58	5MU	y	54	58	-	0/5/25/26	0/2/2/2
56	4SU	w	8	56	-	0/5/25/26	0/2/2/2
56	5MU	w	54	56	-	0/5/25/26	0/2/2/2
58	4SU	y	8	58	-	1/5/25/26	0/2/2/2
56	7MG	w	46	56	-	3/7/37/38	0/3/3/3
56	MIA	w	37	56	-	6/10/31/34	0/3/3/3
57	5MC	x	32	57	-	0/5/25/26	0/2/2/2
58	PSU	y	39	58	-	0/7/25/26	0/2/2/2
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
57	PSU	x	55	57	-	0/7/25/26	0/2/2/2
58	PSU	y	55	58	-	0/7/25/26	0/2/2/2

All (40) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	8	4SU	C5-C4	9.07	1.48	1.38
56	w	37	MIA	C2-S10	-7.24	1.69	1.75
56	w	37	MIA	C13-C14	6.90	1.52	1.32
58	y	8	4SU	C6-N1	6.34	1.43	1.35
56	w	46	7MG	C6-C5	5.47	1.48	1.41
56	w	39	PSU	C5-C1'	-5.06	1.47	1.52
57	x	55	PSU	C5-C1'	-4.83	1.48	1.52
56	w	46	7MG	C5-C4	4.78	1.48	1.39
56	w	32	PSU	C5-C1'	-4.56	1.48	1.52
57	x	32	5MC	C5-C4	4.53	1.48	1.41
58	y	39	PSU	C5-C1'	-4.38	1.48	1.52
58	y	8	4SU	C4-S4	-4.26	1.59	1.67
56	w	8	4SU	C4-S4	-4.06	1.60	1.67
58	y	32	PSU	C4-C5	4.06	1.50	1.41
58	y	8	4SU	C6-C5	4.03	1.47	1.38
57	x	8	4SU	C2-N3	-3.71	1.30	1.38
56	w	55	PSU	C4-C5	3.59	1.49	1.41
58	y	39	PSU	C4-C5	3.55	1.49	1.41
58	y	55	PSU	C4-C5	3.46	1.48	1.41
58	y	54	5MU	C4-C5	3.43	1.48	1.41
56	w	54	5MU	C4-C5	3.38	1.48	1.41
56	w	32	PSU	C4-C5	3.36	1.48	1.41
57	x	55	PSU	C4-C5	3.35	1.48	1.41
56	w	55	PSU	C5-C1'	-3.30	1.49	1.52
58	y	55	PSU	C5-C1'	-3.22	1.49	1.52
56	w	46	7MG	C5-N7	-3.02	1.34	1.39
58	y	37	MIA	C2-N3	3.01	1.36	1.32
58	y	37	MIA	C5-C4	2.91	1.48	1.40
56	w	39	PSU	C4-C5	2.90	1.47	1.41
58	y	32	PSU	C5-C1'	-2.89	1.49	1.52
57	x	54	5MU	C4-C5	2.63	1.47	1.41
57	x	55	PSU	C2-N3	-2.40	1.33	1.38
56	w	46	7MG	C4-N9	-2.27	1.34	1.38
57	x	8	4SU	C4-S4	-2.24	1.63	1.67
56	w	37	MIA	C5-C4	2.17	1.46	1.40
56	w	8	4SU	C2-N3	-2.14	1.33	1.38
58	y	39	PSU	O4'-C1'	-2.13	1.41	1.44
56	w	32	PSU	O4'-C1'	-2.12	1.41	1.44
58	y	55	PSU	O4'-C1'	-2.11	1.41	1.44
57	x	55	PSU	O4'-C1'	-2.08	1.41	1.44

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	x	8	4SU	C2-N3-C4	12.81	133.73	115.15
56	w	55	PSU	N1-C2-N3	-9.23	121.09	128.43
56	w	46	7MG	N3-C4-N9	8.63	137.99	126.91
56	w	39	PSU	N1-C2-N3	-8.60	121.59	128.43
58	y	55	PSU	N1-C2-N3	-8.52	121.65	128.43
58	y	32	PSU	N1-C2-N3	-8.51	121.67	128.43
58	y	39	PSU	N1-C2-N3	-8.40	121.75	128.43
56	w	54	5MU	C4-N3-C2	8.23	122.09	115.14
57	x	55	PSU	N1-C2-N3	-8.22	121.90	128.43
56	w	32	PSU	N1-C2-N3	-8.02	122.06	128.43
56	w	37	MIA	C12-C13-C14	-7.94	111.69	127.14
58	y	54	5MU	C4-N3-C2	7.52	121.49	115.14
58	y	32	PSU	C4-N3-C2	7.17	121.20	115.14
58	y	39	PSU	C4-N3-C2	7.15	121.18	115.14
57	x	8	4SU	C5-C4-N3	-7.15	114.27	123.83
56	w	32	PSU	C4-N3-C2	6.95	121.01	115.14
57	x	54	5MU	C4-N3-C2	6.68	120.78	115.14
56	w	37	MIA	C11-S10-C2	-6.68	97.28	102.27
56	w	55	PSU	C4-N3-C2	6.62	120.73	115.14
57	x	55	PSU	C4-N3-C2	6.54	120.66	115.14
58	y	55	PSU	C4-N3-C2	6.20	120.38	115.14
56	w	39	PSU	C4-N3-C2	5.96	120.17	115.14
57	x	55	PSU	C5-C4-N3	-5.62	118.11	125.36
58	y	39	PSU	C5-C4-N3	-5.52	118.25	125.36
56	w	32	PSU	C5-C4-N3	-5.48	118.30	125.36
58	y	32	PSU	C5-C4-N3	-5.42	118.38	125.36
56	w	46	7MG	C6-N1-C2	5.12	124.06	115.93
56	w	46	7MG	N7-C8-N9	-5.11	96.08	103.38
56	w	39	PSU	C5-C6-N1	-5.07	118.22	124.44
56	w	46	7MG	C5-C4-N3	-4.88	118.53	126.49
56	w	39	PSU	C5-C4-N3	-4.88	119.08	125.36
57	x	55	PSU	C5-C6-N1	-4.86	118.47	124.44
56	w	37	MIA	C16-C14-C13	-4.84	108.65	122.65
58	y	39	PSU	C5-C6-N1	-4.84	118.49	124.44
56	w	8	4SU	C2-N3-C4	4.78	122.08	115.15
56	w	55	PSU	C5-C4-N3	-4.72	119.28	125.36
56	w	55	PSU	C6-N1-C2	4.55	122.87	115.36
58	y	55	PSU	C5-C4-N3	-4.54	119.52	125.36
56	w	32	PSU	C5-C6-N1	-4.49	118.93	124.44
56	w	39	PSU	C6-N1-C2	4.44	122.69	115.36
56	w	32	PSU	C5-C1'-C2'	-4.41	107.44	115.32
56	w	55	PSU	C5-C6-N1	-4.38	119.06	124.44
57	x	55	PSU	C6-N1-C2	4.30	122.45	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	y	55	PSU	C6-N1-C2	4.27	122.41	115.36
58	y	39	PSU	C6-N1-C2	4.19	122.27	115.36
58	y	8	4SU	C2-N3-C4	4.17	121.20	115.15
56	w	39	PSU	C5-C1'-C2'	-4.11	107.98	115.32
58	y	32	PSU	C6-N1-C2	4.04	122.02	115.36
58	y	55	PSU	C5-C6-N1	-3.96	119.57	124.44
56	w	46	7MG	C5-C6-N1	-3.94	115.05	123.14
56	w	37	MIA	C2-N3-C4	3.88	120.67	115.32
56	w	32	PSU	C6-N1-C2	3.82	121.66	115.36
58	y	39	PSU	C5-C1'-C2'	-3.78	108.57	115.32
58	y	55	PSU	C5-C1'-C2'	-3.77	108.59	115.32
56	w	46	7MG	C6-C5-C4	3.75	119.22	115.20
58	y	32	PSU	C5-C6-N1	-3.74	119.84	124.44
56	w	37	MIA	C15-C14-C13	-3.68	112.01	122.65
58	y	37	MIA	N3-C2-N1	-3.62	123.02	128.68
57	x	55	PSU	C5-C1'-C2'	-3.59	108.91	115.32
57	x	32	5MC	C2-N3-C4	3.42	120.14	116.02
56	w	8	4SU	C5-C4-N3	-3.18	119.57	123.83
56	w	37	MIA	C5-C6-N1	-3.10	118.24	120.81
58	y	8	4SU	C5-C6-N1	3.03	127.45	120.68
57	x	32	5MC	N4-C4-N3	2.86	121.07	117.03
56	w	46	7MG	C8-N7-C5	2.71	115.98	108.94
56	w	37	MIA	C2-N1-C6	2.68	121.98	117.19
56	w	37	MIA	C12-N6-C6	-2.57	118.74	122.55
58	y	37	MIA	C4-C5-N7	-2.34	106.96	109.40
57	x	54	5MU	C5-C6-N1	-2.28	119.74	122.19
56	w	37	MIA	N3-C2-N1	-2.27	122.81	126.98
57	x	32	5MC	C5-C6-N1	-2.25	119.77	122.19
58	y	39	PSU	O4'-C1'-C2'	2.23	108.27	104.66
56	w	55	PSU	C5-C1'-C2'	-2.20	111.39	115.32
56	w	46	7MG	CM7-N7-C5	2.19	132.44	124.01
58	y	54	5MU	C5-C6-N1	-2.17	119.85	122.19
56	w	37	MIA	C4-C5-N7	-2.15	107.16	109.40
56	w	46	7MG	C5-C4-N9	-2.11	103.48	106.44
56	w	46	7MG	C2-N3-C4	2.10	119.70	113.89
58	y	55	PSU	O4'-C1'-C5	-2.06	106.74	109.93
56	w	39	PSU	O4'-C1'-C2'	2.06	107.99	104.66

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	y	8	4SU	C2'-C1'-N1-C6
56	w	37	MIA	C5-C6-N6-C12
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
56	w	46	7MG	O4'-C4'-C5'-O5'
56	w	46	7MG	C3'-C4'-C5'-O5'
56	w	37	MIA	N1-C6-N6-C12
58	y	37	MIA	C3'-C4'-C5'-O5'
58	y	32	PSU	C4'-C5'-O5'-P
56	w	37	MIA	N1-C2-S10-C11
58	y	32	PSU	C3'-C4'-C5'-O5'
56	w	37	MIA	N3-C2-S10-C11
56	w	46	7MG	C4'-C5'-O5'-P
58	y	32	PSU	C2'-C1'-C5-C6
58	y	37	MIA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
63	GCP	z	703	60	26,34,34	3.38	9 (34%)	31,54,54	1.45	4 (12%)
62	SF4	d	302	37	0,12,12	0.00	-	-		

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
63	GCP	z	703	60	-	11/18/38/38	0/3/3/3
62	SF4	d	302	37	-	-	0/6/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	703	GCP	C4-N9	-12.62	1.30	1.47
63	z	703	GCP	PB-O2B	-6.34	1.41	1.56
63	z	703	GCP	PG-O3G	-4.32	1.45	1.54
63	z	703	GCP	C8-N9	-4.02	1.31	1.45
63	z	703	GCP	C5-C6	-3.92	1.46	1.52
63	z	703	GCP	C2-N1	-2.78	1.32	1.44
63	z	703	GCP	PB-O1B	2.77	1.58	1.51
63	z	703	GCP	PG-O1G	2.37	1.55	1.50
63	z	703	GCP	PA-O2A	-2.21	1.44	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	703	GCP	C4-C5-N7	3.67	107.32	102.46
63	z	703	GCP	O3'-C3'-C2'	-2.79	102.79	111.82
63	z	703	GCP	O3G-PG-O2G	2.45	115.24	108.08
63	z	703	GCP	O2G-PG-O1G	-2.24	106.47	112.39

There are no chirality outliers.

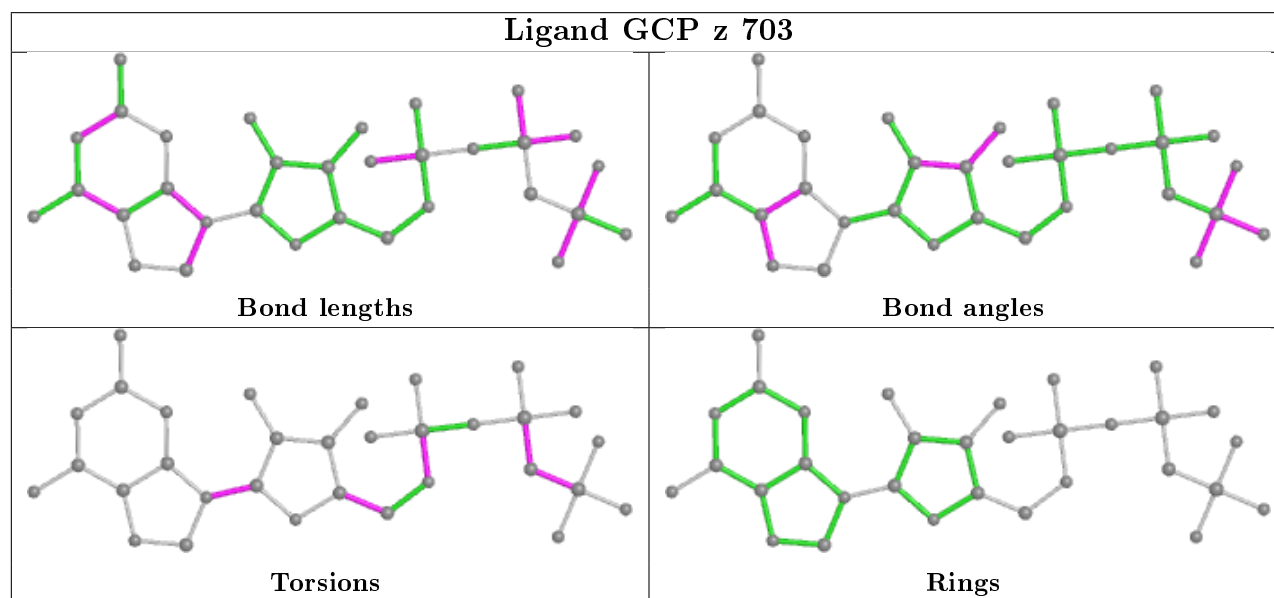
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	z	703	GCP	PB-C3B-PG-O1G
63	z	703	GCP	PB-C3B-PG-O2G
63	z	703	GCP	PG-C3B-PB-O1B
63	z	703	GCP	C5'-O5'-PA-O3A
63	z	703	GCP	O4'-C4'-C5'-O5'
63	z	703	GCP	O4'-C1'-N9-C4
63	z	703	GCP	C2'-C1'-N9-C4
63	z	703	GCP	C3'-C4'-C5'-O5'
63	z	703	GCP	C5'-O5'-PA-O1A
63	z	703	GCP	C5'-O5'-PA-O2A
63	z	703	GCP	PB-C3B-PG-O3G

