



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:32 am GMT

PDB ID : 5LZD
EMDB ID : EMD-4124
Title : Structure of SelB-Sec-tRNA^{Sec} bound to the 70S ribosome in the GTPase activated state (GA)
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : 2016-09-29
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

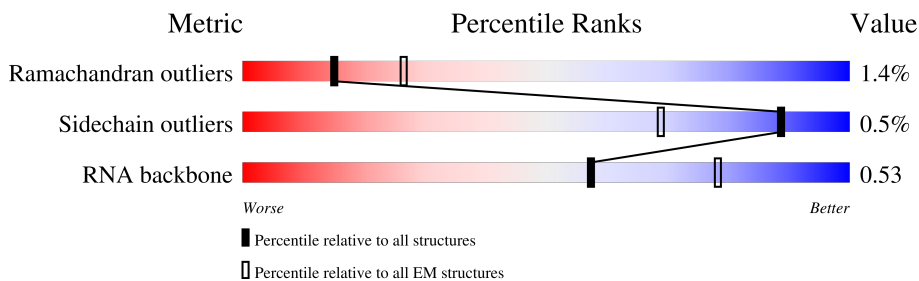
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	1539	
2	b	218	
3	c	206	
4	d	205	
5	e	157	
6	f	100	
7	g	151	
8	h	129	

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Mol	Chain	Length	Quality of chain
9	i	127	9% 94% 5%
10	j	98	17% 93% 6%
11	k	116	96% ..
12	l	123	5% 92% 7%
13	m	114	6% 92% 8%
14	n	100	6% 94% 6%
15	o	88	5% 94% 6%
16	p	82	11% 99% .
17	q	80	90% 10%
18	r	65	11% 94% 6%
19	s	86	12% 93% 6%
20	t	85	6% 98% .
21	u	65	18% 89% 11%
22	v	77	77% 19% .
23	x	48	58% 40% 38% 23%
24	y	95	65% 35%
25	z	614	29% 96% .
26	A	2903	76% 22% .
27	B	120	74% 23% .
28	C	271	97% .
29	D	209	99%
30	E	201	7% 97% .
31	F	177	11% 93% 6% .
32	G	176	6% 96% .
33	I	141	97% 99% .

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Mol	Chain	Length	Quality of chain
34	H	149	73% 96%
35	J	142	99%
36	K	122	97%
37	L	143	5% 97%
38	M	136	99%
39	N	120	98%
40	O	116	5% 99%
41	P	114	98%
42	Q	117	99%
43	R	103	8% 99%
44	S	110	97%
45	T	93	6% 99%
46	U	102	8% 92% 7%
47	V	94	7% 100%
48	W	75	100%
49	X	77	5% 99%
50	Y	63	10% 94% 6%
51	Z	58	5% 98%
52	0	56	5% 96%
53	1	50	8% 94% 6%
54	2	46	100%
55	3	64	97%
56	4	38	92% 8%
57	6	66	27% 94% 5%
58	w	3	67% 100%

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
1	G7M	a	527	X	-	-	-
26	G7M	A	2069	X	-	-	-

2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 153177 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1539	33029	14738	6052	10700	1539	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	218	1705	1081	305	312	7	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	206	1625	1028	305	289	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	205	1643	1026	315	298	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	157	1157	719	218	214	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	100	818	515	148	149	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	151	1182	735	227	216	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	129	979	616	173	184	6	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	127	1022	634	206	179	3	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	98	787	493	150	143	1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	116	870	535	173	159	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	123	955	590	196	165	4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	114	884	546	178	157	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	86	Total	C	N	O	S	0	0
			687	438	131	116	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called fMet-tRNA^{fMet}.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called Sec-tRNA^{Sec}.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	95	Total	C	N	O	P	0	0
			2031	907	357	672	95		

- Molecule 25 is a protein called Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	614	Total	C	N	O	S	0	0
			4853	3043	901	892	17		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2903	Total	C	N	O	P	0	0
			62335	27815	11467	20150	2903		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	J	142	1129	714	212	199	4	0	0

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	K	122	939	587	180	166	6	0	0

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	L	143	1045	649	206	189	1	0	0

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	M	136	1074	686	205	177	6	0	0

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	N	120	961	593	196	167	5	0	0

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	O	116	892	552	178	162	0	0

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	P	114	917	574	179	163	1	0	0

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	U	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 58 is a RNA chain called CCA 3' end of E-site tRNA^{Sec} (low occupancy).

Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 59 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
59	a	1	Total	Cl	0
			1	1	

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

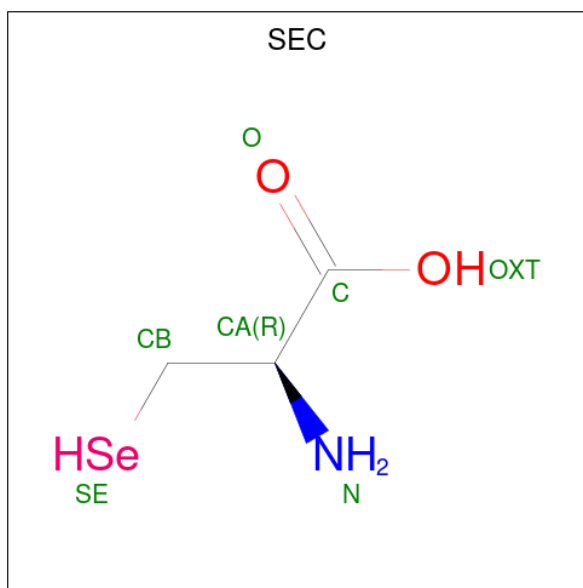
Mol	Chain	Residues	Atoms		AltConf
60	a	30	Total	Mg	0
			30	30	
60	n	1	Total	Mg	0
			1	1	
60	v	1	Total	Mg	0
			1	1	
60	y	1	Total	Mg	0
			1	1	
60	z	1	Total	Mg	0
			1	1	
60	A	111	Total	Mg	0
			111	111	
60	B	2	Total	Mg	0
			2	2	

- Molecule 61 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



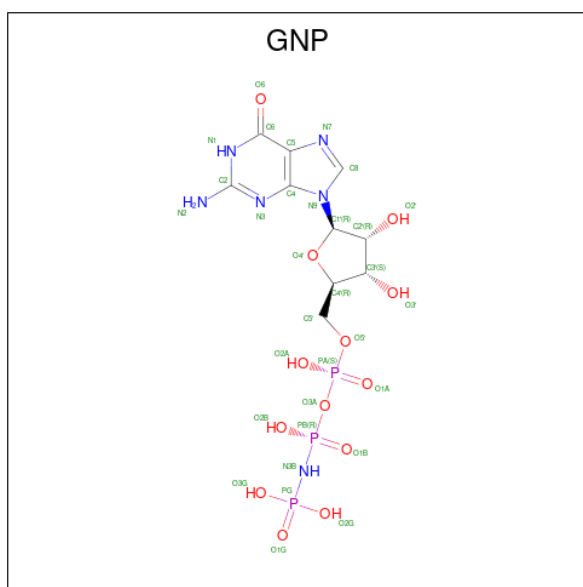
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
61	v	1	10	6	1	2	1	0

- Molecule 62 is SELENOCYSTEINE (three-letter code: SEC) (formula: $C_3H_7NO_2Se$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	Se	
62	y	1	6	3	1	1	1	0

- Molecule 63 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
63	z	1	32	10	6	13	3	0

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
64	4	1	1	1	0
64	6	1	1	1	0

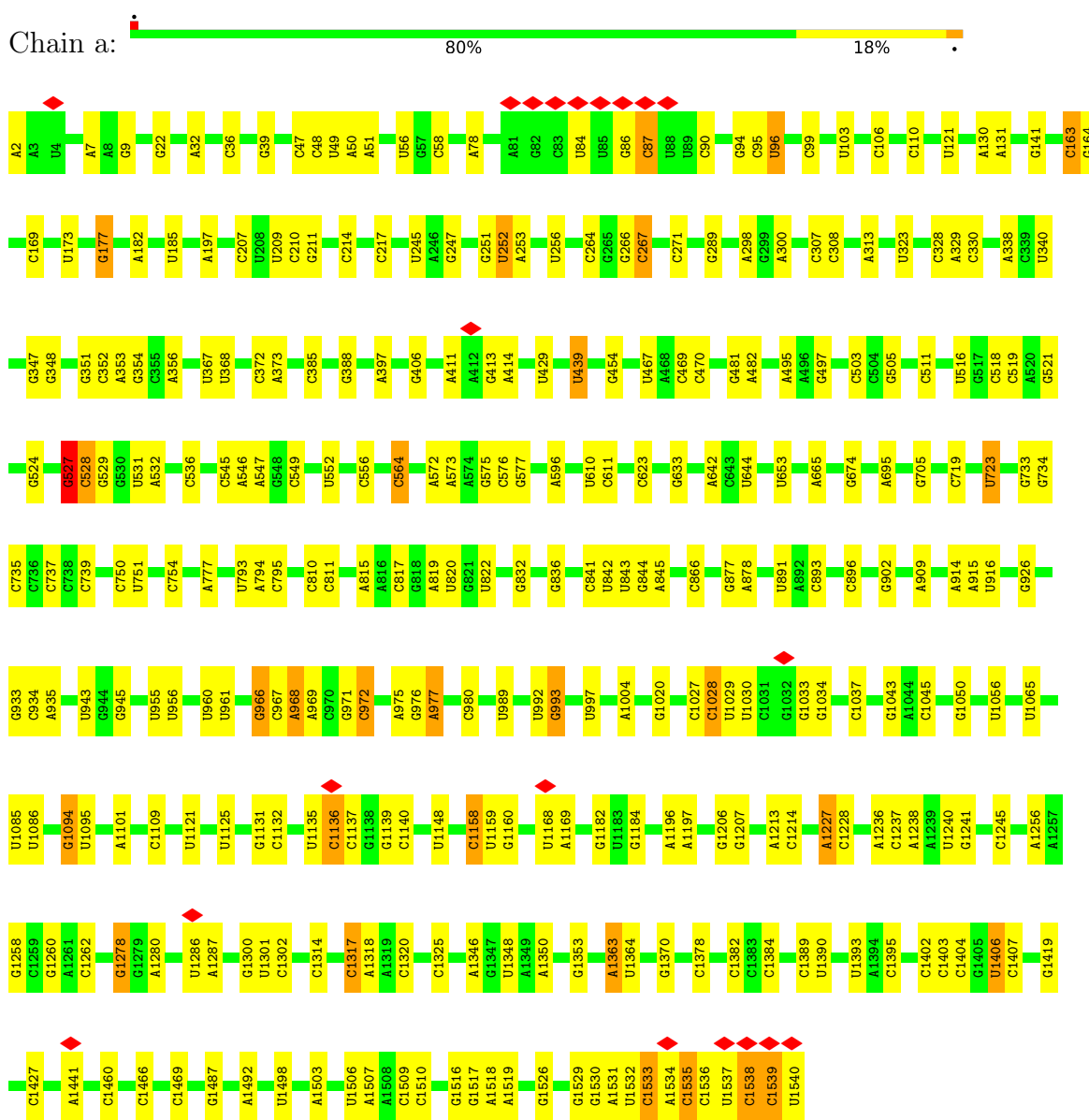
- Molecule 65 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
65	z	2	2	2	0

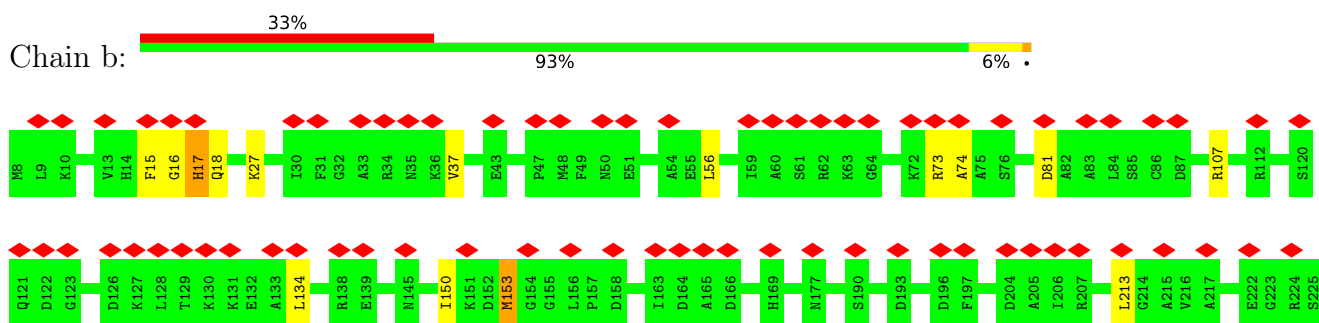
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

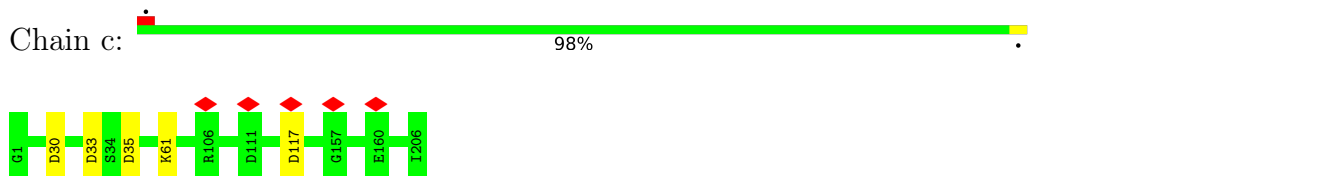
- Molecule 1: 16S ribosomal RNA



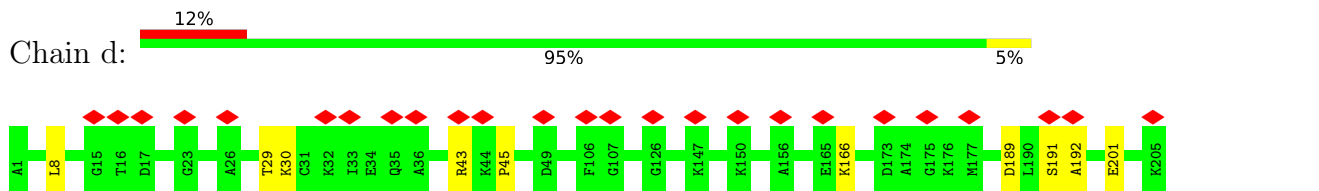
- Molecule 2: 30S ribosomal protein S2



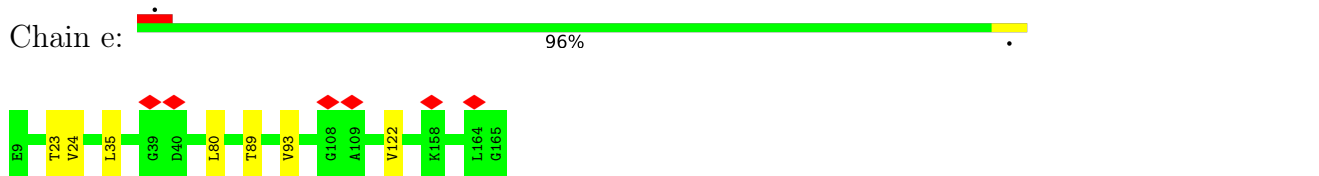
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4



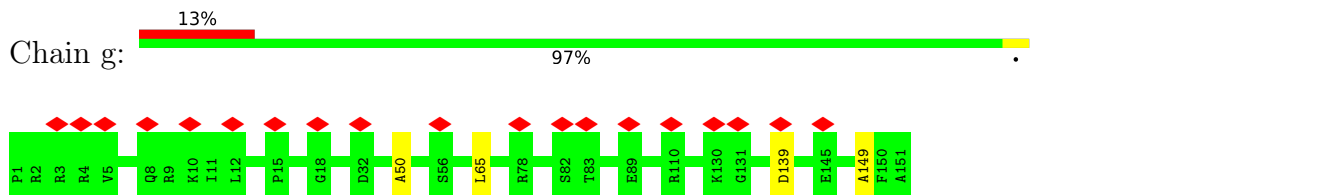
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