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	2874/2915 (98%)	0.19	151 (5%) 26 20	22, 39, 92, 112	465 (16%)
2	B	120/121 (99%)	0.15	0 100 100	36, 57, 73, 93	18 (15%)
3	C	136/228 (59%)	2.05	60 (44%) 0 0	72, 89, 95, 97	104 (76%)
4	D	275/276 (99%)	-0.01	1 (0%) 92 91	18, 37, 49, 69	42 (15%)
5	E	204/206 (99%)	0.18	5 (2%) 57 51	20, 41, 63, 76	38 (18%)
6	F	203/210 (96%)	0.09	3 (1%) 73 70	22, 50, 75, 90	31 (15%)
7	G	181/182 (99%)	0.35	10 (5%) 25 19	42, 58, 78, 84	38 (20%)
8	H	174/180 (96%)	0.30	8 (4%) 32 26	39, 54, 70, 73	30 (17%)
9	J	130/173 (75%)	3.73	89 (68%) 0 0	84, 138, 186, 214	10 (7%)
10	K	139/147 (94%)	4.74	112 (80%) 0 0	93, 102, 107, 110	115 (82%)
11	N	140/140 (100%)	0.07	3 (2%) 63 58	26, 43, 65, 83	27 (19%)
12	O	122/122 (100%)	-0.06	0 100 100	27, 39, 50, 65	7 (5%)
13	P	149/150 (99%)	0.20	3 (2%) 65 60	21, 49, 65, 83	38 (25%)
14	Q	141/141 (100%)	-0.03	3 (2%) 63 58	27, 42, 59, 87	36 (25%)
15	R	118/118 (100%)	0.10	0 100 100	26, 43, 55, 69	16 (13%)
16	S	110/112 (98%)	0.29	1 (0%) 84 82	40, 52, 65, 75	24 (21%)
17	T	131/146 (89%)	0.23	3 (2%) 60 54	34, 45, 72, 92	22 (16%)
18	U	116/118 (98%)	0.13	0 100 100	26, 40, 49, 53	23 (19%)
19	V	101/101 (100%)	0.07	1 (0%) 82 80	28, 48, 59, 66	12 (11%)
20	W	112/113 (99%)	0.15	1 (0%) 84 82	28, 41, 63, 79	24 (21%)
21	X	95/96 (98%)	0.24	3 (3%) 47 40	39, 50, 72, 84	14 (14%)
22	Y	107/110 (97%)	0.44	8 (7%) 14 10	44, 54, 81, 87	24 (22%)
23	Z	94/206 (45%)	0.48	5 (5%) 26 20	42, 59, 74, 97	15 (15%)
24	0	74/85 (87%)	-0.01	0 100 100	26, 39, 52, 65	16 (21%)

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

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

All (803) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	K	92	GLY	15.0
1	A	934	C	14.8
10	K	122	ALA	14.7
10	K	135	GLY	13.9
10	K	139	VAL	12.3
10	K	116	ASN	12.0
10	K	9	LYS	11.7
40	g	82	GLY	11.1
9	J	49	ALA	10.8
9	J	116	ILE	10.7
10	K	52	ILE	10.6
10	K	45	THR	10.6
10	K	43	ALA	10.2
10	K	93	ARG	9.9
10	K	77	LEU	9.8
9	J	97	ALA	9.7
10	K	47	ASN	9.7
10	K	34	ILE	9.2
9	J	130	THR	9.0
10	K	46	ALA	9.0
10	K	4	VAL	9.0
3	C	198	ALA	8.8
9	J	129	PRO	8.7
10	K	140	GLY	8.6
9	J	43	ALA	8.6
3	C	200	LYS	8.6
10	K	17	ALA	8.6
10	K	7	VAL	8.5
9	J	55	LYS	8.4
9	J	39	ALA	8.4
10	K	59	ILE	8.2
9	J	53	VAL	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	935	C	8.1
10	K	18	THR	8.0
34	a	1012	G	8.0
10	K	10	LEU	8.0
10	K	104	VAL	8.0
34	a	984	A	7.9
1	A	938	C	7.8
9	J	118	THR	7.8
10	K	94	GLU	7.7
40	g	81	GLY	7.7
9	J	103	GLY	7.7
1	A	2806	C	7.6
9	J	123	GLU	7.6
40	g	80	VAL	7.6
9	J	121	ASP	7.6
34	a	1014	G	7.5
10	K	49	GLY	7.4
1	A	1220	G	7.4
46	m	120	LYS	7.4
10	K	138	VAL	7.4
58	y	44	G	7.4
9	J	94	VAL	7.4
9	J	117	LEU	7.3
9	J	88	ALA	7.3
34	a	1013	A	7.3
1	A	1219	U	7.3
34	a	1015	G	7.3
10	K	41	PHE	7.2
27	3	2	PRO	7.2
34	a	74	G	7.2
34	a	985	C	7.2
9	J	35	LYS	7.1
9	J	50	ARG	7.1
10	K	25	PRO	7.1
9	J	105	PRO	7.0
1	A	2812	G	7.0
10	K	2	LYS	7.0
9	J	133	GLU	6.9
3	C	205	LYS	6.9
1	A	933	A	6.9
1	A	2167	C	6.8
9	J	46	GLN	6.8

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Mol	Chain	Res	Type	RSRZ
9	J	99	SER	6.8
9	J	100	ASN	6.8
1	A	932	C	6.8
10	K	98	ARG	6.7
9	J	93	LEU	6.7
10	K	3	LYS	6.7
10	K	5	VAL	6.6
10	K	95	LYS	6.6
3	C	209	LEU	6.6
10	K	117	THR	6.5
34	a	982	G	6.5
9	J	85	ASP	6.4
56	w	19	G	6.4
1	A	273	U	6.4
28	4	56	VAL	6.4
10	K	44	ALA	6.4
10	K	13	PRO	6.3
9	J	89	ALA	6.3
9	J	37	THR	6.2
10	K	6	ALA	6.2
1	A	1554	C	6.2
46	m	119	GLY	6.1
9	J	54	ALA	6.1
10	K	118	THR	6.1
10	K	100	THR	6.0
3	C	223	ARG	5.9
10	K	14	ALA	5.9
10	K	54	PRO	5.9
34	a	1005	G	5.9
9	J	101	PRO	5.9
34	a	1004	U	5.9
34	a	211	U	5.8
1	A	217	A	5.8
9	J	87	VAL	5.8
1	A	937	G	5.8
10	K	33	ASN	5.8
10	K	48	MET	5.8
9	J	48	GLY	5.8
9	J	17	LEU	5.7
10	K	62	ASP	5.7
1	A	2805	G	5.7
1	A	2185	C	5.7

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Mol	Chain	Res	Type	RSRZ
10	K	137	GLU	5.7
10	K	37	PHE	5.6
9	J	47	ASN	5.6
34	a	1019	G	5.6
9	J	10	LEU	5.5
23	Z	93	ASP	5.5
9	J	122	VAL	5.5
10	K	53	VAL	5.5
9	J	76	GLY	5.5
28	4	54	GLY	5.5
10	K	30	HIS	5.4
3	C	210	ARG	5.4
1	A	2168	G	5.4
1	A	2813	C	5.4
9	J	75	GLN	5.3
56	w	57	G	5.3
10	K	16	LYS	5.3
1	A	2165	U	5.3
3	C	158	ALA	5.3
10	K	28	GLY	5.3
1	A	1120	C	5.2
1	A	1762	G	5.2
10	K	63	ARG	5.2
1	A	2814	C	5.2
3	C	196	LEU	5.2
9	J	131	MET	5.2
1	A	682	G	5.1
10	K	15	GLY	5.1
3	C	14	VAL	5.1
9	J	98	LYS	5.0
1	A	2166	C	5.0
35	b	234	PRO	5.0
1	A	2804	G	5.0
11	N	8	GLN	5.0
59	z	525	ALA	5.0
9	J	91	LYS	5.0
34	a	986	C	5.0
1	A	1091	A	5.0
9	J	92	THR	5.0
9	J	77	PRO	5.0
3	C	19	ILE	5.0
10	K	8	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	936	A	4.9
56	w	24	G	5.0
1	A	2163	C	4.9
10	K	96	VAL	4.9
1	A	2802	A	4.9
35	b	232	PRO	4.9
10	K	88	ALA	4.9
1	A	1567	G	4.9
9	J	7	VAL	4.8
1	A	696	C	4.8
1	A	297	G	4.8
1	A	678	A	4.8
28	4	57	GLU	4.8
1	A	1774	C	4.8
10	K	50	ASP	4.8
1	A	1123	U	4.8
1	A	569	C	4.8
9	J	72	ASP	4.7
10	K	125	ARG	4.7
10	K	58	THR	4.7
28	4	49	PHE	4.7
56	w	18	G	4.7
9	J	52	PHE	4.7
10	K	136	VAL	4.7
34	a	1022	C	4.7
9	J	23	SER	4.6
9	J	6	ASN	4.6
7	G	50	ALA	4.6
3	C	199	HIS	4.6
1	A	2137	G	4.6
10	K	60	TYR	4.6
23	Z	17	ALA	4.6
51	r	20	ALA	4.6
1	A	2164	C	4.6
10	K	36	GLU	4.6
9	J	14	LYS	4.5
9	J	8	GLU	4.5
1	A	1458	G	4.5
34	a	1002	G	4.5
1	A	2158	C	4.5
34	a	160	C	4.5
59	z	288	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
58	y	20	U	4.5
1	A	695	C	4.5
34	a	1021	C	4.5
10	K	105	LEU	4.5
56	w	51	U	4.5
22	Y	53	PRO	4.4
1	A	929	G	4.4
1	A	1583	G	4.4
3	C	194	ARG	4.4
10	K	38	VAL	4.4
10	K	31	GLY	4.4
43	j	27	ALA	4.4
1	A	2213	G	4.4
34	a	1010	G	4.4
10	K	124	ALA	4.4
9	J	42	GLN	4.4
1	A	939	C	4.4
3	C	29	VAL	4.4
9	J	9	LEU	4.4
1	A	926	G	4.3
1	A	1775	G	4.3
34	a	980	G	4.3
58	y	12	U	4.3
35	b	233	SER	4.3
10	K	101	TRP	4.3
56	w	25	C	4.3
59	z	397	PRO	4.3
9	J	34	ALA	4.3
3	C	11	LEU	4.2
3	C	225	ASN	4.2
7	G	51	ARG	4.2
56	w	58	A	4.2
39	f	15	ASP	4.2
25	1	2	SER	4.2
9	J	36	GLU	4.2
9	J	22	GLY	4.2
34	a	1003	G	4.1
1	A	2188	U	4.1
35	b	126	GLU	4.1
9	J	132	ASP	4.1
10	K	107	ILE	4.1
9	J	11	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
10	K	26	ALA	4.1
10	K	12	LEU	4.1
1	A	2136	G	4.1
10	K	73	PRO	4.1
10	K	102	GLU	4.1
43	j	88	LEU	4.1
34	a	1017	G	4.1
28	4	53	GLU	4.0
34	a	987	C	4.0
58	y	34	G	4.0
34	a	983	A	4.0
28	4	68	ARG	4.0
1	A	298	G	4.0
1	A	927	G	4.0
1	A	2903	U	4.0
34	a	152	G	4.0
34	a	826	C	4.0
3	C	38	ASP	3.9
7	G	48	GLU	3.9
9	J	38	HIS	3.9
10	K	35	MET	3.9
10	K	61	ALA	3.9
56	w	15	G	3.9
1	A	2811	A	3.9
34	a	75	C	3.9
56	w	71	G	3.9
34	a	209	U	3.9
10	K	42	ASN	3.9
1	A	940	U	3.9
10	K	66	THR	3.9
9	J	86	PRO	3.9
9	J	18	GLU	3.9
56	w	20	U	3.9
1	A	2178	G	3.8
28	4	55	ARG	3.8
42	i	94	ALA	3.8
10	K	82	ALA	3.8
3	C	68	LEU	3.8
9	J	44	LEU	3.8
22	Y	93	GLY	3.8
8	H	21	PRO	3.8
34	a	1020	C	3.8

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Mol	Chain	Res	Type	RSRZ
25	1	82	LEU	3.8
1	A	2152	G	3.8
10	K	11	GLN	3.8
10	K	29	GLN	3.8
10	K	76	TYR	3.7
1	A	1763	G	3.7
34	a	825	U	3.7
56	w	56	C	3.7
9	J	56	ASN	3.7
1	A	1222	C	3.7
1	A	2157	C	3.7
34	a	981	G	3.7
34	a	1120	C	3.7
17	T	126	ALA	3.7
34	a	73	C	3.7
10	K	99	ILE	3.7
10	K	121	GLU	3.7
35	b	137	ARG	3.7
10	K	69	THR	3.7
56	w	14	A	3.7
10	K	57	ILE	3.7
43	j	75	ILE	3.7
56	w	3	C	3.7
1	A	1584	G	3.7
3	C	17	ASN	3.6
34	a	1000	G	3.6
56	w	52	G	3.6
10	K	20	ALA	3.6
1	A	1457	A	3.6
3	C	206	GLY	3.6
35	b	119	GLU	3.6
1	A	677	A	3.6
1	A	944	A	3.6
3	C	212	VAL	3.6
10	K	68	VAL	3.6
39	f	40	VAL	3.6
1	A	2905	U	3.6
58	y	47	U	3.6
22	Y	91	GLU	3.6
35	b	129	GLU	3.6
59	z	434	ARG	3.6
56	w	45	U	3.6

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Mol	Chain	Res	Type	RSRZ
17	T	38	ASN	3.6
56	w	10	G	3.6
40	g	85	TYR	3.6
23	Z	94	GLU	3.5
34	a	153	G	3.5
3	C	30	LYS	3.5
9	J	68	LEU	3.5
1	A	681	G	3.5
1	A	1218	A	3.5
10	K	119	ASP	3.5
34	a	1011	C	3.5
35	b	227	GLY	3.5
34	a	76	G	3.5
34	a	89	G	3.5
58	y	45	U	3.5
10	K	132	ARG	3.5
10	K	84	LEU	3.5
1	A	1759	U	3.5
1	A	2189	G	3.5
34	a	158	C	3.5
56	w	73	A	3.5
59	z	394	ALA	3.5
1	A	1773	C	3.4
3	C	55	ASP	3.4
9	J	4	LYS	3.4
59	z	-3	GLU	3.4
34	a	1016	G	3.4
59	z	515	THR	3.4
36	c	132	ARG	3.4
57	x	47	U	3.4
1	A	942	C	3.4
9	J	104	ILE	3.4
34	a	1018	A	3.4
3	C	37	PHE	3.4
28	4	46	GLN	3.4
56	w	44	G	3.4
9	J	124	ALA	3.4
59	z	586	ALA	3.4
37	d	47	ARG	3.4
9	J	120	LYS	3.4
57	x	1	C	3.4
55	v	14	A	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	54	SER	3.3
1	A	385	U	3.3
1	A	1126	U	3.3
34	a	707	U	3.3
10	K	90	LYS	3.3
1	A	2187	G	3.3
10	K	51	ALA	3.3
56	w	6	G	3.3
58	y	28	G	3.3
9	J	84	GLU	3.3
9	J	90	ALA	3.3
10	K	97	GLY	3.3
10	K	27	LEU	3.3
43	j	79	ARG	3.3
34	a	210	U	3.3
46	m	34	LEU	3.3
1	A	2815	G	3.3
9	J	25	PHE	3.3
35	b	236	TYR	3.3
3	C	178	ALA	3.3
10	K	32	ALA	3.3
58	y	22	G	3.3
34	a	1007	C	3.3
6	F	15	SER	3.3
10	K	65	PHE	3.3
1	A	2135	A	3.3
35	b	228	GLY	3.3
1	A	386	G	3.2
1	A	2121	G	3.2
34	a	824	C	3.2
58	y	46	G	3.2
1	A	2120	U	3.2
35	b	231	GLU	3.2
59	z	380	VAL	3.2
1	A	296	C	3.2
3	C	181	PRO	3.2
1	A	2186	G	3.2
3	C	163	PHE	3.2
9	J	24	PHE	3.2
35	b	229	VAL	3.2
1	A	1553	A	3.2
10	K	56	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
57	x	17	C	3.2
10	K	22	PRO	3.2
28	4	45	GLY	3.2
28	4	52	THR	3.2
43	j	36	GLY	3.2
35	b	136	VAL	3.1
46	m	56	LEU	3.1
1	A	928	G	3.1
9	J	96	PHE	3.1
59	z	526	GLU	3.1
1	A	1636	G	3.1
34	a	212	G	3.1
56	w	1	G	3.1
3	C	22	ILE	3.1
43	j	32	ALA	3.1
56	w	23	A	3.1
59	z	289	SER	3.1
34	a	1009	C	3.1
10	K	85	GLU	3.1
40	g	84	ASN	3.1
1	A	2153	U	3.1
1	A	1637	C	3.1
3	C	183	GLU	3.1
9	J	70	GLU	3.1
46	m	40	ASN	3.1
1	A	2133	G	3.1
10	K	21	PRO	3.1
3	C	203	GLY	3.1
43	j	72	VAL	3.1
3	C	63	SER	3.1
58	y	10	G	3.1
9	J	51	LEU	3.1
43	j	33	GLN	3.1
57	x	17(A)	U	3.0
35	b	120	ALA	3.0
3	C	201	PRO	3.0
3	C	224	ILE	3.0
10	K	19	PRO	3.0
3	C	53	ARG	3.0
3	C	162	GLU	3.0
6	F	16	GLY	3.0
52	s	27	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
43	j	26	ALA	3.0
1	A	270	U	3.0
13	P	141	ALA	3.0
42	i	84	ALA	3.0
22	Y	61	ILE	3.0
1	A	1221	A	3.0
1	A	1772	C	2.9
3	C	171	ILE	2.9
3	C	207	THR	2.9
34	a	979	A	2.9
46	m	48	LEU	2.9
40	g	155	ARG	2.9
40	g	156	TRP	2.9
26	2	18	PRO	2.9
1	A	1135	U	2.9
58	y	57	G	2.9
25	1	81	LYS	2.9
35	b	156	LYS	2.9
45	l	18	VAL	2.9
1	A	2138	A	2.9
40	g	50	ILE	2.9
20	W	1	MET	2.9
1	A	1136	G	2.9
3	C	204	ALA	2.9
9	J	119	ALA	2.9
35	b	131	PRO	2.9
1	A	924	A	2.9
1	A	941	A	2.9
59	z	-11	LEU	2.9
56	w	61	C	2.9
10	K	81	ALA	2.9
1	A	1776	G	2.9
35	b	223	ILE	2.9
51	r	25	THR	2.9
7	G	148	MET	2.9
3	C	25	ALA	2.9
58	y	13	C	2.9
5	E	88	GLY	2.9
27	3	36	VAL	2.9
1	A	1635	U	2.9
35	b	144	ARG	2.9
10	K	24	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
59	z	510	ARG	2.9
1	A	287	U	2.8
43	j	35	SER	2.8
1	A	2159	C	2.8
56	w	72	C	2.8
35	b	61	LEU	2.8
46	m	53	VAL	2.8
3	C	65	PRO	2.8
52	s	46	GLY	2.8
8	H	111	HIS	2.8
58	y	56	C	2.8
8	H	20	ALA	2.8
9	J	69	PRO	2.8
34	a	70	G	2.8
56	w	53	G	2.8
10	K	108	ALA	2.8
10	K	75	SER	2.8
7	G	58	GLN	2.8
1	A	2816	G	2.8
1	A	2803	C	2.8
48	o	4	THR	2.8
9	J	125	LEU	2.8
3	C	60	GLY	2.8
53	t	47	GLY	2.8
38	e	108	ALA	2.8
35	b	48	MET	2.8
1	A	945	A	2.8
1	A	2177	G	2.8
10	K	109	LYS	2.8
16	S	81	GLY	2.8
3	C	16	PRO	2.7
21	X	68	ARG	2.7
59	z	599	ALA	2.7
34	a	159	U	2.7
56	w	63	G	2.7
28	4	48	ARG	2.7
40	g	52	GLU	2.7
1	A	2211	G	2.7
3	C	166	ASP	2.7
39	f	17	SER	2.7
1	A	378	G	2.7
1	A	697	G	2.7

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Mol	Chain	Res	Type	RSRZ
9	J	13	LEU	2.7
1	A	312	A	2.7
3	C	179	SER	2.7
59	z	39	ARG	2.7
9	J	126	ALA	2.7
1	A	1761	G	2.7
46	m	54	VAL	2.7
59	z	436	VAL	2.7
59	z	392	ASN	2.7
37	d	168	ARG	2.7
49	p	48	TRP	2.7
31	7	45	ALA	2.6
34	a	88	C	2.6
58	y	23	A	2.6
1	A	1216	G	2.6
13	P	98	GLU	2.6
3	C	59	ARG	2.6
37	d	86	LYS	2.6
59	z	582	LYS	2.6
1	A	1090	A	2.6
22	Y	52	SER	2.6
34	a	91	G	2.6
3	C	197	GLU	2.6
3	C	23	ASP	2.6
56	w	75	C	2.6
1	A	2154	G	2.6
43	j	96	ILE	2.6
9	J	19	ARG	2.6
36	c	92	ALA	2.6
44	k	126	ARG	2.6
58	y	42	C	2.6
9	J	107	VAL	2.6
35	b	230	VAL	2.6
59	z	592	VAL	2.6
1	A	2190	A	2.6
56	w	76	A	2.6
39	f	24	GLU	2.6
59	z	565	GLY	2.6
8	H	112	PRO	2.6
34	a	998	C	2.6
22	Y	90	LEU	2.6
25	1	80	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
10	K	129	GLY	2.6
1	A	8	U	2.5
59	z	290	PRO	2.5
1	A	925	G	2.5
1	A	311	C	2.5
10	K	106	GLU	2.5
1	A	271	U	2.5
59	z	420	TYR	2.5
8	H	99	VAL	2.5
49	p	80	PHE	2.5
4	D	2	ALA	2.5
10	K	74	ALA	2.5
36	c	50	ALA	2.5
5	E	71	GLY	2.5
42	i	93	ARG	2.5
43	j	17	ASP	2.5
31	7	49	ARG	2.5
40	g	79	ARG	2.5
59	z	246	THR	2.5
1	A	310	C	2.5
59	z	225	GLY	2.5
46	m	52	GLU	2.5
34	a	1006	C	2.5
10	K	133	SER	2.5
35	b	235	SER	2.5
14	Q	59	ARG	2.5
43	j	89	ASP	2.5
21	X	92	LEU	2.5
34	a	155	A	2.5
10	K	67	PHE	2.5
1	A	1217	G	2.5
1	A	1127	U	2.4
56	w	21	A	2.4
3	C	31	GLU	2.4
8	H	47	GLU	2.4
56	w	74	C	2.4
52	s	59	PRO	2.4
1	A	1459	G	2.4
23	Z	16	SER	2.4
3	C	9	ALA	2.4
37	d	149	ALA	2.4
1	A	161	G	2.4

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Mol	Chain	Res	Type	RSRZ
34	a	1001	G	2.4
43	j	25	GLU	2.4
59	z	395	ASP	2.4
59	z	523	LYS	2.4
28	4	60	GLN	2.4
56	w	68	C	2.4
34	a	1156	G	2.4
28	4	51	ASP	2.4
34	a	706	A	2.4
3	C	58	VAL	2.4
9	J	67	GLY	2.4
56	w	13	C	2.4
28	4	61	ARG	2.4
39	f	36	ARG	2.4
1	A	1144	G	2.4
1	A	1899	G	2.4
1	A	2169	G	2.4
7	G	60	LEU	2.4
10	K	131	ALA	2.4
59	z	146	LEU	2.4
49	p	52	ASP	2.4
1	A	2134	U	2.4
34	a	90	U	2.4
34	a	1008	C	2.4
59	z	387	GLU	2.4
48	o	9	GLN	2.4
43	j	73	ASP	2.4
35	b	38	GLY	2.4
58	y	29	G	2.4
14	Q	5	ARG	2.4
1	A	1771	C	2.3
11	N	132	ALA	2.3
36	c	41	GLY	2.3
9	J	83	TYR	2.3
10	K	91	PRO	2.3
52	s	47	HIS	2.3
1	A	931	C	2.3
1	A	2132	C	2.3
3	C	45	ALA	2.3
6	F	13	SER	2.3
28	4	23	GLU	2.3
46	m	49	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	679	G	2.3
59	z	398	ASP	2.3
1	A	1465	U	2.3
3	C	211	SER	2.3
9	J	108	LYS	2.3
35	b	63	MET	2.3
1	A	2212	G	2.3
34	a	1114	G	2.3
59	z	239	VAL	2.3
59	z	521	VAL	2.3
34	a	1432	A	2.3
44	k	76	GLY	2.3
35	b	124	SER	2.3
59	z	396	LEU	2.3
35	b	237	ALA	2.3
59	z	291	TYR	2.3
59	z	319	ALA	2.3
34	a	5	U	2.3
7	G	150	ASP	2.3
9	J	73	GLY	2.3
26	2	8	LYS	2.3
1	A	2179	A	2.3
9	J	115	GLN	2.3
46	m	63	THR	2.3
34	a	1023	U	2.3
59	z	-50	VAL	2.3
1	A	680	C	2.3
7	G	146	TYR	2.3
43	j	87	THR	2.3
1	A	1555	A	2.3
19	V	51	VAL	2.3
1	A	637	U	2.2
56	w	60	U	2.2
3	C	226	PRO	2.2
35	b	138	LEU	2.2
8	H	102	ALA	2.2
1	A	308	C	2.2
5	E	59	VAL	2.2
39	f	25	ILE	2.2
28	4	59	PHE	2.2
1	A	2127	G	2.2
59	z	322	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
27	3	58	VAL	2.2
25	1	83	GLU	2.2
27	3	60	GLU	2.2
59	z	237	PHE	2.2
49	p	74	LEU	2.2
59	z	195	PRO	2.2
43	j	18	ALA	2.2
1	A	1760	G	2.2
1	A	2203	G	2.2
7	G	145	THR	2.2
49	p	19	ILE	2.2
59	z	360	ARG	2.2
8	H	168	PRO	2.2
37	d	84	LYS	2.2
22	Y	59	GLY	2.2
34	a	1112	C	2.2
46	m	51	ALA	2.2
1	A	2131	G	2.2
34	a	71	G	2.2
3	C	41	VAL	2.2
59	z	537	ILE	2.2
9	J	30	GLN	2.2
1	A	1551	C	2.2
1	A	1142	U	2.1
59	z	-7	LYS	2.1
34	a	163	G	2.1
3	C	192	PHE	2.1
40	g	62	PHE	2.1
1	A	384	G	2.1
3	C	13	LYS	2.1
1	A	387	A	2.1
59	z	37	SER	2.1
44	k	75	TYR	2.1
37	d	187	ARG	2.1
52	s	38	SER	2.1
39	f	14	LEU	2.1
52	s	42	PRO	2.1
34	a	999	U	2.1
34	a	1109	U	2.1
34	a	1433	C	2.1
9	J	40	LEU	2.1
21	X	69	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2155	A	2.1
34	a	976	G	2.1
34	a	1509	A	2.1
59	z	593	PRO	2.1
3	C	33	ALA	2.1
33	9	12	ASP	2.1
59	z	524	LEU	2.1
5	E	204	ALA	2.1
36	c	160	ALA	2.1
14	Q	60	ARG	2.1
59	z	233	THR	2.1
3	C	180	PHE	2.1
1	A	33	C	2.1
59	z	502	ASP	2.1
22	Y	19	LYS	2.1
35	b	125	PRO	2.1
40	g	58	PRO	2.1
1	A	638	G	2.0
1	A	1143	A	2.1
35	b	79	ASP	2.1
59	z	-49	ASP	2.1
1	A	2226	G	2.0
59	z	542	GLY	2.1
59	z	564	GLY	2.1
3	C	66	HIS	2.0
9	J	80	VAL	2.0
34	a	188	C	2.0
40	g	51	GLN	2.0
13	P	110	TYR	2.0
23	Z	92	SER	2.0
37	d	143	GLY	2.0
59	z	171	GLY	2.0
59	z	-52	GLN	2.0
59	z	435	LEU	2.0
3	C	174	PRO	2.0
7	G	5	VAL	2.0
36	c	141	VAL	2.0
43	j	34	VAL	2.0
1	A	2206	C	2.0
17	T	108	ARG	2.0
41	h	122	ARG	2.0
46	m	35	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
38	e	21	ALA	2.0
10	K	83	GLY	2.0
33	9	11	CYS	2.0
38	e	116	THR	2.0
10	K	89	HIS	2.0
5	E	87	GLU	2.0
11	N	9	VAL	2.0
35	b	127	ILE	2.0
1	A	571	A	2.0
1	A	2901	G	2.0
9	J	62	ALA	2.0
34	a	1146	C	2.0
51	r	76	LEU	2.0
27	3	59	VAL	2.0
52	s	45	VAL	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
56	PSU	w	55	20/21	0.67	0.31	96,105,110,111	13
56	5MU	w	54	21/22	0.68	0.48	94,99,101,104	14
58	PSU	y	39	20/21	0.78	0.23	85,93,96,96	8
56	7MG	w	46	24/25	0.79	0.23	91,97,102,104	13
58	PSU	y	32	20/21	0.82	0.20	92,98,106,108	11
58	PSU	y	55	20/21	0.82	0.21	68,75,84,88	11
58	MIA	y	37	22/30	0.83	0.18	75,84,87,89	8
58	4SU	y	8	20/21	0.83	0.20	78,95,101,102	10
56	4SU	w	8	20/21	0.83	0.24	86,92,95,95	12
58	5MU	y	54	21/22	0.87	0.24	67,72,82,83	11
56	PSU	w	32	20/21	0.93	0.15	54,61,66,72	2
56	PSU	w	39	20/21	0.94	0.27	54,63,69,70	7
57	5MU	x	54	21/22	0.94	0.20	40,51,55,61	10
56	MIA	w	37	27/30	0.94	0.24	42,47,52,52	8
57	PSU	x	55	20/21	0.95	0.18	39,51,54,57	7
57	4SU	x	8	20/21	0.96	0.16	41,49,54,54	7
57	5MC	x	32	21/22	0.96	0.18	33,40,44,46	4