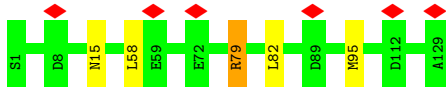


- Molecule 7: 30S ribosomal protein S7

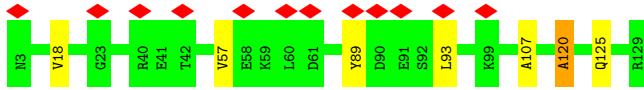
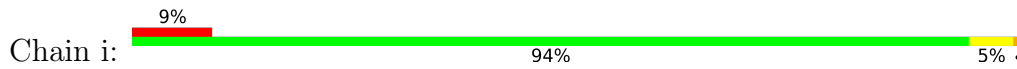


- Molecule 8: 30S ribosomal protein S8

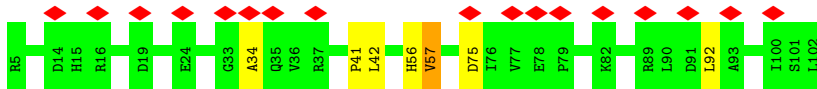
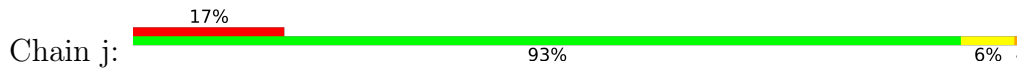




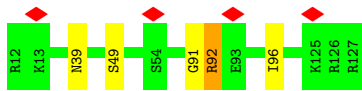
- Molecule 9: 30S ribosomal protein S9



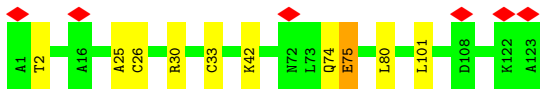
- Molecule 10: 30S ribosomal protein S10



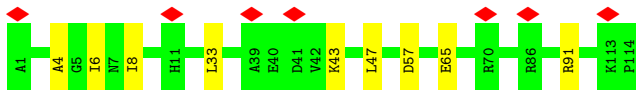
- Molecule 11: 30S ribosomal protein S11



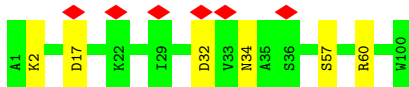
- Molecule 12: 30S ribosomal protein S12



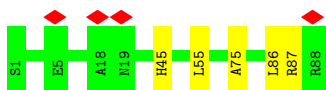
- Molecule 13: 30S ribosomal protein S13



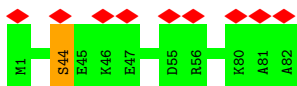
- Molecule 14: 30S ribosomal protein S14



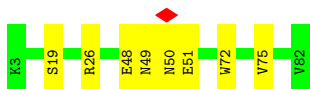
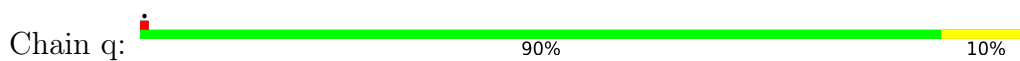
- Molecule 15: 30S ribosomal protein S15



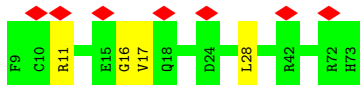
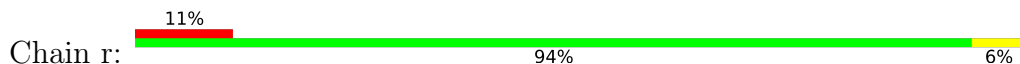
- Molecule 16: 30S ribosomal protein S16



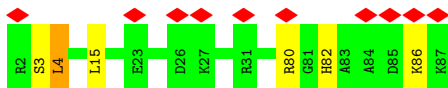
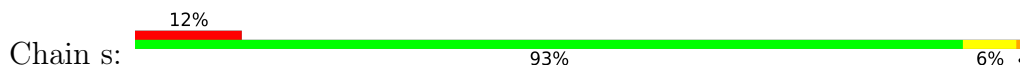
- Molecule 17: 30S ribosomal protein S17



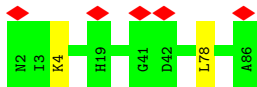
- Molecule 18: 30S ribosomal protein S18



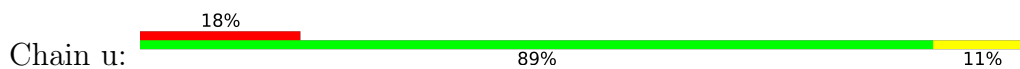
- Molecule 19: 30S ribosomal protein S19

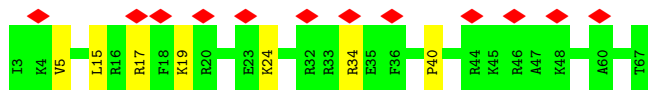


- Molecule 20: 30S ribosomal protein S20

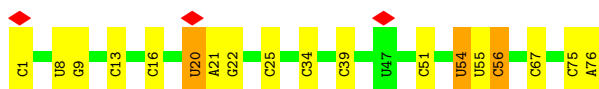
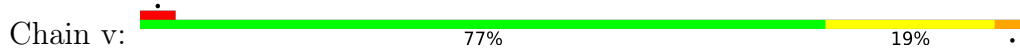


- Molecule 21: 30S ribosomal protein S21





- Molecule 22: fMet-tRNA_fMet



- Molecule 23: SECIS mRNA



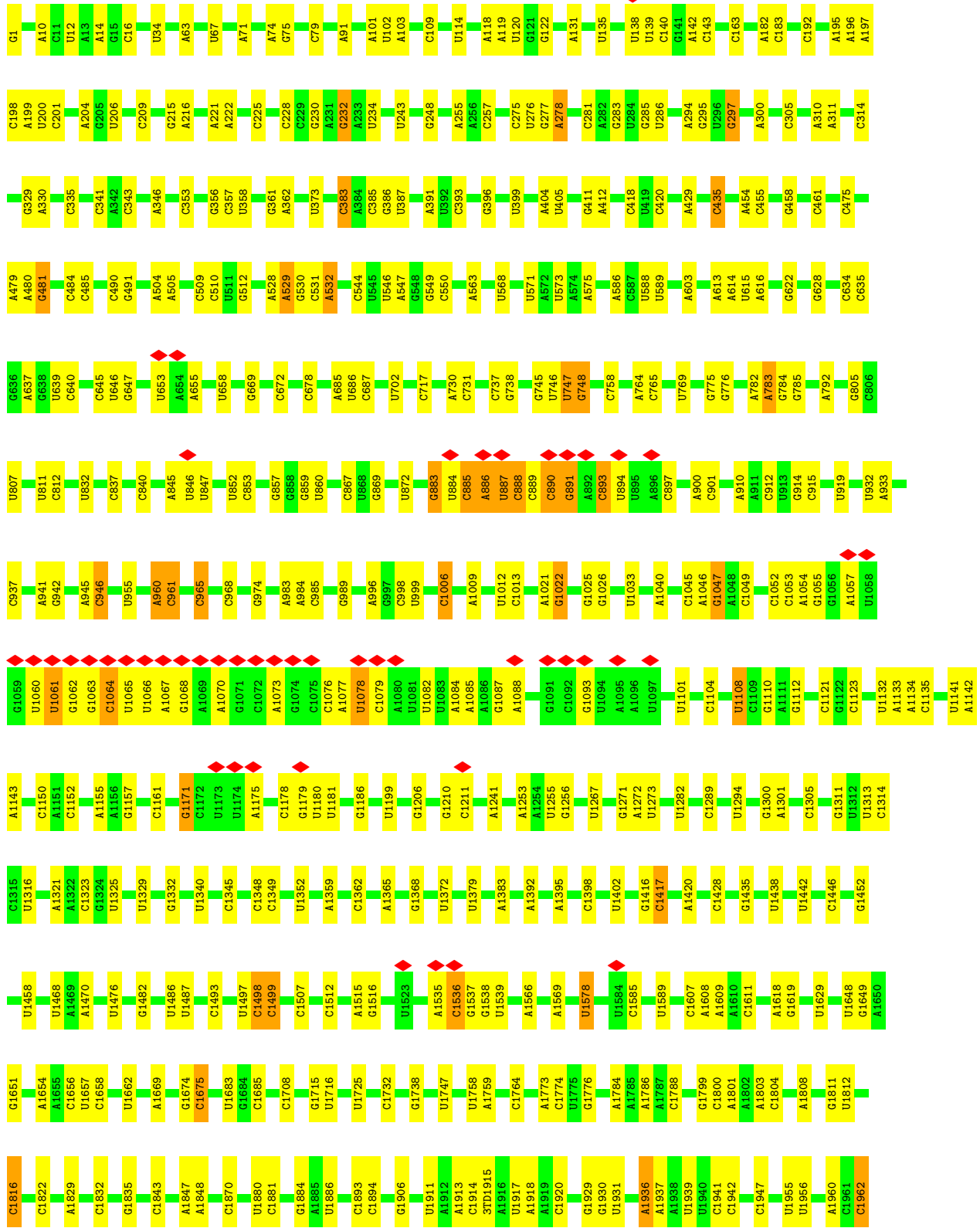
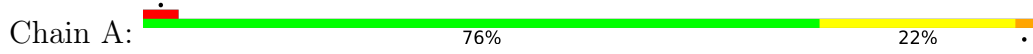
- Molecule 24: Sec-tRNA^{Sec}