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
60	MG	a	1614	1/1	0.29	0.67	75,75,75,75	0
60	MG	a	1705	1/1	0.38	0.37	72,72,72,72	0
60	MG	B	206	1/1	0.39	0.37	86,86,86,86	0
60	MG	A	3234	1/1	0.44	0.54	61,61,61,61	0
60	MG	a	1676	1/1	0.46	0.24	58,58,58,58	0
60	MG	A	3208	1/1	0.49	0.34	60,60,60,60	0
60	MG	A	3252	1/1	0.49	0.18	76,76,76,76	0
60	MG	V	202	1/1	0.51	0.55	73,73,73,73	0
60	MG	A	3155	1/1	0.51	0.28	65,65,65,65	0
60	MG	A	3283	1/1	0.53	0.53	41,41,41,41	0
60	MG	A	3057	1/1	0.54	0.38	72,72,72,72	0
60	MG	a	1638	1/1	0.54	0.42	53,53,53,53	0
60	MG	A	3586	1/1	0.55	0.52	75,75,75,75	0
60	MG	a	1661	1/1	0.56	0.19	69,69,69,69	0
60	MG	a	1701	1/1	0.58	0.18	66,66,66,66	0
60	MG	A	3394	1/1	0.59	0.30	81,81,81,81	0
60	MG	A	3169	1/1	0.59	0.45	44,44,44,44	1
60	MG	A	3274	1/1	0.59	0.23	66,66,66,66	0
60	MG	A	3267	1/1	0.60	0.45	64,64,64,64	0
60	MG	A	3098	1/1	0.60	0.24	61,61,61,61	0
60	MG	a	1604	1/1	0.61	0.25	64,64,64,64	0
60	MG	x	109	1/1	0.62	0.17	77,77,77,77	0
60	MG	A	3117	1/1	0.62	0.30	48,48,48,48	0
60	MG	A	3295	1/1	0.62	0.36	58,58,58,58	0
60	MG	A	3006	1/1	0.62	0.38	52,52,52,52	1
60	MG	a	1689	1/1	0.62	0.24	74,74,74,74	0
60	MG	A	3094	1/1	0.63	0.54	55,55,55,55	0
60	MG	B	204	1/1	0.63	0.24	63,63,63,63	0
60	MG	A	3525	1/1	0.64	0.24	37,37,37,37	0
60	MG	B	215	1/1	0.64	0.28	75,75,75,75	1
60	MG	a	1662	1/1	0.64	0.33	53,53,53,53	0
60	MG	A	3092	1/1	0.65	0.27	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3278	1/1	0.65	0.24	56,56,56,56	0
60	MG	A	3236	1/1	0.65	0.63	47,47,47,47	1
60	MG	A	3557	1/1	0.66	0.28	70,70,70,70	0
60	MG	A	3606	1/1	0.66	0.26	56,56,56,56	0
60	MG	A	3199	1/1	0.67	0.24	45,45,45,45	0
60	MG	A	3585	1/1	0.67	0.25	46,46,46,46	0
60	MG	A	3135	1/1	0.67	0.14	59,59,59,59	0
60	MG	A	3066	1/1	0.67	0.32	58,58,58,58	0
60	MG	A	3055	1/1	0.68	0.22	47,47,47,47	0
60	MG	A	3624	1/1	0.68	0.60	63,63,63,63	0
60	MG	A	3265	1/1	0.69	0.24	64,64,64,64	0
60	MG	A	3237	1/1	0.69	0.43	43,43,43,43	1
60	MG	A	3151	1/1	0.69	0.18	72,72,72,72	0
60	MG	B	209	1/1	0.70	0.32	60,60,60,60	0
60	MG	A	3335	1/1	0.70	0.35	59,59,59,59	1
60	MG	A	3154	1/1	0.70	0.33	67,67,67,67	0
60	MG	R	202	1/1	0.70	0.19	62,62,62,62	0
60	MG	A	3050	1/1	0.70	0.42	60,60,60,60	0
60	MG	A	3014	1/1	0.70	0.32	37,37,37,37	0
60	MG	a	1779	1/1	0.70	0.34	55,55,55,55	0
60	MG	a	1666	1/1	0.70	0.44	68,68,68,68	0
60	MG	a	1698	1/1	0.71	0.22	49,49,49,49	0
60	MG	A	3197	1/1	0.71	0.33	48,48,48,48	1
60	MG	a	1615	1/1	0.71	0.41	54,54,54,54	0
60	MG	A	3255	1/1	0.71	0.39	94,94,94,94	0
60	MG	A	3054	1/1	0.71	0.27	48,48,48,48	0
60	MG	a	1636	1/1	0.71	0.42	59,59,59,59	0
60	MG	B	211	1/1	0.71	0.28	69,69,69,69	0
60	MG	x	106	1/1	0.72	0.45	56,56,56,56	1
60	MG	A	3022	1/1	0.72	0.29	59,59,59,59	0
60	MG	A	3179	1/1	0.72	0.25	61,61,61,61	0
60	MG	A	3049	1/1	0.72	0.32	68,68,68,68	0
60	MG	A	3277	1/1	0.72	0.41	47,47,47,47	1
60	MG	A	3602	1/1	0.72	0.34	48,48,48,48	0
60	MG	A	3127	1/1	0.72	0.33	24,24,24,24	1
60	MG	A	3243	1/1	0.72	0.22	52,52,52,52	0
60	MG	A	3492	1/1	0.73	0.38	64,64,64,64	1
60	MG	a	1641	1/1	0.73	0.34	68,68,68,68	0
60	MG	A	3577	1/1	0.73	0.42	60,60,60,60	0
60	MG	A	3591	1/1	0.73	0.34	39,39,39,39	1
60	MG	A	3100	1/1	0.73	0.50	66,66,66,66	0
60	MG	A	3242	1/1	0.73	0.41	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	a	1703	1/1	0.73	0.24	57,57,57,57	1
60	MG	A	3099	1/1	0.74	0.28	51,51,51,51	0
60	MG	A	3607	1/1	0.74	0.15	54,54,54,54	0
60	MG	A	3227	1/1	0.74	0.34	63,63,63,63	0
60	MG	A	3223	1/1	0.74	0.42	52,52,52,52	0
60	MG	a	1686	1/1	0.74	0.24	61,61,61,61	0
60	MG	a	1643	1/1	0.74	0.46	58,58,58,58	0
60	MG	A	3144	1/1	0.74	0.42	51,51,51,51	0
60	MG	a	1663	1/1	0.74	0.29	60,60,60,60	0
60	MG	A	3630	1/1	0.74	0.38	34,34,34,34	1
60	MG	A	3228	1/1	0.74	0.31	49,49,49,49	0
60	MG	A	3527	1/1	0.74	0.29	45,45,45,45	0
60	MG	A	3052	1/1	0.74	0.26	51,51,51,51	1
60	MG	A	3371	1/1	0.75	0.24	40,40,40,40	0
60	MG	A	3610	1/1	0.75	0.24	62,62,62,62	0
60	MG	P	202	1/1	0.75	0.40	59,59,59,59	0
60	MG	A	3342	1/1	0.75	0.30	58,58,58,58	0
60	MG	A	3097	1/1	0.75	0.29	56,56,56,56	0
60	MG	a	1660	1/1	0.75	0.36	53,53,53,53	0
60	MG	A	3563	1/1	0.75	0.26	46,46,46,46	0
60	MG	x	108	1/1	0.76	0.26	55,55,55,55	0
60	MG	A	3358	1/1	0.76	0.32	46,46,46,46	1
60	MG	a	1691	1/1	0.76	0.29	53,53,53,53	0
60	MG	A	3282	1/1	0.76	0.29	68,68,68,68	0
60	MG	A	3465	1/1	0.76	0.10	59,59,59,59	0
60	MG	a	1606	1/1	0.76	0.12	48,48,48,48	0
60	MG	A	3217	1/1	0.76	0.56	56,56,56,56	1
60	MG	0	102	1/1	0.76	0.26	47,47,47,47	0
60	MG	a	1665	1/1	0.76	0.52	47,47,47,47	1
60	MG	A	3157	1/1	0.76	0.54	40,40,40,40	1
60	MG	B	201	1/1	0.76	0.47	53,53,53,53	1
60	MG	A	3536	1/1	0.76	0.31	57,57,57,57	0
60	MG	A	3521	1/1	0.76	0.23	35,35,35,35	1
60	MG	A	3064	1/1	0.76	0.14	58,58,58,58	0
60	MG	A	3517	1/1	0.77	0.21	85,85,85,85	0
60	MG	A	3449	1/1	0.77	0.31	29,29,29,29	1
60	MG	a	1772	1/1	0.77	0.35	62,62,62,62	0
60	MG	e	201	1/1	0.77	0.15	78,78,78,78	0
60	MG	A	3402	1/1	0.77	0.35	36,36,36,36	0
60	MG	A	3456	1/1	0.77	0.28	46,46,46,46	1
60	MG	A	3599	1/1	0.78	0.20	45,45,45,45	0
60	MG	A	3060	1/1	0.78	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	a	1761	1/1	0.78	0.25	55,55,55,55	1
60	MG	A	3391	1/1	0.78	0.41	56,56,56,56	0
60	MG	A	3579	1/1	0.78	0.25	50,50,50,50	0
60	MG	A	3253	1/1	0.78	0.14	67,67,67,67	0
60	MG	A	3235	1/1	0.78	0.20	43,43,43,43	0
60	MG	A	3142	1/1	0.79	0.23	57,57,57,57	0
60	MG	A	3087	1/1	0.79	0.14	41,41,41,41	0
60	MG	A	3124	1/1	0.79	0.25	32,32,32,32	1
60	MG	A	3085	1/1	0.79	0.24	70,70,70,70	0
60	MG	A	3121	1/1	0.79	0.34	38,38,38,38	1
60	MG	A	3130	1/1	0.79	0.30	55,55,55,55	0
60	MG	A	3333	1/1	0.79	0.24	61,61,61,61	1
60	MG	A	3344	1/1	0.79	0.11	70,70,70,70	0
60	MG	A	3518	1/1	0.79	0.19	39,39,39,39	0
60	MG	A	3037	1/1	0.79	0.18	44,44,44,44	0
60	MG	A	3420	1/1	0.79	0.16	55,55,55,55	0
60	MG	x	103	1/1	0.79	0.10	62,62,62,62	0
60	MG	A	3172	1/1	0.79	0.39	49,49,49,49	0
60	MG	A	3361	1/1	0.79	0.18	64,64,64,64	0
60	MG	A	3004	1/1	0.79	0.41	40,40,40,40	1
60	MG	A	3573	1/1	0.80	0.69	34,34,34,34	1
60	MG	a	1785	1/1	0.80	0.47	53,53,53,53	0
60	MG	A	3581	1/1	0.80	0.10	63,63,63,63	0
60	MG	a	1664	1/1	0.80	0.26	62,62,62,62	0
60	MG	A	3305	1/1	0.80	0.40	38,38,38,38	0
60	MG	a	1611	1/1	0.80	0.18	58,58,58,58	0
60	MG	a	1679	1/1	0.80	0.21	39,39,39,39	0
60	MG	Z	301	1/1	0.80	0.16	61,61,61,61	0
60	MG	A	3644	1/1	0.80	0.23	42,42,42,42	0
60	MG	F	305	1/1	0.80	0.14	46,46,46,46	0
60	MG	a	1718	1/1	0.80	0.41	55,55,55,55	1
60	MG	a	1620	1/1	0.80	0.49	47,47,47,47	0
60	MG	O	201	1/1	0.80	0.23	55,55,55,55	0
60	MG	A	3505	1/1	0.80	0.14	41,41,41,41	0
60	MG	a	1648	1/1	0.80	0.27	58,58,58,58	0
60	MG	A	3611	1/1	0.80	0.20	46,46,46,46	0
60	MG	A	3039	1/1	0.80	0.16	63,63,63,63	0
60	MG	A	3453	1/1	0.80	0.14	57,57,57,57	0
60	MG	A	3015	1/1	0.80	0.18	45,45,45,45	0
60	MG	B	207	1/1	0.80	0.15	76,76,76,76	0
60	MG	A	3316	1/1	0.80	0.37	63,63,63,63	0
60	MG	A	3011	1/1	0.80	0.70	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	P	201	1/1	0.80	0.36	59,59,59,59	0
60	MG	A	3122	1/1	0.80	0.31	51,51,51,51	1
60	MG	A	3259	1/1	0.80	0.31	60,60,60,60	0
60	MG	A	3555	1/1	0.81	0.15	63,63,63,63	0
60	MG	A	3244	1/1	0.81	0.19	53,53,53,53	0
60	MG	A	3141	1/1	0.81	0.32	42,42,42,42	1
60	MG	a	1625	1/1	0.81	0.30	60,60,60,60	0
60	MG	a	1786	1/1	0.81	0.77	38,38,38,38	1
60	MG	A	3510	1/1	0.81	0.33	48,48,48,48	0
60	MG	a	1704	1/1	0.81	0.22	52,52,52,52	0
60	MG	A	3180	1/1	0.81	0.35	44,44,44,44	0
60	MG	A	3068	1/1	0.81	0.38	69,69,69,69	0
60	MG	A	3511	1/1	0.81	0.33	50,50,50,50	0
60	MG	A	3257	1/1	0.81	0.16	52,52,52,52	0
60	MG	A	3438	1/1	0.81	0.13	77,77,77,77	0
60	MG	A	3088	1/1	0.81	0.32	53,53,53,53	0
60	MG	6	101	1/1	0.81	0.35	42,42,42,42	1
60	MG	a	1629	1/1	0.81	0.15	44,44,44,44	0
60	MG	a	1603	1/1	0.81	0.29	67,67,67,67	0
60	MG	A	3263	1/1	0.81	0.21	67,67,67,67	0
60	MG	A	3200	1/1	0.81	0.18	39,39,39,39	0
60	MG	A	3551	1/1	0.81	0.18	71,71,71,71	0
60	MG	A	3209	1/1	0.81	0.30	72,72,72,72	0
60	MG	A	3556	1/1	0.82	0.29	35,35,35,35	1
60	MG	A	3249	1/1	0.82	0.41	72,72,72,72	0
60	MG	A	3029	1/1	0.82	0.30	48,48,48,48	0
60	MG	a	1675	1/1	0.82	0.60	61,61,61,61	0
60	MG	A	3132	1/1	0.82	0.42	43,43,43,43	1
60	MG	A	3597	1/1	0.82	0.34	47,47,47,47	0
60	MG	a	1782	1/1	0.82	0.58	62,62,62,62	0
60	MG	A	3639	1/1	0.82	0.29	36,36,36,36	0
60	MG	A	3270	1/1	0.82	0.19	51,51,51,51	0
60	MG	a	1725	1/1	0.82	0.30	51,51,51,51	0
60	MG	A	3170	1/1	0.82	0.25	33,33,33,33	0
60	MG	A	3284	1/1	0.82	0.28	39,39,39,39	1
60	MG	a	1616	1/1	0.82	0.21	54,54,54,54	0
60	MG	A	3604	1/1	0.82	0.17	64,64,64,64	0
60	MG	A	3167	1/1	0.82	0.37	51,51,51,51	0
60	MG	A	3150	1/1	0.82	0.17	54,54,54,54	0
60	MG	z	702	1/1	0.82	0.07	57,57,57,57	0
60	MG	A	3212	1/1	0.82	0.13	46,46,46,46	0
60	MG	A	3519	1/1	0.82	0.17	48,48,48,48	0