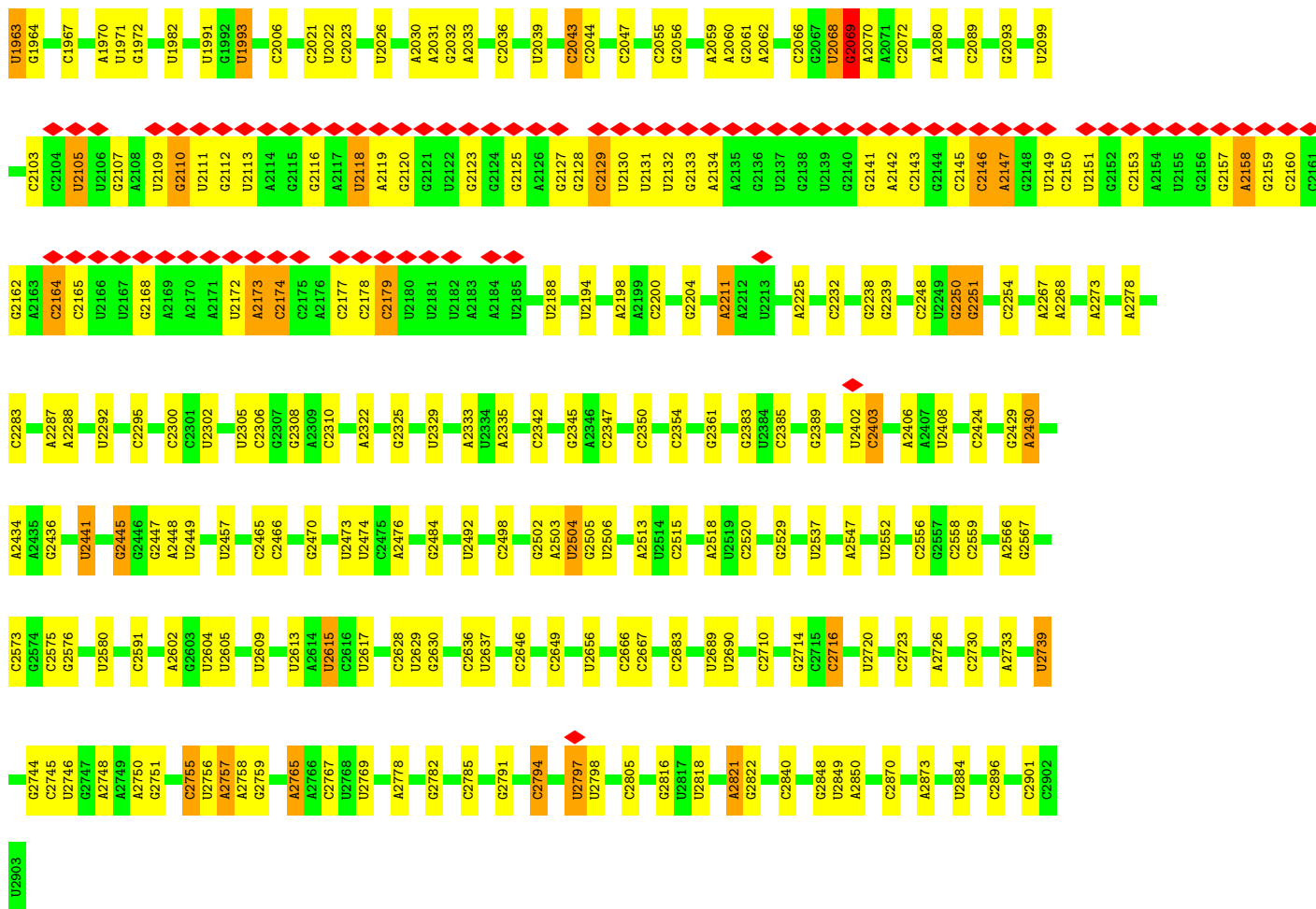


- Molecule 25: Selenocysteine-specific elongation factor

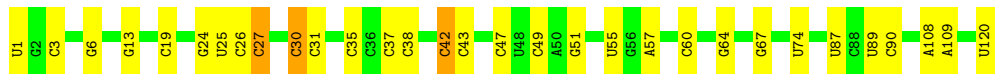


- Molecule 26: 23S ribosomal RNA





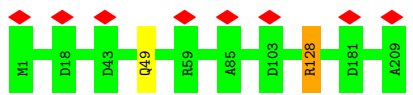
• Molecule 27: 5S ribosomal RNA



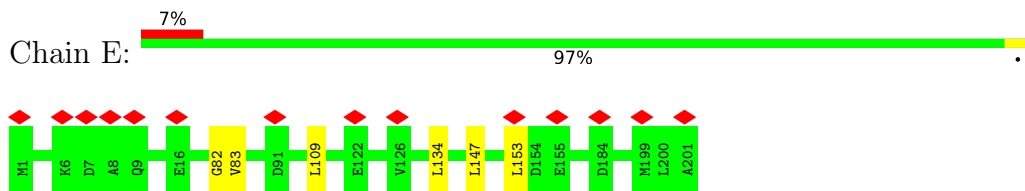
• Molecule 28: 50S ribosomal protein L2



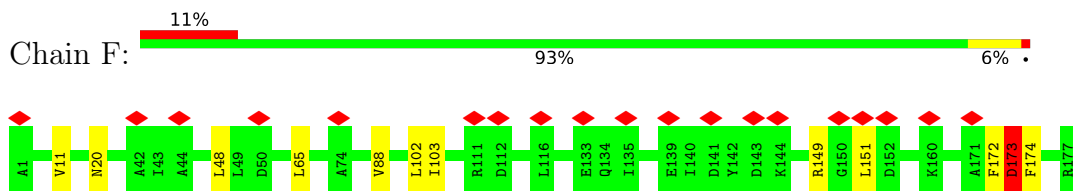
• Molecule 29: 50S ribosomal protein L3



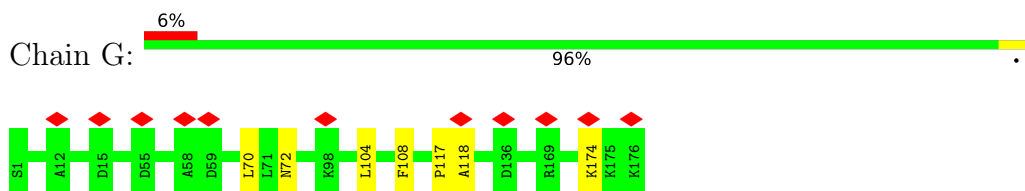
• Molecule 30: 50S ribosomal protein L4



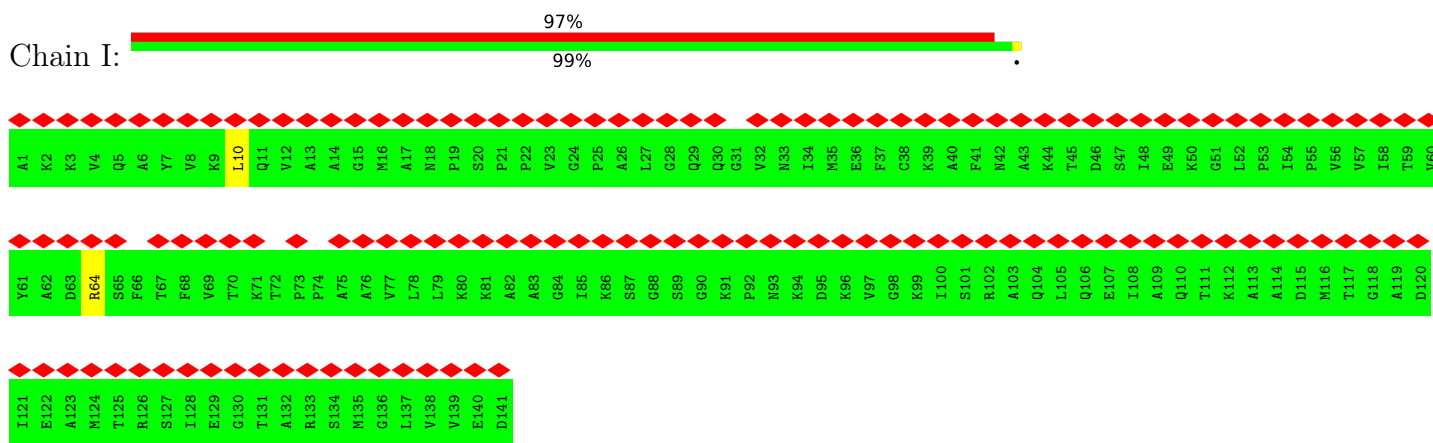
• Molecule 31: 50S ribosomal protein L5



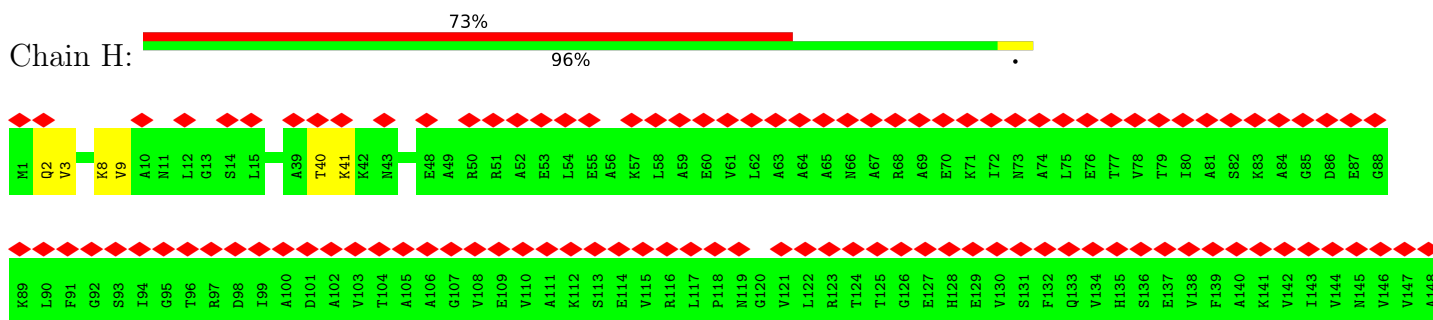
• Molecule 32: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L11

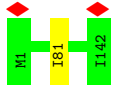


• Molecule 34: 50S ribosomal protein L9

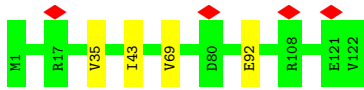




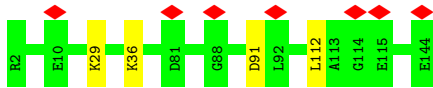
- Molecule 35: 50S ribosomal protein L13



- Molecule 36: 50S ribosomal protein L14



- Molecule 37: 50S ribosomal protein L15



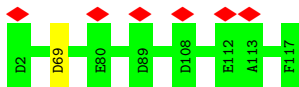
- Molecule 38: 50S ribosomal protein L16



- Molecule 39: 50S ribosomal protein L17



- Molecule 40: 50S ribosomal protein L18



- Molecule 41: 50S ribosomal protein L19

Chain P:  98%



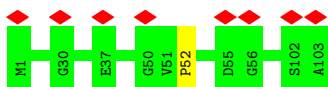
- Molecule 42: 50S ribosomal protein L20

Chain Q:  99%



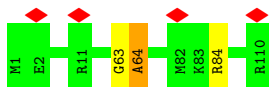
- Molecule 43: 50S ribosomal protein L21

Chain R:  99%



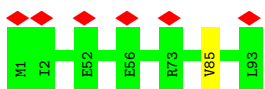
- Molecule 44: 50S ribosomal protein L22

Chain S:  97%

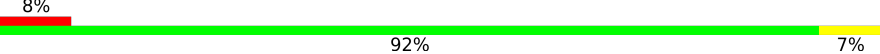


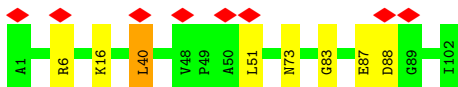
- Molecule 45: 50S ribosomal protein L23

Chain T:  99%



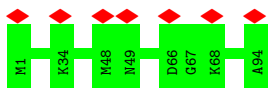
- Molecule 46: 50S ribosomal protein L24

Chain U:  92% 7%



- Molecule 47: 50S ribosomal protein L25

Chain V:  100%



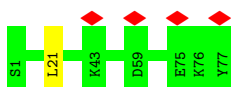
- Molecule 48: 50S ribosomal protein L27

Chain W: 100%



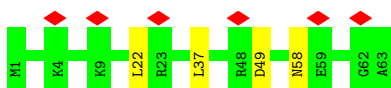
- Molecule 49: 50S ribosomal protein L28

Chain X: 99%



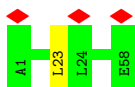
- Molecule 50: 50S ribosomal protein L29

Chain Y: 94%



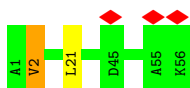
- Molecule 51: 50S ribosomal protein L30

Chain Z: 98%



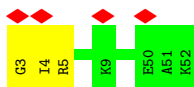
- Molecule 52: 50S ribosomal protein L32

Chain 0: 96%



- Molecule 53: 50S ribosomal protein L33

Chain 1: 94%



- Molecule 54: 50S ribosomal protein L34

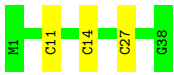
Chain 2: 100%



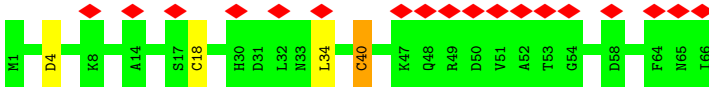
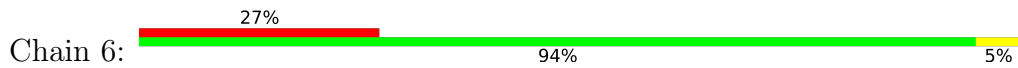
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 57: 50S ribosomal protein L31



- Molecule 58: CCA 3' end of E-site tRNA^{Sec} (low occupancy)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159729	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	4.579	Depositor
Minimum map value	-2.360	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.280	Depositor
Recommended contour level	0.56	Depositor
Map size (\AA)	315.52, 315.52, 315.52	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.16, 1.16, 1.16	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 6IA, 2MA, 4OC, SEC, GNP, OMU, ZN, 5MU, 5MC, OMG, MA6, G7M, PSU, OMC, FME, 6MZ, MG, 4SU, UR3, CL, 2MG, H2U, 1MG

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	0.58	2/36701 (0.0%)	1.18	255/57246 (0.4%)
2	b	0.51	2/1736 (0.1%)	0.90	6/2338 (0.3%)
3	c	0.44	0/1652	0.82	4/2225 (0.2%)
4	d	0.49	0/1665	0.87	2/2227 (0.1%)
5	e	0.51	0/1170	0.88	2/1573 (0.1%)
6	f	0.56	0/836	0.87	2/1128 (0.2%)
7	g	0.48	0/1196	0.81	2/1602 (0.1%)
8	h	0.46	0/989	0.86	5/1326 (0.4%)
9	i	0.55	0/1034	0.97	4/1375 (0.3%)
10	j	0.50	0/797	0.95	1/1077 (0.1%)
11	k	0.53	0/886	0.88	2/1195 (0.2%)
12	l	0.64	2/969 (0.2%)	0.93	3/1300 (0.2%)
13	m	0.52	0/893	0.98	5/1193 (0.4%)
14	n	0.53	0/806	0.90	3/1074 (0.3%)
15	o	0.44	0/722	0.81	3/964 (0.3%)
16	p	0.49	0/659	0.77	0/884
17	q	0.60	0/658	1.07	3/881 (0.3%)
18	r	0.42	0/512	0.82	2/689 (0.3%)
19	s	0.45	0/703	0.89	2/944 (0.2%)
20	t	0.47	0/671	0.81	2/888 (0.2%)
21	u	0.53	0/501	1.06	2/668 (0.3%)
22	v	0.58	1/1745 (0.1%)	1.18	13/2716 (0.5%)
23	x	0.76	2/1145 (0.2%)	1.63	31/1781 (1.7%)
24	y	0.53	1/2168 (0.0%)	1.27	26/3375 (0.8%)
25	z	0.46	1/4952 (0.0%)	0.89	13/6712 (0.2%)
26	A	0.62	10/69240 (0.0%)	1.22	593/108014 (0.5%)
27	B	0.58	1/2873 (0.0%)	1.28	30/4478 (0.7%)
28	C	0.50	1/2122 (0.0%)	0.81	3/2852 (0.1%)
29	D	0.49	0/1586	0.81	2/2134 (0.1%)
30	E	0.47	0/1571	0.81	4/2113 (0.2%)
31	F	0.61	1/1435 (0.1%)	1.00	9/1926 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	G	0.45	0/1343	0.79	2/1816 (0.1%)
33	I	0.40	0/1046	0.73	1/1410 (0.1%)
34	H	0.41	0/1122	0.72	0/1515
35	J	0.46	0/1152	0.72	0/1551
36	K	0.53	1/948 (0.1%)	0.85	1/1268 (0.1%)
37	L	0.42	0/1054	0.78	1/1403 (0.1%)
38	M	0.44	0/1093	0.78	0/1460
39	N	0.50	0/974	0.78	1/1301 (0.1%)
40	O	0.48	0/902	0.75	1/1209 (0.1%)
41	P	0.45	0/929	0.82	3/1242 (0.2%)
42	Q	0.50	0/960	0.68	1/1278 (0.1%)
43	R	0.47	0/829	0.77	0/1107
44	S	0.46	0/864	0.80	2/1156 (0.2%)
45	T	0.45	0/745	0.73	0/994
46	U	0.52	0/788	0.90	3/1051 (0.3%)
47	V	0.47	0/766	0.71	0/1025
48	W	0.46	0/582	0.75	0/769
49	X	0.42	0/635	0.77	1/848 (0.1%)
50	Y	0.52	0/510	0.97	2/677 (0.3%)
51	Z	0.41	0/453	0.78	1/605 (0.2%)
52	0	0.51	1/450 (0.2%)	0.93	2/599 (0.3%)
53	1	0.42	0/417	0.85	1/554 (0.2%)
54	2	0.45	0/380	0.73	0/498
55	3	0.43	0/513	0.73	0/676
56	4	0.75	2/303 (0.7%)	0.93	2/397 (0.5%)
57	6	0.47	0/532	1.00	4/709 (0.6%)
58	w	0.39	0/68	0.94	0/103
All	All	0.57	28/164951 (0.0%)	1.12	1063/246119 (0.4%)

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
1	a	2	0
2	b	0	2
4	d	0	1
6	f	0	1
10	j	0	3
11	k	0	2
12	l	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	p	0	1
17	q	0	2
21	u	0	1
25	z	0	1
26	A	2	0
28	C	0	1
30	E	0	1
31	F	0	2
32	G	0	2
34	H	0	3
44	S	0	1
46	U	0	2
53	1	0	1
55	3	0	1
All	All	4	30

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	1	U	OP3-P	-10.85	1.48	1.61
24	y	1	G	OP3-P	-10.68	1.48	1.61
22	v	1	C	OP3-P	-10.68	1.48	1.61
26	A	1	G	OP3-P	-10.59	1.48	1.61
1	a	2	A	OP3-P	-10.59	1.48	1.61
23	x	87	A	OP3-P	-10.57	1.48	1.61
26	A	571	U	C4-O4	8.50	1.30	1.23
12	l	26	CYS	CB-SG	-8.20	1.68	1.82
1	a	723	U	C4-O4	-7.13	1.18	1.23
31	F	11	VAL	CB-CG1	-7.10	1.38	1.52
26	A	1963	U	C2-O2	-7.07	1.16	1.22
56	4	27	CYS	CB-SG	6.97	1.94	1.82
56	4	11	CYS	CB-SG	6.63	1.93	1.82
52	0	2	VAL	CB-CG2	-6.37	1.39	1.52
36	K	69	VAL	CB-CG1	-5.79	1.40	1.52
2	b	27	LYS	C-N	5.74	1.45	1.34
26	A	2173	A	N9-C4	5.71	1.41	1.37
26	A	278	A	N9-C4	5.58	1.41	1.37
25	z	322	VAL	CB-CG2	-5.54	1.41	1.52
26	A	1936	A	C2-N3	-5.48	1.28	1.33
2	b	37	VAL	CB-CG2	-5.46	1.41	1.52
23	x	128	C	O3'-P	5.46	1.67	1.61
26	A	2211	A	N9-C4	5.26	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	356	G	N7-C5	-5.25	1.36	1.39
12	l	33	CYS	CB-SG	-5.13	1.73	1.81
26	A	571	U	C5-C6	-5.13	1.29	1.34
26	A	1936	A	N3-C4	-5.04	1.31	1.34
28	C	30	ALA	C-N	5.01	1.43	1.34