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3353	1/1	0.85	0.22	60,60,60,60	0
60	MG	a	1609	1/1	0.85	0.55	51,51,51,51	0
60	MG	A	3520	1/1	0.85	0.36	55,55,55,55	0
60	MG	W	201	1/1	0.85	0.29	59,59,59,59	0
60	MG	A	3458	1/1	0.85	0.24	38,38,38,38	0
60	MG	a	1674	1/1	0.85	0.43	50,50,50,50	0
60	MG	B	212	1/1	0.85	0.18	52,52,52,52	0
60	MG	A	3250	1/1	0.85	0.28	64,64,64,64	0
60	MG	A	3206	1/1	0.85	0.31	50,50,50,50	0
60	MG	A	3546	1/1	0.85	0.13	53,53,53,53	0
60	MG	A	3280	1/1	0.85	0.33	46,46,46,46	0
60	MG	a	1669	1/1	0.85	0.27	60,60,60,60	0
60	MG	A	3552	1/1	0.85	0.12	48,48,48,48	0
60	MG	F	306	1/1	0.85	0.33	46,46,46,46	0
60	MG	a	1767	1/1	0.85	0.12	45,45,45,45	0
60	MG	A	3183	1/1	0.85	0.25	21,21,21,21	0
60	MG	a	1763	1/1	0.85	0.27	34,34,34,34	1
60	MG	G	202	1/1	0.85	0.10	48,48,48,48	0
60	MG	a	1693	1/1	0.85	0.32	39,39,39,39	0
60	MG	a	1690	1/1	0.85	0.14	69,69,69,69	0
60	MG	A	3148	1/1	0.85	0.30	47,47,47,47	0
60	MG	A	3082	1/1	0.85	0.31	43,43,43,43	1
60	MG	A	3084	1/1	0.85	0.11	56,56,56,56	0
60	MG	A	3574	1/1	0.85	0.18	39,39,39,39	0
60	MG	A	3528	1/1	0.85	0.51	51,51,51,51	0
60	MG	a	1601	1/1	0.85	0.53	68,68,68,68	0
60	MG	a	1644	1/1	0.85	0.17	46,46,46,46	0
60	MG	A	3059	1/1	0.85	0.22	37,37,37,37	1
60	MG	A	3531	1/1	0.85	0.41	55,55,55,55	0
60	MG	A	3072	1/1	0.85	0.17	46,46,46,46	0
60	MG	A	3433	1/1	0.85	0.20	27,27,27,27	1
60	MG	A	3081	1/1	0.85	0.35	56,56,56,56	0
60	MG	A	3118	1/1	0.85	0.23	64,64,64,64	0
60	MG	A	3161	1/1	0.85	0.29	34,34,34,34	1
60	MG	A	3225	1/1	0.85	0.29	54,54,54,54	0
60	MG	a	1667	1/1	0.85	0.21	55,55,55,55	0
60	MG	A	3423	1/1	0.85	0.20	73,73,73,73	0
60	MG	A	3568	1/1	0.85	0.24	61,61,61,61	0
60	MG	A	3429	1/1	0.86	0.29	45,45,45,45	0
60	MG	f	201	1/1	0.86	0.19	53,53,53,53	0
60	MG	B	216	1/1	0.86	0.11	53,53,53,53	0
60	MG	a	1627	1/1	0.86	0.28	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3448	1/1	0.86	0.43	60,60,60,60	0
60	MG	A	3441	1/1	0.86	0.56	52,52,52,52	0
60	MG	A	3576	1/1	0.86	0.12	59,59,59,59	0
60	MG	A	3384	1/1	0.86	0.23	39,39,39,39	0
60	MG	a	1721	1/1	0.86	0.08	41,41,41,41	0
60	MG	a	1631	1/1	0.86	0.43	42,42,42,42	0
60	MG	A	3067	1/1	0.86	0.18	34,34,34,34	0
60	MG	A	3540	1/1	0.86	0.10	57,57,57,57	0
60	MG	A	3247	1/1	0.86	0.23	46,46,46,46	1
60	MG	A	3633	1/1	0.86	0.31	30,30,30,30	0
60	MG	A	3530	1/1	0.86	0.42	38,38,38,38	1
60	MG	A	3111	1/1	0.86	0.23	46,46,46,46	0
60	MG	A	3356	1/1	0.86	0.40	50,50,50,50	0
60	MG	a	1752	1/1	0.86	0.35	43,43,43,43	0
60	MG	a	1681	1/1	0.86	0.16	55,55,55,55	0
60	MG	A	3443	1/1	0.86	0.28	41,41,41,41	0
60	MG	A	3404	1/1	0.86	0.27	35,35,35,35	0
60	MG	a	1640	1/1	0.86	0.62	68,68,68,68	0
60	MG	D	304	1/1	0.86	0.32	36,36,36,36	1
60	MG	A	3182	1/1	0.86	0.41	43,43,43,43	0
60	MG	A	3350	1/1	0.86	0.12	59,59,59,59	0
60	MG	F	302	1/1	0.86	0.27	32,32,32,32	1
60	MG	A	3043	1/1	0.86	0.24	39,39,39,39	0
60	MG	A	3258	1/1	0.86	0.41	41,41,41,41	0
60	MG	A	3024	1/1	0.86	0.28	40,40,40,40	0
60	MG	A	3063	1/1	0.86	0.29	49,49,49,49	0
60	MG	A	3271	1/1	0.86	0.48	71,71,71,71	0
60	MG	A	3450	1/1	0.87	0.33	58,58,58,58	0
60	MG	A	3110	1/1	0.87	0.27	25,25,25,25	1
60	MG	a	1602	1/1	0.87	0.28	57,57,57,57	0
60	MG	a	1632	1/1	0.87	0.36	42,42,42,42	0
60	MG	A	3073	1/1	0.87	0.21	32,32,32,32	0
60	MG	A	3075	1/1	0.87	0.14	60,60,60,60	1
60	MG	A	3642	1/1	0.87	0.21	38,38,38,38	1
60	MG	a	1775	1/1	0.87	0.18	53,53,53,53	1
60	MG	7	101	1/1	0.87	0.14	63,63,63,63	0
60	MG	A	3291	1/1	0.87	0.40	55,55,55,55	0
60	MG	A	3354	1/1	0.87	0.30	53,53,53,53	0
60	MG	A	3153	1/1	0.87	0.24	45,45,45,45	0
60	MG	U	201	1/1	0.87	0.33	30,30,30,30	1
60	MG	A	3343	1/1	0.87	0.09	64,64,64,64	0
60	MG	a	1694	1/1	0.87	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3571	1/1	0.87	0.30	38,38,38,38	1
60	MG	A	3580	1/1	0.87	0.35	43,43,43,43	0
60	MG	A	3559	1/1	0.87	0.27	38,38,38,38	1
60	MG	a	1709	1/1	0.87	0.12	36,36,36,36	0
60	MG	a	1672	1/1	0.87	0.23	41,41,41,41	0
60	MG	A	3320	1/1	0.87	0.21	62,62,62,62	0
60	MG	A	3436	1/1	0.87	0.21	43,43,43,43	0
60	MG	A	3612	1/1	0.87	0.10	62,62,62,62	0
60	MG	A	3133	1/1	0.87	0.26	36,36,36,36	1
60	MG	a	1653	1/1	0.87	0.42	61,61,61,61	0
60	MG	A	3617	1/1	0.88	0.16	45,45,45,45	0
60	MG	A	3548	1/1	0.88	0.38	65,65,65,65	0
60	MG	a	1713	1/1	0.88	0.45	43,43,43,43	0
60	MG	A	3375	1/1	0.88	0.20	35,35,35,35	0
60	MG	A	3297	1/1	0.88	0.28	35,35,35,35	1
60	MG	a	1657	1/1	0.88	0.14	57,57,57,57	0
60	MG	A	3299	1/1	0.88	0.32	35,35,35,35	0
60	MG	A	3152	1/1	0.88	0.10	48,48,48,48	0
60	MG	A	3276	1/1	0.88	0.20	51,51,51,51	1
60	MG	A	3224	1/1	0.88	0.20	34,34,34,34	0
60	MG	A	3164	1/1	0.88	0.32	31,31,31,31	0
60	MG	A	3514	1/1	0.88	0.15	69,69,69,69	0
60	MG	A	3382	1/1	0.88	0.27	30,30,30,30	0
60	MG	A	3618	1/1	0.88	0.17	57,57,57,57	0
60	MG	A	3025	1/1	0.88	0.28	51,51,51,51	1
60	MG	A	3012	1/1	0.88	0.30	60,60,60,60	0
60	MG	A	3560	1/1	0.88	0.20	58,58,58,58	0
60	MG	A	3254	1/1	0.88	0.30	62,62,62,62	0
60	MG	A	3502	1/1	0.88	0.14	44,44,44,44	0
60	MG	F	304	1/1	0.88	0.70	28,28,28,28	1
60	MG	A	3496	1/1	0.88	0.31	33,33,33,33	1
60	MG	A	3351	1/1	0.88	0.37	33,33,33,33	0
60	MG	a	1654	1/1	0.88	0.16	50,50,50,50	0
60	MG	A	3239	1/1	0.88	0.49	51,51,51,51	0
60	MG	A	3221	1/1	0.88	0.30	49,49,49,49	0
60	MG	a	1759	1/1	0.88	0.13	53,53,53,53	0
60	MG	A	3339	1/1	0.88	0.12	54,54,54,54	0
60	MG	a	1742	1/1	0.88	0.18	58,58,58,58	0
60	MG	A	3544	1/1	0.88	0.33	53,53,53,53	0
60	MG	A	3001	1/1	0.88	0.20	51,51,51,51	0
60	MG	A	3229	1/1	0.88	0.26	39,39,39,39	0
60	MG	A	3129	1/1	0.88	0.19	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3310	1/1	0.88	0.16	37,37,37,37	0
60	MG	A	3592	1/1	0.88	0.48	41,41,41,41	1
60	MG	F	303	1/1	0.88	0.20	53,53,53,53	0
60	MG	A	3620	1/1	0.88	0.18	29,29,29,29	0
60	MG	A	3246	1/1	0.88	0.29	66,66,66,66	0
60	MG	A	3328	1/1	0.88	0.17	62,62,62,62	0
60	MG	A	3532	1/1	0.88	0.20	41,41,41,41	0
60	MG	A	3038	1/1	0.88	0.21	29,29,29,29	0
60	MG	A	3268	1/1	0.89	0.27	52,52,52,52	0
60	MG	a	1765	1/1	0.89	0.13	55,55,55,55	0
60	MG	A	3474	1/1	0.89	0.34	44,44,44,44	0
60	MG	A	3191	1/1	0.89	0.22	51,51,51,51	0
60	MG	A	3290	1/1	0.89	0.20	56,56,56,56	0
60	MG	D	303	1/1	0.89	0.24	24,24,24,24	1
60	MG	a	1659	1/1	0.89	0.27	55,55,55,55	0
60	MG	A	3201	1/1	0.89	0.48	45,45,45,45	0
60	MG	A	3196	1/1	0.89	0.20	51,51,51,51	0
60	MG	A	3181	1/1	0.89	0.40	49,49,49,49	0
60	MG	A	3146	1/1	0.89	0.09	72,72,72,72	0
60	MG	A	3319	1/1	0.89	0.21	43,43,43,43	0
60	MG	a	1656	1/1	0.89	0.10	60,60,60,60	0
60	MG	A	3231	1/1	0.89	0.24	68,68,68,68	0
60	MG	A	3101	1/1	0.89	0.23	47,47,47,47	0
60	MG	a	1673	1/1	0.89	0.24	60,60,60,60	0
60	MG	A	3625	1/1	0.89	0.11	45,45,45,45	0
60	MG	A	3109	1/1	0.89	0.30	25,25,25,25	1
60	MG	A	3545	1/1	0.89	0.42	42,42,42,42	0
60	MG	a	1732	1/1	0.89	0.17	54,54,54,54	0
60	MG	A	3071	1/1	0.89	0.15	61,61,61,61	0
60	MG	A	3102	1/1	0.89	0.31	55,55,55,55	0
60	MG	a	1677	1/1	0.89	0.20	63,63,63,63	0
60	MG	A	3160	1/1	0.89	0.45	57,57,57,57	0
60	MG	A	3537	1/1	0.89	0.16	45,45,45,45	0
60	MG	H	201	1/1	0.89	0.18	62,62,62,62	0
60	MG	A	3374	1/1	0.89	0.22	54,54,54,54	0
60	MG	A	3296	1/1	0.89	0.20	31,31,31,31	0
60	MG	A	3190	1/1	0.89	0.49	58,58,58,58	0
60	MG	V	201	1/1	0.89	0.40	55,55,55,55	0
60	MG	A	3289	1/1	0.89	0.19	59,59,59,59	0
60	MG	A	3636	1/1	0.89	0.32	37,37,37,37	1
60	MG	A	3041	1/1	0.89	0.26	38,38,38,38	0
60	MG	A	3550	1/1	0.89	0.39	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3593	1/1	0.89	0.08	70,70,70,70	0
60	MG	A	3226	1/1	0.89	0.29	45,45,45,45	0
60	MG	A	3251	1/1	0.89	0.15	46,46,46,46	0
60	MG	A	3083	1/1	0.89	0.18	51,51,51,51	0
60	MG	a	1758	1/1	0.89	0.49	72,72,72,72	0
60	MG	A	3065	1/1	0.89	0.29	64,64,64,64	0
60	MG	A	3112	1/1	0.89	0.27	44,44,44,44	0
60	MG	A	3554	1/1	0.89	0.16	67,67,67,67	0
60	MG	A	3269	1/1	0.89	0.20	64,64,64,64	0
60	MG	A	3016	1/1	0.89	0.38	59,59,59,59	0
60	MG	A	3240	1/1	0.90	0.08	56,56,56,56	0
60	MG	A	3336	1/1	0.90	0.10	52,52,52,52	0
60	MG	0	101	1/1	0.90	0.23	39,39,39,39	0
60	MG	A	3589	1/1	0.90	0.14	42,42,42,42	0
60	MG	A	3535	1/1	0.90	0.26	55,55,55,55	0
60	MG	A	3159	1/1	0.90	0.18	45,45,45,45	1
60	MG	A	3338	1/1	0.90	0.29	20,20,20,20	0
60	MG	A	3471	1/1	0.90	0.13	65,65,65,65	0
60	MG	A	3079	1/1	0.90	0.17	18,18,18,18	0
60	MG	A	3609	1/1	0.90	0.21	31,31,31,31	0
60	MG	a	1683	1/1	0.90	0.40	58,58,58,58	0
60	MG	a	1650	1/1	0.90	0.47	47,47,47,47	0
60	MG	A	3114	1/1	0.90	0.39	42,42,42,42	0
60	MG	A	3090	1/1	0.90	0.21	43,43,43,43	0
60	MG	A	3163	1/1	0.90	0.11	26,26,26,26	0
60	MG	A	3202	1/1	0.90	0.09	36,36,36,36	0
60	MG	A	3332	1/1	0.90	0.13	53,53,53,53	0
60	MG	A	3468	1/1	0.90	0.18	37,37,37,37	1
60	MG	A	3010	1/1	0.90	0.36	32,32,32,32	1
60	MG	5	102	1/1	0.90	0.39	58,58,58,58	0
60	MG	a	1622	1/1	0.90	0.21	36,36,36,36	0
60	MG	A	3232	1/1	0.90	0.20	35,35,35,35	0
60	MG	A	3638	1/1	0.90	0.23	38,38,38,38	0
60	MG	E	304	1/1	0.90	0.20	35,35,35,35	0
60	MG	A	3047	1/1	0.90	0.18	29,29,29,29	0
60	MG	R	201	1/1	0.90	0.45	50,50,50,50	0
60	MG	A	3107	1/1	0.90	0.21	55,55,55,55	0
60	MG	A	3003	1/1	0.90	0.24	32,32,32,32	0
60	MG	A	3480	1/1	0.90	0.34	41,41,41,41	0
60	MG	A	3147	1/1	0.90	0.24	50,50,50,50	0
60	MG	A	3042	1/1	0.90	0.38	40,40,40,40	0
60	MG	A	3119	1/1	0.90	0.18	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3220	1/1	0.90	0.29	45,45,45,45	0
60	MG	a	1697	1/1	0.90	0.21	34,34,34,34	0
60	MG	A	3613	1/1	0.90	0.31	67,67,67,67	0
60	MG	a	1626	1/1	0.90	0.42	52,52,52,52	0
60	MG	a	1717	1/1	0.90	0.63	54,54,54,54	0
60	MG	a	1770	1/1	0.90	0.35	56,56,56,56	0
60	MG	F	301	1/1	0.91	0.20	44,44,44,44	0
60	MG	E	303	1/1	0.91	0.31	32,32,32,32	1
60	MG	A	3392	1/1	0.91	0.17	42,42,42,42	0
60	MG	A	3311	1/1	0.91	0.20	41,41,41,41	0
60	MG	a	1736	1/1	0.91	0.07	46,46,46,46	0
60	MG	A	3321	1/1	0.91	0.17	49,49,49,49	0
60	MG	a	1680	1/1	0.91	0.33	60,60,60,60	0
60	MG	a	1769	1/1	0.91	0.12	58,58,58,58	0
60	MG	a	1687	1/1	0.91	0.29	29,29,29,29	0
60	MG	A	3245	1/1	0.91	0.18	45,45,45,45	0
60	MG	A	3165	1/1	0.91	0.34	42,42,42,42	0
60	MG	A	3091	1/1	0.91	0.21	49,49,49,49	0
60	MG	A	3460	1/1	0.91	0.13	41,41,41,41	0
60	MG	a	1751	1/1	0.91	0.14	59,59,59,59	0
60	MG	a	1706	1/1	0.91	0.11	48,48,48,48	0
60	MG	A	3400	1/1	0.91	0.35	42,42,42,42	0
60	MG	n	102	1/1	0.91	0.32	28,28,28,28	0
60	MG	A	3218	1/1	0.91	0.65	52,52,52,52	0
60	MG	A	3035	1/1	0.91	0.40	30,30,30,30	1
60	MG	a	1685	1/1	0.91	0.16	46,46,46,46	0
60	MG	a	1762	1/1	0.91	0.15	52,52,52,52	0
60	MG	A	3058	1/1	0.91	0.21	59,59,59,59	0
60	MG	B	205	1/1	0.91	0.15	52,52,52,52	0
60	MG	a	1712	1/1	0.91	0.25	54,54,54,54	0
60	MG	a	1651	1/1	0.91	0.13	64,64,64,64	0
60	MG	N	201	1/1	0.91	0.24	42,42,42,42	0
60	MG	A	3524	1/1	0.91	0.19	49,49,49,49	1
60	MG	E	301	1/1	0.91	0.17	33,33,33,33	0
60	MG	A	3385	1/1	0.91	0.16	35,35,35,35	0
60	MG	A	3437	1/1	0.91	0.21	30,30,30,30	1
60	MG	A	3312	1/1	0.91	0.18	40,40,40,40	0
60	MG	A	3203	1/1	0.91	0.26	52,52,52,52	0
60	MG	A	3346	1/1	0.91	0.21	57,57,57,57	0
60	MG	a	1628	1/1	0.91	0.20	45,45,45,45	0
60	MG	A	3045	1/1	0.91	0.35	20,20,20,20	0
60	MG	A	3315	1/1	0.91	0.16	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	a	1787	1/1	0.91	0.90	40,40,40,40	1
60	MG	9	101	1/1	0.91	0.31	50,50,50,50	0
60	MG	A	3493	1/1	0.91	0.25	48,48,48,48	1
60	MG	A	3598	1/1	0.91	0.18	29,29,29,29	0
60	MG	A	3176	1/1	0.91	0.13	37,37,37,37	0
60	MG	Q	202	1/1	0.91	0.21	33,33,33,33	0
60	MG	A	3403	1/1	0.91	0.20	37,37,37,37	0
60	MG	A	3499	1/1	0.91	0.19	36,36,36,36	0
60	MG	A	3256	1/1	0.91	0.50	62,62,62,62	0
60	MG	a	1682	1/1	0.91	0.20	45,45,45,45	0
60	MG	A	3435	1/1	0.91	0.33	51,51,51,51	0
60	MG	a	1783	1/1	0.91	0.39	60,60,60,60	0
60	MG	a	1647	1/1	0.91	0.10	35,35,35,35	0
60	MG	A	3370	1/1	0.91	0.38	39,39,39,39	0
60	MG	a	1747	1/1	0.91	0.11	38,38,38,38	0
60	MG	8	101	1/1	0.91	0.21	35,35,35,35	0
60	MG	a	1730	1/1	0.91	0.45	53,53,53,53	0
60	MG	A	3562	1/1	0.91	0.16	67,67,67,67	0
60	MG	A	3461	1/1	0.91	0.22	40,40,40,40	0
60	MG	A	3406	1/1	0.91	0.06	74,74,74,74	0
60	MG	A	3365	1/1	0.91	0.16	35,35,35,35	0
60	MG	a	1740	1/1	0.91	0.24	58,58,58,58	0
60	MG	A	3334	1/1	0.91	0.37	57,57,57,57	0
60	MG	v	101	1/1	0.91	0.36	35,35,35,35	1
60	MG	a	1630	1/1	0.91	0.31	44,44,44,44	0
60	MG	A	3578	1/1	0.91	0.18	60,60,60,60	0
60	MG	A	3614	1/1	0.92	0.19	39,39,39,39	0
60	MG	A	3631	1/1	0.92	0.42	24,24,24,24	1
60	MG	A	3136	1/1	0.92	0.27	32,32,32,32	0
60	MG	A	3538	1/1	0.92	0.27	39,39,39,39	0
60	MG	A	3317	1/1	0.92	0.09	52,52,52,52	0
60	MG	A	3076	1/1	0.92	0.27	33,33,33,33	1
60	MG	a	1719	1/1	0.92	0.20	48,48,48,48	0
60	MG	A	3293	1/1	0.92	0.26	48,48,48,48	0
60	MG	a	1637	1/1	0.92	0.41	54,54,54,54	0
60	MG	A	3569	1/1	0.92	0.18	41,41,41,41	0
60	MG	A	3626	1/1	0.92	0.26	30,30,30,30	1
60	MG	A	3326	1/1	0.92	0.17	32,32,32,32	0
60	MG	a	1671	1/1	0.92	0.22	48,48,48,48	0
60	MG	A	3414	1/1	0.92	0.09	47,47,47,47	0
60	MG	A	3021	1/1	0.92	0.19	34,34,34,34	0
60	MG	A	3307	1/1	0.92	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3125	1/1	0.92	0.30	22,22,22,22	1
60	MG	A	3034	1/1	0.92	0.43	59,59,59,59	0
60	MG	A	3219	1/1	0.92	0.20	50,50,50,50	0
60	MG	A	3488	1/1	0.92	0.24	41,41,41,41	0
60	MG	A	3115	1/1	0.92	0.33	27,27,27,27	1
60	MG	A	3635	1/1	0.92	0.35	29,29,29,29	1
60	MG	a	1639	1/1	0.92	0.15	48,48,48,48	0
60	MG	a	1768	1/1	0.92	0.36	43,43,43,43	0
60	MG	A	3292	1/1	0.92	0.42	47,47,47,47	0
60	MG	A	3009	1/1	0.92	0.14	52,52,52,52	0
60	MG	A	3233	1/1	0.92	0.12	56,56,56,56	0
60	MG	A	3367	1/1	0.92	0.15	40,40,40,40	0
60	MG	A	3222	1/1	0.92	0.15	39,39,39,39	0
60	MG	A	3028	1/1	0.92	0.11	57,57,57,57	0
60	MG	a	1678	1/1	0.92	0.23	36,36,36,36	0
60	MG	a	1773	1/1	0.92	0.14	58,58,58,58	0
60	MG	a	1605	1/1	0.92	0.27	54,54,54,54	0
60	MG	A	3300	1/1	0.92	0.28	42,42,42,42	0
60	MG	A	3379	1/1	0.92	0.15	36,36,36,36	0
60	MG	A	3248	1/1	0.92	0.34	48,48,48,48	1
60	MG	A	3166	1/1	0.92	0.17	40,40,40,40	0
60	MG	A	3377	1/1	0.92	0.29	26,26,26,26	0
60	MG	A	3104	1/1	0.92	0.17	25,25,25,25	0
60	MG	A	3504	1/1	0.92	0.21	25,25,25,25	0
60	MG	D	302	1/1	0.92	0.19	43,43,43,43	0
60	MG	A	3204	1/1	0.92	0.35	39,39,39,39	0
60	MG	A	3442	1/1	0.92	0.44	60,60,60,60	0
60	MG	A	3388	1/1	0.92	0.19	31,31,31,31	0
60	MG	A	3543	1/1	0.92	0.26	51,51,51,51	0
60	MG	a	1695	1/1	0.92	0.41	40,40,40,40	0
60	MG	A	3623	1/1	0.92	0.35	57,57,57,57	0
60	MG	a	1670	1/1	0.92	0.10	57,57,57,57	0
60	MG	A	3288	1/1	0.92	0.24	45,45,45,45	0
60	MG	A	3359	1/1	0.92	0.16	63,63,63,63	0
60	MG	A	3632	1/1	0.92	0.26	35,35,35,35	1
60	MG	A	3103	1/1	0.92	0.17	44,44,44,44	0
60	MG	A	3306	1/1	0.92	0.28	33,33,33,33	0
60	MG	A	3095	1/1	0.92	0.10	32,32,32,32	0
60	MG	A	3194	1/1	0.92	0.12	63,63,63,63	0
60	MG	A	3634	1/1	0.92	0.14	42,42,42,42	1
60	MG	A	3108	1/1	0.92	0.36	60,60,60,60	0
60	MG	A	3329	1/1	0.92	0.21	33,33,33,33	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3390	1/1	0.92	0.13	36,36,36,36	0
60	MG	A	3313	1/1	0.93	0.17	29,29,29,29	0
60	MG	A	3452	1/1	0.93	0.07	69,69,69,69	0
60	MG	D	306	1/1	0.93	0.16	25,25,25,25	0
60	MG	A	3575	1/1	0.93	0.29	39,39,39,39	1
60	MG	A	3500	1/1	0.93	0.20	30,30,30,30	0
60	MG	A	3463	1/1	0.93	0.68	48,48,48,48	0
60	MG	a	1778	1/1	0.93	0.26	53,53,53,53	0
60	MG	A	3019	1/1	0.93	0.31	20,20,20,20	0
60	MG	a	1777	1/1	0.93	0.28	32,32,32,32	1
60	MG	A	3020	1/1	0.93	0.18	26,26,26,26	0
60	MG	A	3427	1/1	0.93	0.20	49,49,49,49	0
60	MG	A	3539	1/1	0.93	0.17	21,21,21,21	0
60	MG	A	3507	1/1	0.93	0.13	42,42,42,42	0
60	MG	A	3566	1/1	0.93	0.44	55,55,55,55	0
60	MG	A	3287	1/1	0.93	0.20	35,35,35,35	0
60	MG	A	3048	1/1	0.93	0.15	35,35,35,35	0
60	MG	A	3409	1/1	0.93	0.16	35,35,35,35	0
60	MG	A	3457	1/1	0.93	0.18	24,24,24,24	0
60	MG	A	3431	1/1	0.93	0.31	52,52,52,52	0
60	MG	A	3211	1/1	0.93	0.23	50,50,50,50	0
60	MG	A	3189	1/1	0.93	0.31	50,50,50,50	0
60	MG	G	201	1/1	0.93	0.21	48,48,48,48	0
60	MG	A	3345	1/1	0.93	0.26	48,48,48,48	0
60	MG	A	3207	1/1	0.93	0.32	61,61,61,61	0
60	MG	a	1754	1/1	0.93	0.12	42,42,42,42	0
60	MG	A	3303	1/1	0.93	0.17	57,57,57,57	0
60	MG	x	107	1/1	0.93	0.09	69,69,69,69	0
60	MG	A	3193	1/1	0.93	0.22	27,27,27,27	0
60	MG	a	1714	1/1	0.93	0.44	54,54,54,54	0
60	MG	A	3195	1/1	0.93	0.47	55,55,55,55	0
60	MG	A	3325	1/1	0.93	0.14	23,23,23,23	0
60	MG	A	3583	1/1	0.93	0.21	46,46,46,46	0
60	MG	A	3428	1/1	0.93	0.19	56,56,56,56	0
60	MG	A	3349	1/1	0.93	0.18	42,42,42,42	0
60	MG	a	1623	1/1	0.93	0.22	46,46,46,46	1
60	MG	A	3149	1/1	0.93	0.08	54,54,54,54	0
60	MG	A	3093	1/1	0.93	0.30	50,50,50,50	0
60	MG	X	101	1/1	0.93	0.25	50,50,50,50	0
60	MG	a	1696	1/1	0.93	0.49	52,52,52,52	0
60	MG	A	3347	1/1	0.93	0.27	37,37,37,37	1
60	MG	A	3476	1/1	0.93	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	a	1649	1/1	0.93	0.43	67,67,67,67	0
60	MG	A	3007	1/1	0.93	0.21	35,35,35,35	0
60	MG	x	101	1/1	0.93	0.33	29,29,29,29	1
60	MG	A	3553	1/1	0.93	0.25	51,51,51,51	1
60	MG	A	3482	1/1	0.93	0.25	38,38,38,38	0
60	MG	A	3210	1/1	0.93	0.56	30,30,30,30	0
60	MG	a	1658	1/1	0.93	0.12	30,30,30,30	0
60	MG	A	3508	1/1	0.93	0.11	68,68,68,68	0
60	MG	a	1755	1/1	0.93	0.08	40,40,40,40	0
60	MG	a	1753	1/1	0.93	0.32	46,46,46,46	0
60	MG	A	3641	1/1	0.93	0.17	32,32,32,32	1
60	MG	A	3156	1/1	0.93	0.19	26,26,26,26	0
60	MG	a	1619	1/1	0.93	0.27	32,32,32,32	0
60	MG	A	3466	1/1	0.93	0.22	49,49,49,49	0
60	MG	A	3561	1/1	0.93	0.20	60,60,60,60	0
60	MG	A	3455	1/1	0.93	0.27	28,28,28,28	0
60	MG	A	3134	1/1	0.93	0.19	25,25,25,25	0
60	MG	A	3596	1/1	0.93	0.25	44,44,44,44	1
60	MG	A	3285	1/1	0.93	0.31	31,31,31,31	0
60	MG	a	1617	1/1	0.93	0.38	47,47,47,47	0
60	MG	A	3494	1/1	0.93	0.20	35,35,35,35	0
60	MG	A	3381	1/1	0.93	0.16	56,56,56,56	0
60	MG	A	3464	1/1	0.93	0.13	56,56,56,56	0
60	MG	5	101	1/1	0.93	0.30	44,44,44,44	1
60	MG	A	3304	1/1	0.94	0.13	53,53,53,53	0
60	MG	a	1613	1/1	0.94	0.26	29,29,29,29	0
60	MG	v	102	1/1	0.94	0.30	42,42,42,42	0
60	MG	a	1710	1/1	0.94	0.34	53,53,53,53	1
60	MG	A	3138	1/1	0.94	0.12	31,31,31,31	0
60	MG	A	3498	1/1	0.94	0.15	68,68,68,68	0
60	MG	n	103	1/1	0.94	0.31	55,55,55,55	0
60	MG	A	3643	1/1	0.94	0.29	34,34,34,34	0
60	MG	A	3053	1/1	0.94	0.27	35,35,35,35	0
60	MG	A	3352	1/1	0.94	0.36	39,39,39,39	0
60	MG	A	3432	1/1	0.94	0.16	54,54,54,54	0
60	MG	A	3584	1/1	0.94	0.13	39,39,39,39	0
60	MG	A	3547	1/1	0.94	0.10	41,41,41,41	0
60	MG	A	3523	1/1	0.94	0.28	31,31,31,31	0
60	MG	A	3386	1/1	0.94	0.24	33,33,33,33	0
60	MG	A	3131	1/1	0.94	0.20	57,57,57,57	0
60	MG	A	3605	1/1	0.94	0.36	50,50,50,50	0
60	MG	a	1774	1/1	0.94	0.14	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3205	1/1	0.94	0.17	53,53,53,53	0
60	MG	a	1634	1/1	0.94	0.35	53,53,53,53	0
60	MG	A	3128	1/1	0.94	0.26	37,37,37,37	0
60	MG	A	3327	1/1	0.94	0.23	30,30,30,30	0
60	MG	A	3364	1/1	0.94	0.10	45,45,45,45	0
60	MG	a	1624	1/1	0.94	0.14	39,39,39,39	0
60	MG	a	1737	1/1	0.94	0.35	46,46,46,46	0
60	MG	A	3526	1/1	0.94	0.20	29,29,29,29	0
60	MG	A	3398	1/1	0.94	0.10	37,37,37,37	0
60	MG	a	1711	1/1	0.94	0.18	48,48,48,48	0
60	MG	A	3533	1/1	0.94	0.41	52,52,52,52	0
60	MG	a	1745	1/1	0.94	0.21	40,40,40,40	0
60	MG	A	3637	1/1	0.94	0.45	37,37,37,37	0
60	MG	A	3478	1/1	0.94	0.34	50,50,50,50	0
60	MG	A	3621	1/1	0.94	0.31	48,48,48,48	0
60	MG	A	3185	1/1	0.94	0.22	32,32,32,32	0
60	MG	x	105	1/1	0.94	0.12	51,51,51,51	0
60	MG	A	3140	1/1	0.94	0.19	48,48,48,48	0
60	MG	a	1618	1/1	0.94	0.54	54,54,54,54	0
60	MG	a	1707	1/1	0.94	0.16	34,34,34,34	0
60	MG	A	3564	1/1	0.94	0.13	52,52,52,52	0
60	MG	A	3363	1/1	0.94	0.21	35,35,35,35	0
60	MG	A	3469	1/1	0.94	0.12	48,48,48,48	0
60	MG	A	3331	1/1	0.94	0.21	31,31,31,31	0
60	MG	A	3175	1/1	0.94	0.19	62,62,62,62	0
60	MG	A	3608	1/1	0.94	0.23	32,32,32,32	0
60	MG	a	1766	1/1	0.94	0.24	49,49,49,49	0