All (1063) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	968	A	N1-C6-N6	-23.76	104.34	118.60
1	a	1158	C	N1-C2-O2	18.14	129.78	118.90
26	A	2059	A	N1-C2-N3	-17.84	120.38	129.30
1	a	1158	C	N3-C2-O2	-17.55	109.61	121.90
1	a	529	G	C5-C6-O6	-15.48	119.31	128.60
1	a	968	A	C5-C6-N6	15.15	135.82	123.70
26	A	890	C	C2-N1-C1'	14.01	134.21	118.80
26	A	887	U	N1-C2-O2	13.17	132.02	122.80
26	A	887	U	N3-C2-O2	-13.10	113.03	122.20
26	A	2059	A	C6-N1-C2	12.82	126.29	118.60
1	a	207	C	N3-C2-O2	-12.33	113.27	121.90
26	A	1963	U	N1-C2-N3	12.26	122.26	114.90
26	A	1941	C	N1-C2-O2	12.21	126.23	118.90
1	a	1158	C	C6-N1-C2	-12.03	115.49	120.30
26	A	890	C	C6-N1-C1'	-12.01	106.39	120.80
26	A	1313	U	N1-C2-O2	12.01	131.21	122.80
1	a	529	G	N1-C6-O6	12.00	127.10	119.90
26	A	890	C	N1-C2-O2	11.90	126.04	118.90
1	a	968	A	N9-C4-C5	11.84	110.54	105.80
26	A	1313	U	N3-C2-O2	-11.44	114.19	122.20
31	F	151	LEU	CB-CG-CD2	-11.43	91.56	111.00
26	A	888	C	C6-N1-C2	-11.15	115.84	120.30
26	A	886	A	P-O3'-C3'	11.10	133.02	119.70
25	z	373	LEU	CB-CG-CD1	-11.04	92.23	111.00
26	A	1963	U	C6-N1-C2	-10.93	114.44	121.00
17	q	26	ARG	NE-CZ-NH2	10.89	125.75	120.30
1	a	207	C	N1-C2-O2	10.89	125.43	118.90
26	A	2179	C	N3-C2-O2	-10.84	114.31	121.90
26	A	894	U	C5-C6-N1	10.75	128.07	122.70
26	A	961	C	O5'-P-OP1	-10.64	96.12	105.70
1	a	968	A	C6-C5-N7	10.64	139.75	132.30
26	A	1498	C	C2-N1-C1'	10.43	130.27	118.80
1	a	1027	C	N1-C2-O2	10.39	125.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2805	C	C5-C6-N1	10.36	126.18	121.00
25	z	398	LEU	CB-CG-CD2	-10.30	93.50	111.00
26	A	1941	C	N3-C2-O2	-10.17	114.78	121.90
26	A	893	C	C6-N1-C2	-10.16	116.24	120.30
23	x	114	C	N1-C2-O2	10.16	124.99	118.90
1	a	307	C	N1-C2-O2	10.07	124.94	118.90
27	B	60	C	C5-C6-N1	9.96	125.98	121.00
26	A	1348	C	N1-C2-O2	9.94	124.86	118.90
26	A	2143	C	C6-N1-C2	-9.93	116.33	120.30
26	A	2473	U	N1-C2-O2	9.91	129.74	122.80
17	q	26	ARG	NE-CZ-NH1	-9.90	115.35	120.30
26	A	2805	C	C6-N1-C2	-9.75	116.40	120.30
26	A	893	C	C5-C6-N1	9.69	125.85	121.00
23	x	131	C	C6-N1-C2	-9.60	116.46	120.30
26	A	2757	A	C6-N1-C2	9.59	124.35	118.60
26	A	640	C	C5-C6-N1	9.45	125.72	121.00
26	A	2683	C	N1-C2-O2	9.44	124.56	118.90
1	a	1314	C	O5'-P-OP2	-9.41	97.23	105.70
26	A	2473	U	N3-C2-O2	-9.41	115.61	122.20
1	a	556	C	C5-C6-N1	9.39	125.69	121.00
26	A	571	U	O4'-C1'-N1	-9.32	100.74	108.20
26	A	341	C	C6-N1-C2	-9.30	116.58	120.30
26	A	1956	U	N1-C2-O2	9.26	129.28	122.80
26	A	901	C	N1-C2-O2	9.23	124.44	118.90
26	A	550	C	C5-C6-N1	9.22	125.61	121.00
1	a	207	C	C6-N1-C2	-9.21	116.62	120.30
1	a	529	G	N9-C4-C5	-9.20	101.72	105.40
1	a	90	C	C6-N1-C2	-9.16	116.63	120.30
26	A	1936	A	N1-C2-N3	9.14	133.87	129.30
27	B	30	C	C6-N1-C2	-9.12	116.65	120.30
49	X	21	LEU	CA-CB-CG	9.11	136.25	115.30
26	A	2179	C	N1-C2-O2	9.10	124.36	118.90
1	a	1158	C	C2-N1-C1'	9.05	128.76	118.80
26	A	528	A	C8-N9-C4	-9.05	102.18	105.80
26	A	1313	U	C2-N1-C1'	9.03	128.53	117.70
1	a	968	A	O4'-C1'-N9	9.02	115.42	108.20
1	a	529	G	C4-C5-N7	8.94	114.37	110.80
32	G	104	LEU	CA-CB-CG	8.90	135.77	115.30
26	A	278	A	C2-N3-C4	8.82	115.01	110.60
26	A	571	U	C5-C4-O4	8.81	131.19	125.90
1	a	87	C	C5-C6-N1	8.80	125.40	121.00
1	a	968	A	C4-C5-N7	-8.78	106.31	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	42	C	N1-C2-O2	8.77	124.16	118.90
26	A	639	U	C5-C6-N1	8.74	127.07	122.70
25	z	79	LEU	CA-CB-CG	8.72	135.36	115.30
27	B	60	C	C6-N1-C2	-8.70	116.82	120.30
1	a	1393	U	N3-C2-O2	-8.68	116.12	122.20
1	a	1538	C	C6-N1-C2	-8.67	116.83	120.30
26	A	2072	C	C6-N1-C2	-8.61	116.86	120.30
23	x	114	C	C2-N1-C1'	8.60	128.26	118.80
26	A	183	C	N3-C2-O2	-8.53	115.93	121.90
26	A	2150	C	C6-N1-C2	-8.51	116.90	120.30
26	A	984	A	C2-N3-C4	8.51	114.85	110.60
1	a	1245	C	C5-C6-N1	8.49	125.25	121.00
24	y	40	C	C6-N1-C2	-8.47	116.91	120.30
26	A	550	C	C6-N1-C2	-8.45	116.92	120.30
26	A	847	U	N3-C2-O2	-8.44	116.30	122.20
26	A	283	G	N3-C2-N2	-8.40	114.02	119.90
1	a	1317	C	N1-C2-O2	8.38	123.93	118.90
1	a	307	C	N3-C2-O2	-8.36	116.05	121.90
21	u	15	LEU	CA-CB-CG	8.35	134.50	115.30
26	A	885	C	N1-C2-O2	-8.34	113.90	118.90
31	F	174	PHE	CB-CG-CD1	8.33	126.63	120.80
1	a	556	C	C6-N1-C2	-8.32	116.97	120.30
26	A	1348	C	N3-C2-O2	-8.31	116.08	121.90
26	A	2043	C	C6-N1-C2	-8.29	116.98	120.30
26	A	1941	C	C2-N1-C1'	8.26	127.89	118.80
26	A	2174	C	N1-C2-O2	8.26	123.86	118.90
26	A	968	C	C6-N1-C2	-8.20	117.02	120.30
26	A	2211	A	C2-N3-C4	8.19	114.70	110.60
26	A	2637	U	C5-C6-N1	8.18	126.79	122.70
26	A	2043	C	C5-C6-N1	8.16	125.08	121.00
25	z	427	LEU	CB-CG-CD2	-8.16	97.12	111.00
26	A	894	U	C6-N1-C2	-8.16	116.11	121.00
26	A	837	C	N3-C2-O2	-8.14	116.20	121.90
26	A	1305	C	C6-N1-C2	-8.14	117.04	120.30
26	A	2646	C	C5-C6-N1	8.12	125.06	121.00
27	B	26	C	N1-C2-O2	8.12	123.77	118.90
1	a	723	U	N3-C4-C5	8.11	119.47	114.60
1	a	1537	U	C2-N1-C1'	8.11	127.43	117.70
1	a	968	A	N9-C1'-C2'	-8.11	103.08	112.00
26	A	183	C	C6-N1-C2	-8.08	117.07	120.30
26	A	2105	U	C5-C6-N1	8.07	126.73	122.70
26	A	2302	U	N3-C2-O2	-8.07	116.55	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	217	C	C6-N1-C2	-8.05	117.08	120.30
1	a	1537	U	N3-C2-O2	-8.04	116.57	122.20
1	a	909	A	O5'-P-OP1	-8.03	98.47	105.70
26	A	343	C	C6-N1-C2	-8.03	117.09	120.30
26	A	2173	A	C2-N3-C4	7.99	114.59	110.60
53	1	5	ARG	NE-CZ-NH1	-7.99	116.30	120.30
26	A	234	U	N3-C2-O2	-7.98	116.62	122.20
26	A	1507	C	C6-N1-C2	-7.98	117.11	120.30
26	A	1314	C	C6-N1-C2	-7.96	117.12	120.30
1	a	217	C	C5-C6-N1	7.96	124.98	121.00
26	A	887	U	C2-N1-C1'	7.96	127.25	117.70
26	A	634	C	C6-N1-C2	-7.96	117.12	120.30
26	A	2188	U	C5-C6-N1	7.95	126.68	122.70
51	Z	23	LEU	CB-CG-CD1	-7.95	97.49	111.00
1	a	1245	C	C6-N1-C2	-7.92	117.13	120.30
1	a	90	C	C5-C6-N1	7.85	124.92	121.00
26	A	198	C	C5-C6-N1	7.85	124.92	121.00
26	A	1267	U	N1-C2-O2	7.84	128.29	122.80
1	a	413	G	C5-C6-O6	-7.84	123.90	128.60
1	a	96	U	C5-C6-N1	7.84	126.62	122.70
26	A	1052	C	C5-C6-N1	7.83	124.91	121.00
26	A	571	U	N3-C4-C5	-7.82	109.91	114.60
26	A	1669	A	C2-N3-C4	7.79	114.49	110.60
26	A	2473	U	C2-N1-C1'	7.79	127.04	117.70
26	A	2646	C	C6-N1-C2	-7.78	117.19	120.30
26	A	1956	U	N3-C2-O2	-7.78	116.75	122.20
23	x	127	U	P-O3'-C3'	7.76	129.01	119.70
26	A	358	U	N3-C2-O2	-7.75	116.77	122.20
13	m	8	ILE	CG1-CB-CG2	-7.74	94.37	111.40
26	A	1022	G	N1-C6-O6	-7.74	115.26	119.90
26	A	1499	C	C2-N1-C1'	7.74	127.31	118.80
12	l	75	GLU	N-CA-CB	-7.72	96.71	110.60
26	A	640	C	C6-N1-C2	-7.72	117.21	120.30
56	4	14	CYS	CA-CB-SG	7.71	127.89	114.00
24	y	16	C	C6-N1-C2	-7.70	117.22	120.30
26	A	2292	U	C5-C6-N1	7.70	126.55	122.70
26	A	1063	G	N7-C8-N9	7.70	116.95	113.10
26	A	2617	U	N3-C2-O2	-7.69	116.82	122.20
26	A	2683	C	N3-C2-O2	-7.68	116.52	121.90
26	A	2129	C	O5'-P-OP1	7.68	119.91	110.70
26	A	1963	U	C6-N1-C1'	7.67	131.94	121.20
26	A	528	A	N7-C8-N9	7.67	117.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	32	C	C5-C6-N1	7.67	124.83	121.00
1	a	1537	U	N1-C2-O2	7.67	128.17	122.80
26	A	341	C	C5-C6-N1	7.66	124.83	121.00
1	a	87	C	C6-N1-C2	-7.66	117.23	120.30
26	A	1683	U	C5-C6-N1	7.64	126.52	122.70
26	A	1052	C	C6-N1-C2	-7.64	117.25	120.30
26	A	1920	C	C5-C6-N1	7.63	124.82	121.00
26	A	109	C	C5-C6-N1	7.63	124.81	121.00
27	B	120	U	N3-C2-O2	-7.63	116.86	122.20
1	a	1037	C	C6-N1-C2	-7.57	117.27	120.30
57	6	18	CYS	CA-CB-SG	-7.57	100.38	114.00
23	x	96	C	C6-N1-C2	-7.57	117.27	120.30
26	A	2026	U	C5-C6-N1	7.57	126.48	122.70
26	A	1171	G	C8-N9-C4	-7.55	103.38	106.40
1	a	330	C	N1-C2-O2	7.54	123.42	118.90
26	A	343	C	N1-C2-O2	7.53	123.42	118.90
24	y	40	C	C5-C6-N1	7.52	124.76	121.00
31	F	151	LEU	CB-CG-CD1	7.52	123.79	111.00
26	A	1362	C	C5-C6-N1	7.52	124.76	121.00
26	A	2666	C	N1-C2-O2	7.51	123.41	118.90
26	A	2174	C	N3-C2-O2	-7.51	116.64	121.90
27	B	47	C	N1-C2-O2	7.50	123.40	118.90
1	a	1389	C	C2-N1-C1'	7.49	127.04	118.80
2	b	150	ILE	CG1-CB-CG2	-7.49	94.93	111.40
4	d	189	ASP	CB-CG-OD1	7.46	125.01	118.30
1	a	177	G	C2-N3-C4	7.43	115.61	111.90
26	A	1362	C	C6-N1-C2	-7.43	117.33	120.30
1	a	735	C	C6-N1-C2	-7.43	117.33	120.30
26	A	2305	U	C6-N1-C2	7.41	125.44	121.00
23	x	117	C	O5'-P-OP2	7.41	119.59	110.70
26	A	783	A	C2-N3-C4	7.40	114.30	110.60
26	A	1941	C	C6-N1-C2	-7.39	117.34	120.30
1	a	78	A	N7-C8-N9	7.38	117.49	113.80
26	A	890	C	OP1-P-O3'	7.38	121.43	105.20
26	A	1708	C	C6-N1-C2	-7.38	117.35	120.30
26	A	901	C	N3-C2-O2	-7.36	116.75	121.90
26	A	357	C	C6-N1-C2	-7.36	117.36	120.30
1	a	989	U	N3-C2-O2	-7.35	117.06	122.20
26	A	1435	G	C8-N9-C4	-7.35	103.46	106.40
26	A	183	C	N1-C2-O2	7.34	123.31	118.90
26	A	1021	A	C2-N3-C4	7.34	114.27	110.60
3	c	35	ASP	CB-CG-OD1	7.33	124.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	837	C	N1-C2-O2	7.33	123.30	118.90
26	A	1063	G	C8-N9-C4	-7.33	103.47	106.40
25	z	359	LEU	CB-CG-CD2	7.30	123.41	111.00
26	A	2896	C	C5-C6-N1	7.30	124.65	121.00
26	A	2656	U	C5-C6-N1	7.30	126.35	122.70
1	a	1027	C	N3-C2-O2	-7.29	116.80	121.90
26	A	888	C	N3-C2-O2	-7.29	116.80	121.90
1	a	1109	C	N1-C2-O2	7.27	123.26	118.90
26	A	2250	G	C8-N9-C4	-7.27	103.49	106.40
26	A	2723	C	C5-C6-N1	7.26	124.63	121.00
26	A	1498	C	C5-C6-N1	7.25	124.62	121.00
12	l	80	LEU	CA-CB-CG	7.25	131.97	115.30
25	z	26	ASP	CB-CG-OD1	7.24	124.81	118.30
50	Y	49	ASP	CB-CG-OD1	7.21	124.79	118.30
26	A	234	U	N1-C2-O2	7.21	127.85	122.80
1	a	1406	U	N3-C2-O2	-7.21	117.16	122.20
6	f	98	GLU	N-CA-CB	-7.19	97.66	110.60
26	A	1186	G	O5'-P-OP1	-7.18	99.23	105.70
1	a	1045	C	C5-C6-N1	7.18	124.59	121.00
26	A	669	G	N3-C4-N9	7.17	130.30	126.00
26	A	847	U	N1-C2-O2	7.17	127.81	122.80
26	A	2151	U	C5-C6-N1	7.16	126.28	122.70
26	A	356	G	N7-C8-N9	7.15	116.68	113.10
26	A	358	U	C5-C6-N1	7.15	126.28	122.70
26	A	1708	C	C5-C6-N1	7.15	124.58	121.00
26	A	1920	C	C6-N1-C2	-7.15	117.44	120.30
1	a	1382	C	N1-C2-O2	7.15	123.19	118.90
26	A	669	G	N3-C4-C5	-7.15	125.03	128.60
1	a	439	U	N3-C2-O2	-7.14	117.20	122.20
23	x	125	G	N9-C1'-C2'	-7.14	104.14	112.00
26	A	2179	C	C6-N1-C2	-7.14	117.44	120.30
26	A	2072	C	C5-C6-N1	7.14	124.57	121.00
26	A	1936	A	C2-N3-C4	-7.14	107.03	110.60
1	a	723	U	N3-C4-O4	-7.13	114.41	119.40
26	A	1498	C	C6-N1-C1'	-7.13	112.25	120.80
26	A	2757	A	N1-C2-N3	-7.11	125.74	129.30
1	a	1027	C	C5-C6-N1	7.11	124.56	121.00
27	B	26	C	N3-C2-O2	-7.11	116.92	121.90
26	A	634	C	C5-C6-N1	7.09	124.55	121.00
1	a	611	C	N1-C2-O2	7.09	123.15	118.90
1	a	1427	C	C6-N1-C2	-7.08	117.47	120.30
26	A	314	C	C5-C6-N1	7.08	124.54	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1150	C	C6-N1-C2	-7.08	117.47	120.30
26	A	305	C	C6-N1-C2	-7.07	117.47	120.30
26	A	2739	U	N3-C2-O2	-7.06	117.25	122.20
26	A	1267	U	N3-C2-O2	-7.06	117.26	122.20
1	a	968	A	C8-N9-C4	-7.06	102.98	105.80
26	A	1498	C	C6-N1-C2	-7.06	117.48	120.30
26	A	2723	C	C6-N1-C2	-7.05	117.48	120.30
26	A	891	G	C5-C6-O6	-7.05	124.37	128.60
1	a	1466	C	N1-C2-O2	7.05	123.13	118.90
3	c	33	ASP	CB-CG-OD1	7.04	124.64	118.30
26	A	890	C	C5-C6-N1	7.03	124.51	121.00
26	A	571	U	C5-C6-N1	-7.02	119.19	122.70
23	x	121	U	C2-N1-C1'	7.01	126.11	117.70
26	A	1321	A	C2-N3-C4	7.01	114.10	110.60
15	o	55	LEU	CA-CB-CG	7.00	131.41	115.30
1	a	90	C	N1-C2-O2	7.00	123.10	118.90
26	A	1435	G	N7-C8-N9	7.00	116.60	113.10
26	A	2006	C	C5-C6-N1	7.00	124.50	121.00
26	A	901	C	C2-N1-C1'	7.00	126.50	118.80
26	A	2840	C	C5-C6-N1	7.00	124.50	121.00
1	a	56	U	C5-C6-N1	6.99	126.20	122.70
26	A	901	C	C6-N1-C2	-6.99	117.50	120.30
27	B	27	C	N1-C2-O2	6.98	123.09	118.90
26	A	1963	U	N1-C2-O2	-6.98	117.92	122.80
1	a	503	C	C6-N1-C2	-6.97	117.51	120.30
27	B	37	C	N3-C2-O2	-6.97	117.02	121.90
1	a	1109	C	N3-C2-O2	-6.97	117.02	121.90
9	i	120	ALA	N-CA-CB	6.97	119.85	110.10
1	a	737	C	C6-N1-C2	-6.96	117.52	120.30
26	A	1499	C	N1-C2-O2	6.95	123.07	118.90
1	a	1389	C	C6-N1-C2	-6.95	117.52	120.30
26	A	358	U	C6-N1-C2	-6.95	116.83	121.00
26	A	361	G	N1-C6-O6	6.94	124.06	119.90
1	a	90	C	N3-C2-O2	-6.94	117.04	121.90
2	b	153	MET	CG-SD-CE	-6.93	89.11	100.20
26	A	2656	U	N1-C2-O2	6.93	127.65	122.80
37	L	112	LEU	CA-CB-CG	6.93	131.24	115.30
26	A	867	C	N1-C2-O2	6.93	123.06	118.90
26	A	243	U	N1-C2-O2	6.92	127.64	122.80
26	A	343	C	C2-N1-C1'	6.91	126.40	118.80
26	A	1963	U	C2-N3-C4	-6.91	122.86	127.00
26	A	1340	U	N3-C2-O2	-6.90	117.37	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	16	C	C5-C6-N1	6.90	124.45	121.00
26	A	2069	G7M	P-O3'-C3'	6.89	127.97	119.70
1	a	1403	C	N1-C2-O2	6.89	123.04	118.90
33	I	10	LEU	CA-CB-CG	6.89	131.15	115.30
26	A	314	C	C6-N1-C2	-6.89	117.55	120.30
1	a	1027	C	C6-N1-C2	-6.88	117.55	120.30
26	A	1314	C	C5-C6-N1	6.87	124.44	121.00
1	a	1404	C	C6-N1-C2	-6.87	117.55	120.30
1	a	58	C	C6-N1-C2	-6.87	117.55	120.30
1	a	1466	C	N3-C2-O2	-6.86	117.09	121.90
26	A	297	G	O5'-P-OP1	6.86	118.93	110.70
31	F	102	LEU	CA-CB-CG	6.86	131.08	115.30
1	a	1045	C	C6-N1-C2	-6.85	117.56	120.30
1	a	1469	C	N1-C2-O2	6.85	123.01	118.90
27	B	55	U	N3-C2-O2	-6.85	117.41	122.20
27	B	120	U	N1-C2-O2	6.83	127.58	122.80
26	A	1656	C	C5-C6-N1	6.81	124.41	121.00
1	a	968	A	N1-C2-N3	6.81	132.71	129.30
26	A	2110	G	C5-C6-O6	6.81	132.68	128.60
24	y	32	C	C6-N1-C2	-6.79	117.58	120.30
27	B	37	C	N1-C2-O2	6.78	122.97	118.90
26	A	1294	U	N3-C2-O2	-6.78	117.46	122.20
1	a	980	C	N1-C2-O2	6.76	122.96	118.90
25	z	49	ASP	CB-CG-OD1	6.76	124.39	118.30
26	A	2066	C	C6-N1-C2	-6.75	117.60	120.30
1	a	1389	C	C5-C6-N1	6.75	124.38	121.00
27	B	47	C	N3-C2-O2	-6.75	117.18	121.90
26	A	669	G	C2-N3-C4	6.75	115.27	111.90
26	A	2466	C	O5'-P-OP1	-6.75	99.63	105.70
1	a	413	G	C8-N9-C4	6.74	109.10	106.40
22	v	1	C	N1-C2-O2	6.74	122.94	118.90
1	a	977	A	C2-N3-C4	6.74	113.97	110.60
26	A	2066	C	C5-C6-N1	6.73	124.37	121.00
26	A	885	C	N3-C4-N4	6.73	122.71	118.00
21	u	5	VAL	CG1-CB-CG2	-6.73	100.14	110.90
26	A	1507	C	C5-C6-N1	6.73	124.36	121.00
1	a	207	C	C2-N1-C1'	6.72	126.19	118.80
26	A	1348	C	C6-N1-C2	-6.72	117.61	120.30
1	a	1406	U	N1-C2-O2	6.71	127.50	122.80
1	a	610	U	N3-C2-O2	-6.71	117.50	122.20
31	F	174	PHE	CB-CG-CD2	-6.70	116.11	120.80
26	A	232	G	C8-N9-C4	-6.69	103.72	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	571	U	C4-C5-C6	6.68	123.71	119.70
26	A	889	C	C2-N3-C4	6.68	123.24	119.90
26	A	2666	C	N3-C2-O2	-6.68	117.22	121.90
1	a	1533	C	C6-N1-C2	-6.68	117.63	120.30
1	a	1086	U	N3-C2-O2	-6.67	117.53	122.20
26	A	1774	C	C6-N1-C2	-6.67	117.63	120.30
26	A	1305	C	C5-C6-N1	6.67	124.33	121.00
3	c	117	ASP	CB-CG-OD1	6.64	124.28	118.30
7	g	139	ASP	CB-CG-OD1	6.64	124.28	118.30
1	a	439	U	N1-C2-O2	6.63	127.44	122.80
26	A	2072	C	O4'-C1'-N1	6.63	113.50	108.20
1	a	1056	U	N3-C2-O2	-6.63	117.56	122.20
26	A	399	U	N3-C2-O2	-6.62	117.57	122.20
26	A	1716	U	N1-C2-O2	6.62	127.43	122.80
23	x	114	C	N3-C2-O2	-6.62	117.27	121.90
26	A	589	U	C5-C6-N1	6.61	126.00	122.70
26	A	140	C	C6-N1-C2	-6.59	117.66	120.30
6	f	72	ASP	CB-CG-OD1	6.59	124.23	118.30
1	a	1037	C	C5-C6-N1	6.58	124.29	121.00
26	A	1314	C	C2-N1-C1'	6.58	126.04	118.80
26	A	1442	U	C5-C6-N1	6.57	125.99	122.70
26	A	1061	U	OP2-P-O3'	6.57	119.65	105.20
1	a	549	C	C5-C6-N1	6.56	124.28	121.00
13	m	57	ASP	CB-CG-OD1	6.55	124.20	118.30
1	a	413	G	N9-C4-C5	-6.55	102.78	105.40
19	s	4	LEU	CB-CG-CD1	-6.54	99.87	111.00
1	a	564	C	N1-C2-O2	6.53	122.82	118.90
26	A	283	G	C6-N1-C2	-6.53	121.18	125.10
57	6	34	LEU	CB-CG-CD1	-6.53	99.90	111.00
1	a	527	G7M	P-O3'-C3'	6.53	127.53	119.70
26	A	2617	U	N1-C2-O2	6.52	127.37	122.80
10	j	75	ASP	CB-CG-OD1	6.52	124.17	118.30
1	a	1240	U	C4-C5-C6	6.51	123.61	119.70
26	A	198	C	C6-N1-C2	-6.51	117.70	120.30
1	a	989	U	N1-C2-O2	6.51	127.36	122.80
26	A	143	C	C6-N1-C2	-6.50	117.70	120.30
1	a	1539	C	N1-C2-O2	-6.50	115.00	118.90
26	A	635	C	C6-N1-C2	-6.50	117.70	120.30
26	A	182	A	N7-C8-N9	6.50	117.05	113.80
26	A	2329	U	C5-C6-N1	6.49	125.95	122.70
26	A	1656	C	C6-N1-C2	-6.49	117.70	120.30
26	A	2250	G	N7-C8-N9	6.49	116.34	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	413	G	C4-C5-N7	6.49	113.39	110.80
26	A	2822	G	C5-C6-O6	-6.48	124.71	128.60
26	A	885	C	C5-C4-N4	-6.48	115.67	120.20
26	A	1498	C	N1-C2-O2	6.46	122.77	118.90
26	A	2558	C	C5-C6-N1	6.46	124.23	121.00
1	a	611	C	N3-C2-O2	-6.45	117.38	121.90
26	A	933	A	C2-N3-C4	6.45	113.83	110.60
26	A	361	G	C5-C6-O6	-6.45	124.73	128.60
26	A	890	C	N3-C2-O2	-6.45	117.38	121.90
1	a	1317	C	N3-C2-O2	-6.45	117.39	121.90
1	a	968	A	N3-C4-N9	-6.44	122.25	127.40
1	a	1028	C	N1-C2-O2	6.44	122.77	118.90
26	A	2305	U	C5-C4-O4	-6.44	122.04	125.90
1	a	110	C	N1-C2-O2	6.43	122.76	118.90
1	a	811	C	N1-C2-O2	6.43	122.76	118.90
23	x	114	C	C6-N1-C1'	-6.42	113.09	120.80
26	A	1886	U	N3-C2-O2	-6.42	117.70	122.20
1	a	795	C	C5-C6-N1	6.42	124.21	121.00
26	A	1947	C	C6-N1-C2	-6.42	117.73	120.30
26	A	2515	C	C5-C6-N1	6.42	124.21	121.00
14	n	32	ASP	CB-CG-OD1	6.41	124.07	118.30
30	E	134	LEU	CA-CB-CG	6.41	130.03	115.30
1	a	529	G	C6-C5-N7	-6.40	126.56	130.40
26	A	358	U	N1-C2-O2	6.39	127.27	122.80
26	A	343	C	N3-C2-O2	-6.38	117.43	121.90
17	q	75	VAL	CA-CB-CG2	6.38	120.47	110.90
1	a	610	U	N1-C2-O2	6.38	127.26	122.80
26	A	628	G	C4-N9-C1'	6.38	134.79	126.50
26	A	1816	C	N1-C2-O2	6.38	122.73	118.90
26	A	888	C	O4'-C1'-N1	6.35	113.28	108.20
1	a	529	G	C8-N9-C4	6.35	108.94	106.40
1	a	735	C	C5-C6-N1	6.35	124.17	121.00
2	b	81	ASP	CB-CG-OD1	6.34	124.01	118.30
26	A	305	C	C5-C6-N1	6.34	124.17	121.00
26	A	758	C	C6-N1-C2	-6.33	117.77	120.30
1	a	1393	U	N1-C2-O2	6.33	127.23	122.80
26	A	1446	C	C5-C6-N1	6.33	124.16	121.00
26	A	2118	U	C5-C4-O4	-6.33	122.10	125.90
26	A	2254	C	N1-C2-O2	6.32	122.69	118.90
26	A	2150	C	C5-C6-N1	6.31	124.16	121.00
26	A	1402	U	N3-C2-O2	-6.31	117.78	122.20
26	A	67	U	N3-C4-O4	6.31	123.82	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1537	U	C5-C6-N1	6.31	125.85	122.70
2	b	134	LEU	CA-CB-CG	6.30	129.79	115.30
26	A	2559	C	C6-N1-C2	-6.30	117.78	120.30
26	A	2248	C	N1-C2-O2	6.29	122.68	118.90
40	O	69	ASP	CB-CG-OD1	6.29	123.96	118.30
26	A	2637	U	N1-C2-O2	6.29	127.20	122.80
26	A	399	U	N1-C2-O2	6.29	127.20	122.80
1	a	106	C	C6-N1-C2	-6.28	117.79	120.30
26	A	999	U	N3-C2-O2	-6.28	117.81	122.20
22	v	67	C	C6-N1-C2	-6.28	117.79	120.30
26	A	1446	C	C6-N1-C2	-6.27	117.79	120.30
24	y	70	U	N3-C2-O2	-6.26	117.82	122.20
26	A	912	C	N1-C2-O2	6.25	122.65	118.90
26	A	2656	U	C2-N1-C1'	6.25	125.19	117.70
46	U	51	LEU	CA-CB-CG	6.24	129.66	115.30
26	A	1880	U	N3-C2-O2	-6.24	117.83	122.20
25	z	107	LEU	CB-CG-CD2	-6.24	100.40	111.00
1	a	177	G	N3-C4-C5	-6.24	125.48	128.60
26	A	853	C	C5-C6-N1	6.24	124.12	121.00
52	0	2	VAL	CG1-CB-CG2	-6.24	100.92	110.90
24	y	73	G	N3-C4-C5	6.23	131.71	128.60
26	A	1104	C	C6-N1-C2	-6.23	117.81	120.30
30	E	109	LEU	CA-CB-CG	6.23	129.62	115.30
41	P	71	ARG	CG-CD-NE	-6.23	98.72	111.80
26	A	960	A	OP1-P-O3'	6.22	118.89	105.20
46	U	40	LEU	CA-CB-CG	6.22	129.60	115.30
1	a	1382	C	N3-C2-O2	-6.22	117.55	121.90
9	i	93	LEU	CA-CB-CG	6.22	129.60	115.30
26	A	2254	C	N3-C2-O2	-6.21	117.55	121.90
26	A	832	U	N3-C2-O2	-6.21	117.85	122.20
26	A	2637	U	N3-C2-O2	-6.20	117.86	122.20
14	n	60	ARG	CG-CD-NE	-6.19	98.79	111.80
1	a	545	C	C6-N1-C2	-6.19	117.82	120.30
1	a	750	C	C6-N1-C2	-6.19	117.82	120.30
1	a	1325	C	C6-N1-C2	-6.19	117.82	120.30
1	a	955	U	N1-C2-O2	6.18	127.13	122.80
25	z	610	LEU	CA-CB-CG	6.18	129.51	115.30
26	A	2043	C	C2-N1-C1'	6.17	125.59	118.80
26	A	206	U	N1-C2-O2	6.17	127.12	122.80
1	a	397	A	C2-N3-C4	6.17	113.68	110.60
1	a	1350	A	O5'-P-OP1	-6.17	100.15	105.70
26	A	2300	C	C6-N1-C2	-6.17	117.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	356	G	C8-N9-C4	-6.16	103.94	106.40
26	A	243	U	N3-C2-O2	-6.16	117.89	122.20
26	A	206	U	N3-C2-O2	-6.15	117.89	122.20
23	x	104	U	N3-C2-O2	-6.15	117.89	122.20
26	A	2739	U	N1-C2-O2	6.15	127.11	122.80
26	A	1352	U	N3-C2-O2	-6.15	117.90	122.20
26	A	965	C	C6-N1-C2	-6.14	117.84	120.30
1	a	968	A	C4-C5-C6	-6.14	113.93	117.00
26	A	1486	U	C5-C6-N1	6.14	125.77	122.70
26	A	2756	U	OP1-P-O3'	6.13	118.69	105.20
1	a	552	U	C6-N1-C2	-6.13	117.32	121.00
26	A	2248	C	C5-C6-N1	6.13	124.06	121.00
1	a	1509	C	C6-N1-C2	-6.12	117.85	120.30
1	a	896	C	C6-N1-C2	-6.12	117.85	120.30
1	a	1237	C	OP1-P-O3'	6.12	118.66	105.20
24	y	27	C	C6-N1-C2	-6.12	117.85	120.30
1	a	1469	C	N3-C2-O2	-6.12	117.62	121.90
1	a	1403	C	N3-C2-O2	-6.11	117.62	121.90
1	a	300	A	C8-N9-C4	-6.11	103.36	105.80
26	A	628	G	C8-N9-C1'	-6.11	119.06	127.00
26	A	2302	U	C6-N1-C2	-6.11	117.33	121.00
26	A	192	C	N1-C2-O2	6.11	122.56	118.90
27	B	49	C	C6-N1-C2	-6.11	117.86	120.30
1	a	340	U	N3-C2-O2	-6.11	117.93	122.20
1	a	368	U	N1-C2-N3	6.11	118.56	114.90
1	a	893	C	C6-N1-C2	-6.10	117.86	120.30
1	a	1029	U	C5-C6-N1	6.10	125.75	122.70
41	P	113	LEU	CA-CB-CG	6.09	129.31	115.30
26	A	2492	U	N1-C2-O2	6.08	127.06	122.80
26	A	2188	U	C6-N1-C2	-6.08	117.35	121.00
26	A	2615	U	N1-C2-O2	6.08	127.06	122.80
1	a	267	C	O5'-P-OP2	-6.08	100.23	105.70
26	A	919	U	N3-C2-O2	-6.07	117.95	122.20
1	a	252	U	N3-C2-O2	-6.07	117.95	122.20
23	x	114	C	C5-C6-N1	6.07	124.04	121.00
26	A	2759	G	N1-C6-O6	-6.07	116.26	119.90
26	A	2797	U	C5-C6-N1	6.07	125.73	122.70
26	A	1487	U	C5-C6-N1	6.06	125.73	122.70
26	A	1886	U	N1-C2-O2	6.06	127.04	122.80
26	A	2649	C	C5-C6-N1	6.06	124.03	121.00
1	a	214	C	C6-N1-C2	-6.05	117.88	120.30
26	A	2656	U	N3-C2-O2	-6.05	117.96	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	888	C	C5-C6-N1	6.04	124.02	121.00
26	A	1499	C	C5-C6-N1	6.04	124.02	121.00
23	x	96	C	C5-C6-N1	6.04	124.02	121.00
26	A	2758	A	N1-C6-N6	-6.04	114.97	118.60
26	A	1289	C	C2-N1-C1'	6.04	125.44	118.80
1	a	993	G	N3-C4-N9	6.04	129.62	126.00
26	A	2248	C	C6-N1-C2	-6.03	117.89	120.30
1	a	1532	U	C5-C6-N1	6.03	125.71	122.70
26	A	356	G	C6-C5-N7	-6.03	126.78	130.40
26	A	2730	C	C6-N1-C2	-6.03	117.89	120.30
26	A	1499	C	C6-N1-C2	-6.02	117.89	120.30
1	a	1535	C	N1-C2-O2	6.02	122.51	118.90
1	a	1466	C	C6-N1-C2	-6.02	117.89	120.30
1	a	842	U	C5-C6-N1	6.02	125.71	122.70
1	a	307	C	C6-N1-C2	-6.02	117.89	120.30
26	A	748	G	OP2-P-O3'	6.02	118.44	105.20
26	A	2769	U	N3-C2-O2	-6.01	117.99	122.20
26	A	1104	C	C5-C6-N1	6.01	124.01	121.00
23	x	128	C	C3'-C2'-C1'	6.01	106.31	101.50
26	A	67	U	C5-C4-O4	-6.00	122.30	125.90
26	A	867	C	N3-C2-O2	-6.00	117.70	121.90
26	A	901	C	C5-C6-N1	6.00	124.00	121.00
1	a	338	A	N7-C8-N9	5.99	116.80	113.80
1	a	564	C	N3-C2-O2	-5.99	117.70	121.90
26	A	546	U	C6-N1-C2	-5.99	117.40	121.00
26	A	1199	U	C5-C6-N1	5.99	125.70	122.70
57	6	4	ASP	CB-CG-OD1	5.99	123.69	118.30
1	a	36	C	C5-C6-N1	5.99	123.99	121.00
26	A	2720	U	N3-C2-O2	-5.98	118.01	122.20
52	0	21	LEU	CA-CB-CG	5.98	129.06	115.30
1	a	754	C	N3-C2-O2	-5.97	117.72	121.90
24	y	68	C	C6-N1-C2	-5.97	117.91	120.30
26	A	1150	C	C5-C6-N1	5.97	123.98	121.00
1	a	340	U	N1-C2-O2	5.96	126.97	122.80
26	A	2300	C	C2-N1-C1'	5.96	125.36	118.80
26	A	2408	U	C5-C6-N1	5.95	125.67	122.70
26	A	1931	U	N3-C2-O2	-5.95	118.04	122.20
26	A	2047	C	C6-N1-C2	-5.94	117.92	120.30