60	MG	A	3214	1/1	0.94	0.52	44,44,44,44	1
60	MG	A	3372	1/1	0.94	0.20	41,41,41,41	0
60	MG	0	103	1/1	0.94	0.08	53,53,53,53	0
60	MG	a	1739	1/1	0.94	0.17	42,42,42,42	0
60	MG	A	3516	1/1	0.94	0.19	25,25,25,25	1
60	MG	A	3139	1/1	0.94	0.30	37,37,37,37	0
60	MG	A	3078	1/1	0.94	0.33	27,27,27,27	1
60	MG	A	3393	1/1	0.94	0.28	41,41,41,41	0
60	MG	x	102	1/1	0.94	0.07	77,77,77,77	0
60	MG	A	3192	1/1	0.94	0.18	26,26,26,26	0
60	MG	6	103	1/1	0.94	0.17	41,41,41,41	0
60	MG	A	3126	1/1	0.94	0.28	28,28,28,28	1
60	MG	A	3174	1/1	0.95	0.26	25,25,25,25	0
60	MG	a	1668	1/1	0.95	0.18	30,30,30,30	0
60	MG	A	3622	1/1	0.95	0.35	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3567	1/1	0.95	0.15	38,38,38,38	1
60	MG	A	3074	1/1	0.95	0.15	29,29,29,29	0
60	MG	A	3434	1/1	0.95	0.23	41,41,41,41	0
61	ZN	6	102	1/1	0.95	0.25	72,72,72,72	0
61	ZN	4	501	1/1	0.95	0.06	79,79,79,79	0
60	MG	A	3454	1/1	0.95	0.42	44,44,44,44	0
60	MG	A	3033	1/1	0.95	0.26	59,59,59,59	1
60	MG	A	3294	1/1	0.95	0.18	25,25,25,25	1
60	MG	A	3467	1/1	0.95	0.21	37,37,37,37	0
60	MG	A	3426	1/1	0.95	0.15	36,36,36,36	0
60	MG	A	3629	1/1	0.95	0.17	21,21,21,21	0
60	MG	a	1750	1/1	0.95	0.22	41,41,41,41	0
60	MG	A	3481	1/1	0.95	0.13	46,46,46,46	0
60	MG	A	3417	1/1	0.95	0.28	43,43,43,43	0
60	MG	A	3105	1/1	0.95	0.25	28,28,28,28	1
60	MG	A	3595	1/1	0.95	0.27	27,27,27,27	0
62	SF4	d	302	8/8	0.95	0.05	60,65,70,71	2
60	MG	A	3389	1/1	0.95	0.10	33,33,33,33	0
60	MG	a	1771	1/1	0.95	0.13	67,67,67,67	0
60	MG	A	3286	1/1	0.95	0.49	48,48,48,48	0
60	MG	A	3357	1/1	0.95	0.48	36,36,36,36	0
60	MG	0	104	1/1	0.95	0.40	36,36,36,36	1
60	MG	a	1646	1/1	0.95	0.20	52,52,52,52	0
60	MG	A	3368	1/1	0.95	0.21	36,36,36,36	0
60	MG	A	3570	1/1	0.95	0.17	54,54,54,54	0
60	MG	A	3408	1/1	0.95	0.27	33,33,33,33	0
60	MG	A	3485	1/1	0.95	0.16	59,59,59,59	0
60	MG	A	3405	1/1	0.95	0.29	32,32,32,32	0
60	MG	A	3410	1/1	0.95	0.23	44,44,44,44	0
60	MG	A	3616	1/1	0.95	0.18	45,45,45,45	0
60	MG	a	1655	1/1	0.95	0.40	47,47,47,47	0
60	MG	l	201	1/1	0.95	0.22	31,31,31,31	0
60	MG	A	3168	1/1	0.95	0.22	23,23,23,23	0
60	MG	A	3522	1/1	0.95	0.21	28,28,28,28	0
60	MG	a	1760	1/1	0.95	0.17	38,38,38,38	0
60	MG	A	3601	1/1	0.95	0.24	33,33,33,33	0
60	MG	A	3215	1/1	0.95	0.42	44,44,44,44	0
60	MG	A	3473	1/1	0.95	0.18	27,27,27,27	0
60	MG	A	3416	1/1	0.95	0.17	31,31,31,31	0
60	MG	D	305	1/1	0.95	0.43	43,43,43,43	0
60	MG	A	3069	1/1	0.95	0.24	30,30,30,30	0
60	MG	B	208	1/1	0.95	0.08	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	a	1749	1/1	0.95	0.33	54,54,54,54	0
60	MG	A	3061	1/1	0.95	0.28	43,43,43,43	0
60	MG	A	3187	1/1	0.95	0.40	31,31,31,31	0
60	MG	A	3027	1/1	0.95	0.14	62,62,62,62	0
60	MG	A	3279	1/1	0.95	0.29	30,30,30,30	1
60	MG	a	1684	1/1	0.95	0.14	31,31,31,31	0
60	MG	A	3241	1/1	0.95	0.22	20,20,20,20	0
60	MG	B	218	1/1	0.95	0.27	49,49,49,49	0
60	MG	A	3301	1/1	0.95	0.29	54,54,54,54	0
60	MG	A	3186	1/1	0.95	0.13	33,33,33,33	0
60	MG	A	3515	1/1	0.95	0.28	47,47,47,47	0
60	MG	A	3397	1/1	0.95	0.27	38,38,38,38	0
60	MG	A	3323	1/1	0.95	0.15	72,72,72,72	0
60	MG	A	3123	1/1	0.95	0.22	30,30,30,30	1
60	MG	A	3628	1/1	0.95	0.30	35,35,35,35	0
60	MG	A	3513	1/1	0.95	0.18	58,58,58,58	0
60	MG	a	1757	1/1	0.95	0.24	46,46,46,46	0
60	MG	a	1652	1/1	0.95	0.18	20,20,20,20	0
60	MG	a	1621	1/1	0.96	0.10	64,64,64,64	0
60	MG	Q	201	1/1	0.96	0.45	47,47,47,47	0
60	MG	a	1645	1/1	0.96	0.20	42,42,42,42	0
60	MG	a	1780	1/1	0.96	0.23	54,54,54,54	0
60	MG	A	3340	1/1	0.96	0.24	45,45,45,45	0
60	MG	A	3440	1/1	0.96	0.13	45,45,45,45	0
60	MG	A	3472	1/1	0.96	0.47	25,25,25,25	0
60	MG	A	3490	1/1	0.96	0.12	40,40,40,40	0
60	MG	A	3529	1/1	0.96	0.12	59,59,59,59	0
60	MG	A	3077	1/1	0.96	0.31	24,24,24,24	1
60	MG	a	1735	1/1	0.96	0.15	37,37,37,37	0
60	MG	A	3113	1/1	0.96	0.25	29,29,29,29	1
60	MG	B	213	1/1	0.96	0.17	52,52,52,52	0
60	MG	a	1729	1/1	0.96	0.35	50,50,50,50	0
60	MG	A	3298	1/1	0.96	0.20	34,34,34,34	0
60	MG	A	3046	1/1	0.96	0.15	29,29,29,29	0
60	MG	a	1746	1/1	0.96	0.09	49,49,49,49	0
60	MG	A	3412	1/1	0.96	0.21	44,44,44,44	0
60	MG	A	3330	1/1	0.96	0.34	37,37,37,37	1
60	MG	A	3419	1/1	0.96	0.26	30,30,30,30	1
60	MG	A	3337	1/1	0.96	0.29	48,48,48,48	0
60	MG	A	3558	1/1	0.96	0.24	53,53,53,53	0
60	MG	A	3030	1/1	0.96	0.18	33,33,33,33	0
60	MG	O	202	1/1	0.96	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	E	302	1/1	0.96	0.29	32,32,32,32	0
60	MG	a	1756	1/1	0.96	0.15	52,52,52,52	0
60	MG	A	3640	1/1	0.96	0.14	30,30,30,30	1
60	MG	A	3459	1/1	0.96	0.24	33,33,33,33	0
60	MG	A	3005	1/1	0.96	0.17	31,31,31,31	1
63	GCP	z	703	32/32	0.96	0.15	47,57,62,63	13
60	MG	A	3366	1/1	0.96	0.15	19,19,19,19	1
60	MG	A	3116	1/1	0.96	0.24	47,47,47,47	0
60	MG	A	3470	1/1	0.96	0.22	51,51,51,51	0
60	MG	a	1700	1/1	0.96	0.25	50,50,50,50	0
60	MG	A	3489	1/1	0.96	0.26	27,27,27,27	0
61	ZN	Y	501	1/1	0.96	0.05	63,63,63,63	0
60	MG	a	1722	1/1	0.96	0.15	51,51,51,51	0
60	MG	A	3506	1/1	0.96	0.33	41,41,41,41	0
60	MG	A	3230	1/1	0.96	0.26	40,40,40,40	0
60	MG	A	3422	1/1	0.96	0.20	52,52,52,52	0
60	MG	A	3395	1/1	0.96	0.29	51,51,51,51	0
60	MG	A	3360	1/1	0.96	0.19	54,54,54,54	0
60	MG	A	3373	1/1	0.96	0.25	34,34,34,34	0
60	MG	B	203	1/1	0.96	0.07	56,56,56,56	0
60	MG	a	1692	1/1	0.96	0.25	41,41,41,41	0
60	MG	a	1743	1/1	0.96	0.31	45,45,45,45	0
60	MG	A	3495	1/1	0.96	0.16	35,35,35,35	0
60	MG	a	1716	1/1	0.96	0.16	36,36,36,36	0
60	MG	B	214	1/1	0.96	0.07	59,59,59,59	0
60	MG	m	201	1/1	0.96	0.22	38,38,38,38	1
60	MG	a	1633	1/1	0.96	0.21	32,32,32,32	0
60	MG	A	3479	1/1	0.96	0.10	41,41,41,41	0
60	MG	A	3023	1/1	0.96	0.17	34,34,34,34	0
60	MG	a	1723	1/1	0.96	0.27	48,48,48,48	0
60	MG	A	3162	1/1	0.96	0.19	29,29,29,29	0
60	MG	A	3619	1/1	0.96	0.30	16,16,16,16	0
60	MG	A	3198	1/1	0.97	0.10	20,20,20,20	0
60	MG	A	3413	1/1	0.97	0.13	35,35,35,35	0
60	MG	D	301	1/1	0.97	0.26	21,21,21,21	0
60	MG	a	1744	1/1	0.97	0.16	46,46,46,46	0
60	MG	A	3380	1/1	0.97	0.18	45,45,45,45	0
60	MG	A	3477	1/1	0.97	0.22	21,21,21,21	0
60	MG	A	3600	1/1	0.97	0.08	53,53,53,53	0
60	MG	A	3447	1/1	0.97	0.21	47,47,47,47	0
60	MG	a	1733	1/1	0.97	0.28	51,51,51,51	0
60	MG	A	3439	1/1	0.97	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3177	1/1	0.97	0.37	39,39,39,39	0
60	MG	a	1781	1/1	0.97	0.23	46,46,46,46	0
60	MG	A	3216	1/1	0.97	0.38	31,31,31,31	0
60	MG	m	202	1/1	0.97	0.31	56,56,56,56	0
60	MG	B	202	1/1	0.97	0.14	52,52,52,52	0
60	MG	A	3376	1/1	0.97	0.14	31,31,31,31	0
60	MG	A	3120	1/1	0.97	0.33	26,26,26,26	0
60	MG	A	3324	1/1	0.97	0.11	38,38,38,38	0
60	MG	a	1738	1/1	0.97	0.17	35,35,35,35	0
60	MG	A	3378	1/1	0.97	0.31	41,41,41,41	0
60	MG	a	1748	1/1	0.97	0.07	46,46,46,46	0
60	MG	A	3062	1/1	0.97	0.16	41,41,41,41	0
60	MG	A	3031	1/1	0.97	0.20	33,33,33,33	0
60	MG	B	210	1/1	0.97	0.13	44,44,44,44	0
60	MG	A	3582	1/1	0.97	0.19	21,21,21,21	1
60	MG	A	3451	1/1	0.97	0.29	45,45,45,45	0
61	ZN	5	103	1/1	0.97	0.08	54,54,54,54	0
60	MG	B	217	1/1	0.97	0.13	40,40,40,40	0
60	MG	A	3032	1/1	0.97	0.27	50,50,50,50	0
60	MG	A	3421	1/1	0.97	0.14	57,57,57,57	0
61	ZN	9	102	1/1	0.97	0.19	49,49,49,49	1
60	MG	A	3594	1/1	0.97	0.34	85,85,85,85	0
60	MG	A	3261	1/1	0.97	0.19	46,46,46,46	0
60	MG	A	3445	1/1	0.97	0.26	42,42,42,42	1
60	MG	A	3173	1/1	0.97	0.65	37,37,37,37	0
60	MG	A	3355	1/1	0.97	0.17	61,61,61,61	0
60	MG	A	3145	1/1	0.97	0.41	61,61,61,61	0
60	MG	A	3491	1/1	0.97	0.34	39,39,39,39	0
60	MG	A	3017	1/1	0.97	0.28	41,41,41,41	0
60	MG	a	1728	1/1	0.97	0.13	33,33,33,33	0
60	MG	A	3475	1/1	0.97	0.15	41,41,41,41	0
60	MG	a	1726	1/1	0.97	0.10	43,43,43,43	0
60	MG	A	3446	1/1	0.97	0.24	26,26,26,26	0
60	MG	A	3178	1/1	0.97	0.40	56,56,56,56	0
60	MG	A	3487	1/1	0.97	0.21	35,35,35,35	0
60	MG	P	203	1/1	0.97	0.28	45,45,45,45	1
60	MG	A	3383	1/1	0.97	0.10	28,28,28,28	0
60	MG	a	1776	1/1	0.97	0.25	52,52,52,52	0
60	MG	a	1702	1/1	0.97	0.48	42,42,42,42	0
60	MG	A	3411	1/1	0.97	0.15	39,39,39,39	0
60	MG	A	3415	1/1	0.97	0.11	34,34,34,34	0
60	MG	A	3590	1/1	0.97	0.29	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3302	1/1	0.97	0.15	22,22,22,22	0
60	MG	A	3322	1/1	0.97	0.18	42,42,42,42	1
60	MG	A	3086	1/1	0.98	0.31	21,21,21,21	0
60	MG	A	3407	1/1	0.98	0.17	30,30,30,30	0
60	MG	A	3501	1/1	0.98	0.15	24,24,24,24	0
60	MG	A	3486	1/1	0.98	0.17	44,44,44,44	0
60	MG	A	3483	1/1	0.98	0.21	31,31,31,31	0
60	MG	A	3424	1/1	0.98	0.33	20,20,20,20	0
60	MG	a	1727	1/1	0.98	0.13	49,49,49,49	0
60	MG	A	3512	1/1	0.98	0.22	44,44,44,44	0
60	MG	a	1734	1/1	0.98	0.09	33,33,33,33	0
60	MG	a	1610	1/1	0.98	0.29	32,32,32,32	1
60	MG	A	3314	1/1	0.98	0.09	48,48,48,48	0
60	MG	A	3171	1/1	0.98	0.19	31,31,31,31	0
60	MG	A	3096	1/1	0.98	0.14	27,27,27,27	0
60	MG	a	1699	1/1	0.98	0.26	56,56,56,56	0
60	MG	x	104	1/1	0.98	0.30	43,43,43,43	0
60	MG	A	3213	1/1	0.98	0.10	34,34,34,34	1
60	MG	A	3238	1/1	0.98	0.31	38,38,38,38	0
60	MG	A	3348	1/1	0.98	0.24	30,30,30,30	0
60	MG	A	3497	1/1	0.98	0.25	38,38,38,38	1
60	MG	A	3018	1/1	0.98	0.25	27,27,27,27	0
60	MG	A	3051	1/1	0.98	0.31	54,54,54,54	0
60	MG	A	3369	1/1	0.98	0.14	31,31,31,31	0
60	MG	A	3503	1/1	0.98	0.21	53,53,53,53	0
60	MG	a	1788	1/1	0.98	0.10	43,43,43,43	1
60	MG	A	3309	1/1	0.98	0.20	49,49,49,49	0
60	MG	A	3444	1/1	0.98	0.31	39,39,39,39	0
60	MG	A	3036	1/1	0.98	0.25	25,25,25,25	1
60	MG	A	3509	1/1	0.98	0.37	45,45,45,45	0
60	MG	A	3565	1/1	0.98	0.12	35,35,35,35	0
60	MG	A	3401	1/1	0.98	0.37	36,36,36,36	0
60	MG	A	3587	1/1	0.98	0.28	23,23,23,23	1
60	MG	A	3534	1/1	0.98	0.23	35,35,35,35	0
60	MG	a	1764	1/1	0.98	0.49	37,37,37,37	0
60	MG	A	3425	1/1	0.98	0.28	54,54,54,54	0
60	MG	A	3070	1/1	0.98	0.27	10,10,10,10	0
60	MG	A	3308	1/1	0.98	0.23	14,14,14,14	0
60	MG	a	1708	1/1	0.98	0.11	40,40,40,40	0
60	MG	A	3013	1/1	0.98	0.23	24,24,24,24	0
60	MG	a	1720	1/1	0.98	0.22	48,48,48,48	0
60	MG	A	3318	1/1	0.98	0.17	42,42,42,42	1