23	x	131	C	C5-C6-N1	5.94	123.97	121.00
26	A	1438	U	N3-C2-O2	-5.94	118.05	122.20
26	A	1078	U	OP1-P-OP2	-5.93	110.70	119.60
1	a	385	C	C6-N1-C2	-5.93	117.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	143	C	C5-C6-N1	5.93	123.96	121.00
26	A	1313	U	C6-N1-C1'	-5.93	112.90	121.20
26	A	2636	C	N1-C2-O2	5.92	122.45	118.90
27	B	74	U	N3-C2-O2	-5.92	118.06	122.20
26	A	1539	U	C5-C6-N1	5.92	125.66	122.70
31	F	48	LEU	CA-CB-CG	5.92	128.91	115.30
26	A	639	U	C6-N1-C2	-5.91	117.45	121.00
26	A	1963	U	O4'-C1'-N1	5.91	112.93	108.20
26	A	278	A	N3-C4-C5	-5.91	122.66	126.80
26	A	1788	C	C6-N1-C2	-5.91	117.94	120.30
26	A	2103	C	N1-C2-O2	5.91	122.44	118.90
1	a	972	C	N3-C2-O2	-5.91	117.77	121.90
23	x	129	U	C5'-C4'-C3'	5.91	125.45	116.00
1	a	529	G	N3-C4-N9	5.90	129.54	126.00
1	a	1227	A	N9-C1'-C2'	-5.90	105.52	112.00
1	a	1395	C	N1-C2-O2	5.89	122.44	118.90
18	r	16	GLY	N-CA-C	-5.89	98.36	113.10
2	b	56	LEU	CA-CB-CG	5.89	128.85	115.30
1	a	516	PSU	O3'-P-O5'	-5.88	92.82	104.00
26	A	1658	C	C6-N1-C2	-5.88	117.95	120.30
26	A	2044	C	C6-N1-C2	-5.88	117.95	120.30
26	A	2142	A	C8-N9-C4	-5.88	103.45	105.80
1	a	1314	C	C6-N1-C2	-5.88	117.95	120.30
26	A	1093	G	C5-C6-O6	-5.88	125.07	128.60
26	A	2474	U	N3-C2-O2	-5.88	118.09	122.20
1	a	891	U	N1-C2-O2	5.87	126.91	122.80
26	A	1585	C	N1-C2-O2	5.87	122.42	118.90
26	A	2765	A	C2-N3-C4	5.87	113.53	110.60
27	B	42	C	N3-C2-O2	-5.87	117.79	121.90
1	a	1262	C	N1-C2-O2	5.86	122.42	118.90
1	a	300	A	N7-C8-N9	5.86	116.73	113.80
1	a	1240	U	C5-C6-N1	-5.85	119.77	122.70
26	A	2615	U	N3-C2-O2	-5.85	118.10	122.20
26	A	1716	U	N3-C2-O2	-5.85	118.11	122.20
1	a	1427	C	C5-C6-N1	5.85	123.92	121.00
26	A	1123	C	C6-N1-C2	-5.84	117.96	120.30
26	A	1848	A	N7-C8-N9	5.84	116.72	113.80
26	A	1064	C	C6-N1-C2	-5.84	117.97	120.30
39	N	79	LEU	CA-CB-CG	5.84	128.73	115.30
26	A	200	U	N1-C2-O2	5.84	126.89	122.80
26	A	2515	C	C6-N1-C2	-5.84	117.97	120.30
26	A	1171	G	N7-C8-N9	5.83	116.02	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	Q	108	LEU	CA-CB-CG	5.83	128.71	115.30
1	a	1148	U	N1-C2-O2	5.83	126.88	122.80
1	a	1348	U	N1-C2-O2	5.83	126.88	122.80
20	t	4	LYS	N-CA-CB	5.82	121.08	110.60
24	y	67(A)	U	C5-C6-N1	5.82	125.61	122.70
23	x	133	C	N1-C2-O2	5.82	122.39	118.90
1	a	896	C	C5-C6-N1	5.82	123.91	121.00
26	A	2142	A	N7-C8-N9	5.82	116.71	113.80
26	A	2821	A	O5'-P-OP2	-5.82	100.46	105.70
26	A	1931	U	N1-C2-O2	5.81	126.87	122.80
26	A	2896	C	C6-N1-C2	-5.81	117.98	120.30
1	a	470	C	C6-N1-C2	-5.80	117.98	120.30
22	v	1	C	N3-C2-O2	-5.80	117.84	121.90
26	A	672	C	C6-N1-C2	-5.80	117.98	120.30
25	z	397	LEU	CB-CG-CD1	5.80	120.86	111.00
1	a	719	C	N3-C2-O2	-5.79	117.84	121.90
26	A	1776	G	C4-N9-C1'	5.79	134.03	126.50
26	A	356	G	C4-N9-C1'	5.79	134.02	126.50
26	A	672	C	C5-C6-N1	5.79	123.89	121.00
1	a	58	C	C5-C6-N1	5.78	123.89	121.00
26	A	2575	C	C6-N1-C2	-5.77	117.99	120.30
26	A	857	G	N7-C8-N9	5.77	115.98	113.10
1	a	1278	G	C2-N3-C4	5.77	114.78	111.90
26	A	702	U	N1-C2-O2	5.77	126.84	122.80
26	A	1372	U	N3-C2-O2	-5.76	118.17	122.20
1	a	754	C	C2-N1-C1'	5.76	125.14	118.80
1	a	997	U	C5-C6-N1	5.76	125.58	122.70
26	A	1055	G	C2-N3-C4	5.76	114.78	111.90
26	A	1087	G	N7-C8-N9	5.76	115.98	113.10
26	A	1629	U	N3-C2-O2	-5.76	118.17	122.20
26	A	2667	C	C6-N1-C2	-5.76	118.00	120.30
26	A	731	C	C6-N1-C2	-5.75	118.00	120.30
26	A	998	C	C6-N1-C2	-5.75	118.00	120.30
1	a	353	A	OP2-P-O3'	5.75	117.85	105.20
26	A	738	G	N3-C2-N2	-5.75	115.88	119.90
26	A	1774	C	N3-C2-O2	-5.75	117.88	121.90
26	A	2146	C	N1-C2-O2	5.74	122.35	118.90
26	A	889	C	N1-C2-O2	5.74	122.34	118.90
26	A	2465	C	C6-N1-C2	-5.74	118.00	120.30
1	a	1317	C	C2-N1-C1'	5.73	125.11	118.80
1	a	1148	U	N3-C2-O2	-5.73	118.19	122.20
1	a	307	C	C2-N1-C1'	5.73	125.10	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	195	A	OP1-P-O3'	5.73	117.81	105.20
26	A	2716	C	C6-N1-C2	-5.73	118.01	120.30
26	A	2110	G	N3-C4-N9	-5.73	122.56	126.00
26	A	669	G	C4-N9-C1'	5.72	133.94	126.50
26	A	1936	A	N3-C4-N9	-5.72	122.82	127.40
1	a	1403	C	C6-N1-C2	-5.72	118.01	120.30
27	B	27	C	N3-C2-O2	-5.72	117.89	121.90
26	A	2637	U	C2-N1-C1'	5.72	124.56	117.70
14	n	17	ASP	CB-CG-OD1	5.72	123.44	118.30
26	A	2147	A	C8-N9-C4	-5.72	103.51	105.80
26	A	942	G	N1-C6-O6	-5.71	116.47	119.90
26	A	393	C	C6-N1-C2	-5.71	118.02	120.30
26	A	182	A	C8-N9-C4	-5.71	103.52	105.80
26	A	114	U	N3-C2-O2	-5.71	118.21	122.20
2	b	213	LEU	CB-CG-CD1	5.71	120.70	111.00
26	A	281	C	C6-N1-C2	-5.70	118.02	120.30
26	A	937	C	C6-N1-C2	-5.70	118.02	120.30
26	A	2637	U	C6-N1-C2	-5.70	117.58	121.00
26	A	965	C	C5-C6-N1	5.70	123.85	121.00
23	x	87	A	OP1-P-O3'	5.69	117.73	105.20
26	A	919	U	N1-C2-O2	5.69	126.79	122.80
26	A	109	C	C6-N1-C2	-5.69	118.02	120.30
1	a	469	C	N1-C2-O2	5.69	122.31	118.90
1	a	1241	G	C2-N3-C4	5.69	114.74	111.90
26	A	853	C	C6-N1-C2	-5.69	118.03	120.30
1	a	256	U	C5-C6-N1	5.68	125.54	122.70
26	A	2537	U	N3-C2-O2	-5.68	118.22	122.20
1	a	611	C	C6-N1-C2	-5.68	118.03	120.30
26	A	884	U	N1-C2-O2	-5.68	118.82	122.80
26	A	885	C	C6-N1-C2	-5.68	118.03	120.30
26	A	343	C	C5-C6-N1	5.68	123.84	121.00
26	A	2158	A	C8-N9-C4	-5.68	103.53	105.80
26	A	278	A	N3-C4-N9	5.67	131.94	127.40
41	P	71	ARG	NE-CZ-NH1	-5.67	117.47	120.30
23	x	121	U	N1-C2-O2	5.67	126.77	122.80
26	A	2558	C	C6-N1-C2	-5.67	118.03	120.30
1	a	795	C	C6-N1-C2	-5.67	118.03	120.30
1	a	78	A	C8-N9-C4	-5.66	103.53	105.80
23	x	113	C	OP1-P-O3'	5.66	117.65	105.20
24	y	40	C	C2-N1-C1'	5.66	125.02	118.80
26	A	310	A	O5'-P-OP1	-5.66	100.61	105.70
26	A	546	U	N3-C2-O2	-5.66	118.24	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1086	U	N1-C2-O2	5.65	126.76	122.80
26	A	2710	C	C6-N1-C2	-5.65	118.04	120.30
26	A	1152	C	C6-N1-C2	-5.65	118.04	120.30
1	a	1538	C	C5-C6-N1	5.65	123.82	121.00
26	A	420	C	C6-N1-C2	-5.65	118.04	120.30
26	A	886	A	O3'-P-O5'	5.65	114.73	104.00
11	k	96	ILE	CG1-CB-CG2	-5.65	98.98	111.40
26	A	2769	U	N1-C2-O2	5.64	126.75	122.80
26	A	658	U	C5-C6-N1	5.64	125.52	122.70
26	A	1470	A	N7-C8-N9	5.64	116.62	113.80
26	A	2746	U	C5-C6-N1	5.64	125.52	122.70
1	a	1537	U	C6-N1-C2	-5.64	117.62	121.00
26	A	2066	C	O4'-C1'-N1	5.64	112.71	108.20
23	x	130	G	N9-C1'-C2'	-5.64	105.80	112.00
26	A	852	U	C5-C6-N1	5.63	125.52	122.70
24	y	35	C	C6-N1-C2	-5.63	118.05	120.30
26	A	1323	C	O5'-P-OP1	-5.63	100.63	105.70
13	m	47	LEU	CA-CB-CG	5.63	128.25	115.30
26	A	353	C	C6-N1-C2	-5.63	118.05	120.30
26	A	2870	C	C6-N1-C2	-5.63	118.05	120.30
27	B	49	C	C5-C6-N1	5.63	123.81	121.00
26	A	418	C	C6-N1-C2	-5.62	118.05	120.30
1	a	943	U	N3-C2-O2	-5.62	118.27	122.20
26	A	840	C	C6-N1-C2	-5.62	118.05	120.30
26	A	883	G	C6-C5-N7	-5.62	127.03	130.40
30	E	153	LEU	CA-CB-CG	5.62	128.23	115.30
1	a	313	A	N7-C8-N9	5.62	116.61	113.80
26	A	79	C	C6-N1-C2	-5.62	118.05	120.30
26	A	915	C	C2-N1-C1'	5.61	124.97	118.80
26	A	1832	C	C5-C6-N1	5.61	123.81	121.00
5	e	35	LEU	CB-CG-CD1	-5.61	101.46	111.00
26	A	335	C	C6-N1-C2	-5.61	118.06	120.30
26	A	2591	C	C6-N1-C2	-5.61	118.06	120.30
26	A	2267	A	N1-C2-N3	-5.61	126.50	129.30
1	a	915	A	N1-C6-N6	-5.60	115.24	118.60
26	A	1880	U	N1-C2-O2	5.60	126.72	122.80
26	A	2109	U	C5-C6-N1	5.60	125.50	122.70
36	K	92	GLU	CA-CB-CG	5.60	125.72	113.40
1	a	1094	G	O4'-C1'-N9	5.60	112.68	108.20
26	A	1759	A	C2-N3-C4	5.60	113.40	110.60
26	A	2430	A	O5'-P-OP2	5.60	117.42	110.70
1	a	163	C	N1-C2-O2	5.59	122.26	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	73	G	N3-C4-N9	-5.59	122.64	126.00
1	a	264	C	C6-N1-C2	-5.59	118.06	120.30
26	A	135	U	C5-C6-N1	5.59	125.49	122.70
26	A	1047	G	O4'-C1'-N9	5.59	112.67	108.20
26	A	897	C	C6-N1-C2	-5.58	118.07	120.30
26	A	353	C	C5-C6-N1	5.58	123.79	121.00
24	y	56	C	C6-N1-C2	-5.58	118.07	120.30
24	y	36	A	C2-N3-C4	5.57	113.39	110.60
24	y	47(P)	C	C6-N1-C2	-5.57	118.07	120.30
26	A	2006	C	C6-N1-C2	-5.57	118.07	120.30
26	A	2295	C	C6-N1-C2	-5.57	118.07	120.30
1	a	866	C	C6-N1-C2	-5.57	118.07	120.30
26	A	628	G	C6-C5-N7	-5.57	127.06	130.40
26	A	1685	C	C6-N1-C2	-5.56	118.07	120.30
22	v	39	C	C5-C6-N1	5.56	123.78	121.00
26	A	454	A	OP2-P-O3'	5.56	117.44	105.20
24	y	69	U	C5-C6-N1	5.56	125.48	122.70
26	A	2248	C	C2-N1-C1'	5.56	124.91	118.80
26	A	275	C	N1-C2-O2	5.55	122.23	118.90
26	A	479	A	OP1-P-O3'	5.55	117.42	105.20
26	A	1804	C	C6-N1-C2	-5.55	118.08	120.30
26	A	1578	U	N3-C2-O2	-5.55	118.31	122.20
26	A	2153	C	C6-N1-C2	-5.55	118.08	120.30
1	a	552	U	C5-C6-N1	5.55	125.47	122.70
26	A	2179	C	C5-C4-N4	5.55	124.08	120.20
26	A	2164	C	N1-C2-O2	5.54	122.22	118.90
26	A	888	C	C2-N1-C1'	5.53	124.89	118.80
1	a	1028	C	N3-C2-O2	-5.53	118.03	121.90
26	A	2683	C	C2-N1-C1'	5.53	124.88	118.80
1	a	99	C	C6-N1-C2	-5.53	118.09	120.30
1	a	470	C	C5-C6-N1	5.53	123.76	121.00
26	A	281	C	C5-C6-N1	5.53	123.76	121.00
1	a	891	U	N3-C2-O2	-5.53	118.33	122.20
26	A	2173	A	N3-C4-C5	-5.53	122.93	126.80
1	a	368	U	C2-N3-C4	-5.52	123.69	127.00
26	A	544	C	C6-N1-C2	-5.52	118.09	120.30
28	C	83	ASP	CB-CG-OD1	5.52	123.27	118.30
1	a	1158	C	C5-C6-N1	5.51	123.76	121.00
26	A	1282	U	C5-C6-N1	5.51	125.46	122.70
12	l	25	ALA	N-CA-CB	5.51	117.82	110.10
26	A	1658	C	C5-C6-N1	5.51	123.76	121.00
1	a	820	U	OP2-P-O3'	5.51	117.32	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	810	C	N1-C2-O2	5.51	122.20	118.90
26	A	353	C	C2-N1-C1'	5.51	124.86	118.80
24	y	40	C	N1-C2-O2	5.51	122.20	118.90
26	A	2130	U	N1-C2-O2	5.51	126.66	122.80
26	A	2492	U	N3-C2-O2	-5.51	118.34	122.20
26	A	2430	A	C2-N3-C4	5.51	113.35	110.60
26	A	200	U	N3-C2-O2	-5.50	118.35	122.20
26	A	1843	C	C6-N1-C2	-5.50	118.10	120.30
9	i	89	TYR	CA-CB-CG	5.49	123.84	113.40
1	a	811	C	N3-C2-O2	-5.49	118.06	121.90
26	A	2200	C	C5-C6-N1	5.49	123.75	121.00
26	A	1398	C	C5-C6-N1	5.49	123.74	121.00
26	A	1157	G	C4-N9-C1'	5.49	133.63	126.50
44	S	84	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	a	644	U	N3-C2-O2	-5.48	118.36	122.20
26	A	985	C	C6-N1-C2	-5.48	118.11	120.30
32	G	70	LEU	CA-CB-CG	5.48	127.91	115.30
26	A	2840	C	C6-N1-C2	-5.48	118.11	120.30
27	B	37	C	C6-N1-C2	-5.48	118.11	120.30
26	A	737	C	C6-N1-C2	-5.47	118.11	120.30
28	C	153	LEU	CB-CG-CD1	5.47	120.31	111.00
1	a	163	C	N3-C2-O2	-5.47	118.07	121.90
26	A	887	U	C6-N1-C2	-5.47	117.72	121.00
1	a	1384	C	C2-N1-C1'	5.46	124.81	118.80
26	A	12	U	N3-C2-O2	-5.46	118.37	122.20
26	A	2822	G	C4-C5-N7	5.46	112.99	110.80
27	B	26	C	C6-N1-C2	-5.46	118.11	120.30
8	h	58	LEU	CA-CB-CG	5.46	127.86	115.30
26	A	872	U	C5-C6-N1	5.46	125.43	122.70
1	a	737	C	C5-C6-N1	5.46	123.73	121.00
26	A	2194	U	C5-C6-N1	5.46	125.43	122.70
1	a	214	C	C5-C6-N1	5.46	123.73	121.00
1	a	1184	G	N3-C4-C5	-5.46	125.87	128.60
26	A	912	C	C2-N1-C1'	5.46	124.80	118.80
1	a	454	G	N7-C8-N9	5.46	115.83	113.10
26	A	2757	A	C5-C6-N1	-5.45	114.97	117.70
27	B	55	U	N1-C2-O2	5.45	126.62	122.80
1	a	1027	C	C2-N1-C1'	5.45	124.79	118.80
1	a	1404	C	C5-C6-N1	5.45	123.72	121.00
26	A	1349	C	C6-N1-C2	-5.45	118.12	120.30
26	A	2716	C	C5-C6-N1	5.45	123.72	121.00
26	A	512	G	O4'-C1'-N9	5.45	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	t	78	LEU	CB-CG-CD2	-5.44	101.75	111.00
25	z	107	LEU	CA-CB-CG	5.44	127.81	115.30
26	A	475	C	C6-N1-C2	-5.44	118.12	120.30
31	F	65	LEU	CA-CB-CG	5.44	127.81	115.30
8	h	79	ARG	NE-CZ-NH2	5.44	123.02	120.30
26	A	1087	G	C8-N9-C4	-5.44	104.23	106.40
23	x	118	G	C5'-C4'-O4'	5.43	115.62	109.10
1	a	308	C	C5-C6-N1	5.42	123.71	121.00
1	a	1348	U	N3-C2-O2	-5.42	118.41	122.20
1	a	1384	C	C6-N1-C2	-5.42	118.13	120.30
26	A	968	C	C5-C6-N1	5.42	123.71	121.00
26	A	1348	C	C2-N1-C1'	5.41	124.75	118.80
56	4	27	CYS	CA-CB-SG	5.41	123.74	114.00
26	A	143	C	C2-N1-C1'	5.41	124.75	118.80
23	x	131	C	N1-C1'-C2'	-5.41	106.05	112.00
26	A	122	G	C6-C5-N7	-5.41	127.16	130.40
26	A	1629	U	C6-N1-C2	-5.40	117.76	121.00
1	a	313	A	C8-N9-C4	-5.40	103.64	105.80
1	a	469	C	N3-C2-O2	-5.40	118.12	121.90
26	A	257	C	N1-C2-O2	5.40	122.14	118.90
1	a	956	U	N3-C2-O2	-5.39	118.42	122.20
26	A	2822	G	N1-C6-O6	5.39	123.14	119.90
26	A	1121	C	C6-N1-C2	-5.39	118.14	120.30
26	A	2636	C	C2-N1-C1'	5.39	124.73	118.80
1	a	723	U	N1-C2-O2	5.39	126.57	122.80
26	A	999	U	N1-C2-O2	5.39	126.57	122.80
1	a	623	C	C6-N1-C2	-5.39	118.14	120.30
26	A	2068	U	C5-C6-N1	5.38	125.39	122.70
26	A	702	U	C2-N1-C1'	5.38	124.16	117.70
26	A	1438	U	C5-C6-N1	5.38	125.39	122.70
1	a	1531	A	N7-C8-N9	5.37	116.49	113.80
26	A	529	A	O5'-P-OP2	-5.37	100.86	105.70
26	A	1352	U	N1-C2-O2	5.37	126.56	122.80
26	A	1747	U	C5-C6-N1	5.37	125.38	122.70
1	a	271	C	C6-N1-C2	-5.37	118.15	120.30
26	A	201	C	N3-C2-O2	-5.37	118.14	121.90
26	A	2901	C	C2-N1-C1'	5.37	124.70	118.80
23	x	131	C	C3'-C2'-C1'	5.36	105.79	101.50
26	A	532	A	C2-N3-C4	5.36	113.28	110.60
26	A	2103	C	N3-C2-O2	-5.36	118.15	121.90
28	C	100	ARG	NE-CZ-NH1	-5.36	117.62	120.30
26	A	1438	U	N1-C2-O2	5.36	126.55	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1662	U	N3-C2-O2	-5.36	118.45	122.20
50	Y	37	LEU	CA-CB-CG	5.35	127.61	115.30
24	y	73	G	C4-N9-C1'	-5.35	119.55	126.50
1	a	330	C	N3-C2-O2	-5.35	118.16	121.90
1	a	972	C	C6-N1-C2	-5.35	118.16	120.30
26	A	257	C	N3-C2-O2	-5.35	118.16	121.90
26	A	1085	A	C8-N9-C4	-5.34	103.66	105.80
26	A	2267	A	C2-N3-C4	5.34	113.27	110.60
27	B	30	C	C2-N1-C1'	5.34	124.68	118.80
30	E	147	LEU	CA-CB-CG	5.34	127.59	115.30
26	A	481	G	N9-C4-C5	-5.34	103.26	105.40
23	x	120	U	OP1-P-O3'	5.34	116.94	105.20
1	a	323	U	C5-C6-N1	5.34	125.37	122.70
26	A	2816	G	N3-C2-N2	-5.34	116.16	119.90
26	A	1022	G	C5-C6-O6	5.33	131.80	128.60
26	A	1843	C	C5-C6-N1	5.33	123.67	121.00
26	A	2785	C	C6-N1-C2	-5.33	118.17	120.30
1	a	1131	G	N7-C8-N9	5.33	115.76	113.10
23	x	129	U	P-O5'-C5'	5.32	129.42	120.90
26	A	886	A	O4'-C1'-N9	5.32	112.46	108.20
8	h	79	ARG	CA-CB-CG	5.32	125.10	113.40
1	a	1510	C	C6-N1-C2	-5.32	118.17	120.30
8	h	95	MET	CA-CB-CG	5.32	122.33	113.30
9	i	93	LEU	CB-CG-CD2	-5.32	101.96	111.00
26	A	2110	G	N1-C6-O6	-5.32	116.71	119.90
26	A	2720	U	N1-C2-O2	5.31	126.52	122.80
26	A	1941	C	C5-C6-N1	5.31	123.66	121.00
26	A	1956	U	C5-C6-N1	5.31	125.36	122.70
25	z	397	LEU	CB-CG-CD2	-5.31	101.97	111.00
26	A	635	C	C5-C6-N1	5.31	123.66	121.00
26	A	283	G	N9-C4-C5	5.31	107.52	105.40
26	A	1936	A	N9-C4-C5	5.31	107.92	105.80
26	A	286	U	C5-C6-N1	5.30	125.35	122.70
1	a	955	U	N3-C2-O2	-5.30	118.49	122.20
26	A	2745	C	C6-N1-C2	-5.30	118.18	120.30
26	A	2767	C	C6-N1-C2	-5.30	118.18	120.30
1	a	185	U	C5-C6-N1	5.29	125.35	122.70
1	a	103	U	N3-C2-O2	-5.29	118.50	122.20
1	a	1125	U	C5-C4-O4	-5.29	122.73	125.90
26	A	2173	A	N3-C4-N9	5.29	131.63	127.40
29	D	49	GLN	CA-CB-CG	5.29	125.03	113.40
26	A	687	C	N1-C2-O2	5.29	122.07	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2147	A	N7-C8-N9	5.29	116.44	113.80
23	x	133	C	C2-N1-C1'	5.28	124.61	118.80
26	A	885	C	OP1-P-O3'	5.28	116.82	105.20
26	A	886	A	OP1-P-OP2	-5.28	111.68	119.60
4	d	8	LEU	CA-CB-CG	5.28	127.45	115.30
22	v	1	C	C6-N1-C2	-5.28	118.19	120.30
22	v	75	C	C6-N1-C2	-5.28	118.19	120.30
26	A	1348	C	C5-C6-N1	5.28	123.64	121.00
26	A	1417	C	N1-C2-O2	5.27	122.06	118.90
26	A	2165	C	N3-C2-O2	-5.27	118.21	121.90
22	v	56	C	C6-N1-C2	-5.27	118.19	120.30
26	A	915	C	N1-C2-O2	5.27	122.06	118.90
26	A	2089	C	C6-N1-C2	-5.27	118.19	120.30
26	A	2141	G	C8-N9-C4	-5.27	104.29	106.40
1	a	1533	C	C5-C6-N1	5.27	123.64	121.00
1	a	945	G	N3-C4-N9	5.27	129.16	126.00
22	v	67	C	C2-N1-C1'	5.27	124.60	118.80
26	A	1108	U	C5-C6-N1	5.27	125.33	122.70
31	F	173	ASP	N-CA-C	-5.27	96.78	111.00
26	A	998	C	C5-C6-N1	5.26	123.63	121.00
26	A	1053	C	C6-N1-C2	-5.26	118.19	120.30
26	A	1398	C	C6-N1-C2	-5.26	118.19	120.30
26	A	1669	A	N3-C4-C5	-5.26	123.12	126.80
1	a	674	G	N7-C8-N9	5.26	115.73	113.10
26	A	1316	U	N3-C2-O2	-5.26	118.52	122.20
26	A	1941	C	C6-N1-C1'	-5.26	114.49	120.80
27	B	31	C	C2-N1-C1'	5.26	124.58	118.80
26	A	885	C	C5'-C4'-O4'	5.25	115.41	109.10
1	a	1109	C	C6-N1-C2	-5.25	118.20	120.30
22	v	34	C	N1-C2-O2	5.25	122.05	118.90
26	A	209	C	C6-N1-C2	-5.25	118.20	120.30
27	B	64	G	N9-C4-C5	-5.25	103.30	105.40
23	x	133	C	N3-C2-O2	-5.25	118.23	121.90
26	A	1536	C	P-O3'-C3'	5.25	125.99	119.70
26	A	2782	G	C6-C5-N7	-5.25	127.25	130.40
1	a	754	C	N1-C2-O2	5.24	122.05	118.90
26	A	1881	C	C6-N1-C2	-5.24	118.20	120.30
26	A	1893	C	N1-C2-O2	5.24	122.05	118.90
1	a	169	C	N1-C2-O2	5.24	122.05	118.90
23	x	104	U	N1-C2-O2	5.24	126.47	122.80
26	A	897	C	N1-C2-O2	5.24	122.05	118.90
26	A	2123	G	C8-N9-C4	-5.24	104.31	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	51	C	C5-C6-N1	5.24	123.62	121.00
5	e	80	LEU	CA-CB-CG	5.23	127.33	115.30
26	A	1816	C	N3-C2-O2	-5.23	118.24	121.90
1	a	877	G	O4'-C1'-N9	5.23	112.38	108.20
24	y	19	H2U	P-O3'-C3'	5.23	125.97	119.70
24	y	56	C	C5-C6-N1	5.23	123.61	121.00
26	A	1675	C	C6-N1-C2	-5.23	118.21	120.30
26	A	1894	C	C6-N1-C2	-5.22	118.21	120.30
26	A	888	C	N3-C4-C5	-5.22	119.81	121.90
13	m	91	ARG	CB-CG-CD	-5.22	98.03	111.60
24	y	48	G	C5-C6-O6	-5.21	125.47	128.60
26	A	1499	C	C6-N1-C1'	-5.21	114.55	120.80
1	a	56	U	C6-N1-C2	-5.21	117.87	121.00
26	A	2089	C	C5-C6-N1	5.21	123.60	121.00
7	g	65	LEU	CA-CB-CG	5.21	127.28	115.30
26	A	2211	A	N3-C4-C5	-5.21	123.16	126.80
26	A	946	C	C6-N1-C2	-5.20	118.22	120.30
26	A	2403	C	C6-N1-C2	-5.20	118.22	120.30
1	a	169	C	N3-C2-O2	-5.20	118.26	121.90
3	c	30	ASP	CB-CG-OD1	5.20	122.98	118.30
1	a	1132	C	N1-C2-O2	5.19	122.02	118.90
27	B	19	C	C5-C6-N1	5.19	123.60	121.00
15	o	86	LEU	C-N-CA	5.18	134.66	121.70
26	A	890	C	C4-C5-C6	-5.18	114.81	117.40
26	A	2130	U	N3-C2-O2	-5.18	118.57	122.20
26	A	2305	U	C5-C6-N1	-5.18	120.11	122.70
26	A	2165	C	N1-C2-O2	5.18	122.01	118.90
27	B	30	C	C5-C6-N1	5.18	123.59	121.00
46	U	83	GLY	N-CA-C	-5.18	100.15	113.10
26	A	458	G	O4'-C1'-N9	5.18	112.34	108.20
26	A	1685	C	C5-C6-N1	5.18	123.59	121.00
26	A	2151	U	C6-N1-C2	-5.17	117.90	121.00
1	a	1121	U	C5-C6-N1	5.17	125.29	122.70
1	a	110	C	N3-C2-O2	-5.17	118.28	121.90
26	A	2628	C	C6-N1-C2	-5.17	118.23	120.30
1	a	536	C	C2-N1-C1'	5.17	124.48	118.80
1	a	1395	C	N3-C2-O2	-5.17	118.28	121.90
26	A	1589	U	C5-C6-N1	5.16	125.28	122.70
26	A	2200	C	C6-N1-C2	-5.16	118.23	120.30
27	B	3	C	C5-C6-N1	5.16	123.58	121.00
26	A	2556	C	N1-C2-O2	5.16	122.00	118.90
26	A	1006	C	C6-N1-C2	-5.16	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	x	130	G	C3'-C2'-C1'	5.16	105.63	101.50
26	A	897	C	N3-C2-O2	-5.16	118.29	121.90
1	a	751	U	N3-C2-O2	-5.16	118.59	122.20
26	A	1161	C	O4'-C1'-N1	5.15	112.32	108.20
26	A	2036	C	C5-C6-N1	5.15	123.58	121.00
26	A	1157	G	N3-C4-N9	5.15	129.09	126.00
26	A	1055	G	N3-C4-C5	-5.14	126.03	128.60
26	A	2302	U	N1-C2-N3	5.14	117.99	114.90
1	a	163	C	C6-N1-C2	-5.14	118.24	120.30
26	A	209	C	C5-C6-N1	5.14	123.57	121.00
26	A	2306	C	C6-N1-C2	-5.14	118.24	120.30
26	A	1402	U	N1-C2-O2	5.14	126.40	122.80
26	A	1803	A	N7-C8-N9	5.14	116.37	113.80
26	A	1822	C	C6-N1-C2	-5.14	118.24	120.30
26	A	356	G	C4-C5-C6	5.14	121.88	118.80
26	A	2232	C	C5-C6-N1	5.14	123.57	121.00
18	r	28	LEU	CA-CB-CG	5.13	127.11	115.30
1	a	916	U	N3-C2-O2	-5.13	118.61	122.20
31	F	88	VAL	CG1-CB-CG2	-5.13	102.69	110.90
26	A	1725	U	N3-C2-O2	-5.13	118.61	122.20
26	A	890	C	C5-C4-N4	-5.13	116.61	120.20
26	A	2755	C	C6-N1-C2	-5.13	118.25	120.30
27	B	3	C	C6-N1-C2	-5.12	118.25	120.30
1	a	1318	A	C8-N9-C4	5.12	107.85	105.80
26	A	391	A	C2-N3-C4	5.12	113.16	110.60
26	A	2141	G	N7-C8-N9	5.12	115.66	113.10
26	A	114	U	C2-N1-C1'	5.12	123.84	117.70
26	A	1486	U	C6-N1-C2	-5.12	117.93	121.00
11	k	92	ARG	N-CA-CB	-5.12	101.39	110.60
26	A	1289	C	N1-C2-O2	5.12	121.97	118.90
26	A	1993	U	N3-C2-O2	-5.12	118.62	122.20
26	A	2044	C	C5-C6-N1	5.12	123.56	121.00
1	a	822	U	N3-C2-O2	-5.11	118.62	122.20
26	A	1512	C	C6-N1-C2	-5.11	118.26	120.30
26	A	1788	C	C5-C6-N1	5.11	123.56	121.00
26	A	807	U	N3-C2-O2	-5.11	118.63	122.20
26	A	276	U	OP2-P-O3'	5.10	116.42	105.20
8	h	82	LEU	CA-CB-CG	5.10	127.02	115.30
22	v	25	C	N1-C2-O2	5.10	121.96	118.90
26	A	485	C	C6-N1-C2	-5.10	118.26	120.30
15	o	55	LEU	CB-CG-CD2	-5.09	102.34	111.00
26	A	361	G	N7-C8-N9	5.09	115.65	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	891	G	OP1-P-OP2	-5.09	111.96	119.60
26	A	960	A	P-O3'-C3'	5.09	125.81	119.70
26	A	2099	U	C5-C6-N1	5.09	125.24	122.70
26	A	1052	C	N1-C2-O2	5.09	121.95	118.90
26	A	2576	G	C2-N3-C4	5.08	114.44	111.90
1	a	980	C	N3-C2-O2	-5.08	118.34	121.90
25	z	167	ARG	CA-CB-CG	-5.08	102.22	113.40
1	a	252	U	N1-C2-O2	5.08	126.35	122.80
13	m	33	LEU	CA-CB-CG	-5.08	103.62	115.30
26	A	225	C	C6-N1-C2	-5.07	118.27	120.30
29	D	128	ARG	CG-CD-NE	5.07	122.46	111.80
22	v	16	C	C5-C6-N1	5.07	123.54	121.00
1	a	623	C	C5-C6-N1	5.07	123.53	121.00
1	a	1390	U	N3-C2-O2	-5.07	118.65	122.20
26	A	16	C	C6-N1-C2	-5.07	118.27	120.30
26	A	769	U	C6-N1-C2	-5.06	117.96	121.00
44	S	64	ALA	N-CA-CB	5.06	117.19	110.10
1	a	1136	C	N1-C2-O2	5.06	121.94	118.90
23	x	109	C	P-O3'-C3'	5.06	125.78	119.70
1	a	1460	C	C6-N1-C2	-5.06	118.28	120.30
24	y	71	C	C6-N1-C2	-5.06	118.28	120.30
1	a	1526	G	OP2-P-O3'	5.06	116.33	105.20
19	s	15	LEU	CA-CB-CG	5.06	126.93	115.30
26	A	461	C	C6-N1-C2	-5.05	118.28	120.30
26	A	1157	G	C8-N9-C1'	-5.05	120.43	127.00
26	A	1848	A	C8-N9-C4	-5.05	103.78	105.80
26	A	2188	U	N3-C4-O4	5.05	122.94	119.40
1	a	739	C	C6-N1-C2	-5.05	118.28	120.30
26	A	1657	U	N3-C2-O2	-5.05	118.66	122.20
22	v	34	C	C2-N1-C1'	5.05	124.36	118.80
26	A	373	U	N1-C2-O2	5.05	126.33	122.80
26	A	2473	U	C5-C6-N1	5.05	125.22	122.70
26	A	860	U	N1-C2-O2	5.05	126.33	122.80
26	A	243	U	C2-N1-C1'	5.04	123.75	117.70
26	A	702	U	N3-C2-O2	-5.04	118.67	122.20
26	A	1812	U	N3-C2-O2	-5.04	118.67	122.20
26	A	2794	C	N1-C2-O2	5.04	121.93	118.90
26	A	900	A	N1-C6-N6	-5.04	115.58	118.60
26	A	1049	C	N1-C2-O2	5.04	121.92	118.90
26	A	1914	C	N1-C2-O2	5.04	121.92	118.90
26	A	889	C	C2-N1-C1'	5.04	124.34	118.80
26	A	2232	C	C6-N1-C2	-5.03	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	47(N)	C	C6-N1-C2	-5.02	118.29	120.30
26	A	383	C	N1-C2-O2	5.02	121.91	118.90
57	6	40	CYS	CB-CA-C	-5.02	100.36	110.40
26	A	1585	C	N3-C2-O2	-5.01	118.39	121.90
26	A	2039	U	N3-C2-O2	-5.01	118.69	122.20
26	A	2441	U	N3-C2-O2	-5.01	118.69	122.20
26	A	2751	G	N3-C4-C5	-5.01	126.09	128.60
24	y	71	C	C5-C6-N1	5.01	123.51	121.00
26	A	484	C	C5-C6-N1	5.01	123.51	121.00
26	A	1049	C	C2-N1-C1'	5.01	124.31	118.80
27	B	6	G	N3-C2-N2	-5.01	116.39	119.90
1	a	385	C	C5-C6-N1	5.01	123.50	121.00
26	A	1611	C	C2-N1-C1'	5.01	124.31	118.80
26	A	1803	A	N1-C2-N3	5.01	131.80	129.30
26	A	2248	C	N3-C2-O2	-5.01	118.39	121.90
1	a	528	C	C6-N1-C2	-5.01	118.30	120.30
1	a	1363	A	C2-N3-C4	5.01	113.10	110.60
26	A	2556	C	N3-C2-O2	-5.01	118.39	121.90
1	a	705	G	N3-C4-C5	-5.00	126.10	128.60
26	A	2143	C	N3-C2-O2	-5.00	118.40	121.90
26	A	435	C	N3-C2-O2	-5.00	118.40	121.90
26	A	2109	U	C6-N1-C2	-5.00	118.00	121.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3',C4'
26	A	2069	G7M	C3',C4'