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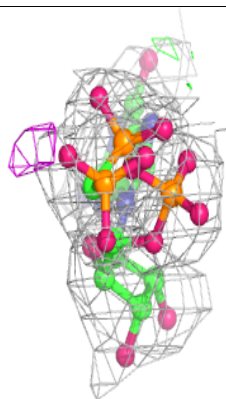
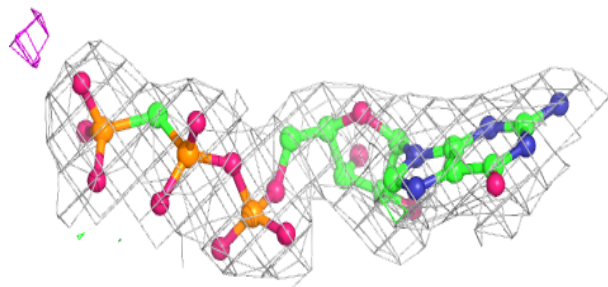
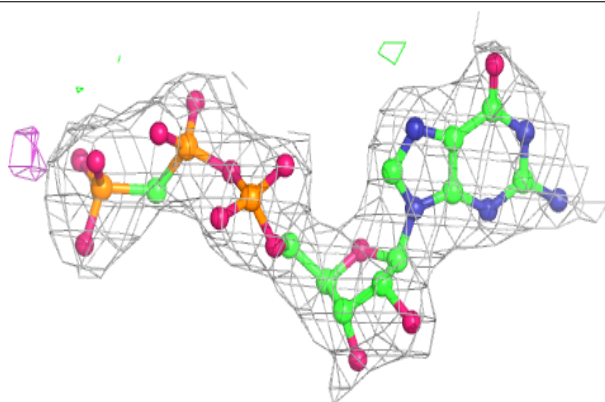
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A	3430	1/1	0.98	0.22	43,43,43,43	0
60	MG	a	1688	1/1	0.98	0.22	32,32,32,32	0
60	MG	A	3484	1/1	0.98	0.40	41,41,41,41	0
60	MG	E	305	1/1	0.99	0.16	23,23,23,23	1
61	ZN	n	104	1/1	0.99	0.15	44,44,44,44	0
60	MG	A	3399	1/1	0.99	0.28	44,44,44,44	0
60	MG	a	1724	1/1	0.99	0.34	42,42,42,42	0
60	MG	a	1608	1/1	0.99	0.29	23,23,23,23	0
60	MG	A	3273	1/1	0.99	0.34	37,37,37,37	1
60	MG	A	3396	1/1	0.99	0.18	26,26,26,26	0
60	MG	A	3184	1/1	0.99	0.42	30,30,30,30	0
60	MG	a	1607	1/1	0.99	0.35	42,42,42,42	1
60	MG	A	3615	1/1	0.99	0.14	34,34,34,34	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 GCP z 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.