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	1	3	GLY	Peptide
55	3	30	HIS	Peptide
28	C	120	ASP	Peptide
30	E	82	GLY	Peptide
31	F	172	PHE	Peptide
31	F	173	ASP	Mainchain
32	G	117	PRO	Peptide
32	G	174	LYS	Mainchain
34	H	2	GLN	Peptide
34	H	40	THR	Peptide

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Mol	Chain	Res	Type	Group
34	H	8	LYS	Mainchain
44	S	63	GLY	Peptide
46	U	16	LYS	Peptide
46	U	87	GLU	Peptide
2	b	16	GLY	Peptide
2	b	17	HIS	Mainchain
4	d	30	LYS	Mainchain
6	f	97	THR	Peptide
10	j	41	PRO	Peptide
10	j	56	HIS	Peptide
10	j	57	VAL	Mainchain
11	k	49	SER	Peptide
11	k	91	GLY	Peptide
12	l	42	LYS	Peptide
12	l	74	GLN	Peptide
16	p	44	SER	Mainchain
17	q	48	GLU	Peptide
17	q	50	ASN	Peptide
21	u	40	PRO	Mainchain
25	z	190	LEU	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
2	b	216/218 (99%)	184 (85%)	26 (12%)	6 (3%)	5	24
3	c	204/206 (99%)	191 (94%)	12 (6%)	1 (0%)	29	61
4	d	203/205 (99%)	185 (91%)	13 (6%)	5 (2%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	155/157 (99%)	138 (89%)	12 (8%)	5 (3%)	4	22
6	f	98/100 (98%)	81 (83%)	14 (14%)	3 (3%)	4	23
7	g	149/151 (99%)	136 (91%)	11 (7%)	2 (1%)	12	39
8	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
9	i	125/127 (98%)	105 (84%)	16 (13%)	4 (3%)	4	22
10	j	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	3	18
11	k	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	17	49
12	l	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	5	26
13	m	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	5	26
14	n	98/100 (98%)	86 (88%)	9 (9%)	3 (3%)	4	23
15	o	86/88 (98%)	71 (83%)	12 (14%)	3 (4%)	3	21
16	p	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	12	39
17	q	78/80 (98%)	68 (87%)	7 (9%)	3 (4%)	3	19
18	r	63/65 (97%)	55 (87%)	6 (10%)	2 (3%)	4	22
19	s	84/86 (98%)	74 (88%)	5 (6%)	5 (6%)	1	10
20	t	83/85 (98%)	76 (92%)	7 (8%)	0	100	100
21	u	63/65 (97%)	51 (81%)	9 (14%)	3 (5%)	2	15
25	z	612/614 (100%)	581 (95%)	24 (4%)	7 (1%)	14	44
28	C	269/271 (99%)	247 (92%)	20 (7%)	2 (1%)	22	55
29	D	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
30	E	199/201 (99%)	186 (94%)	12 (6%)	1 (0%)	29	61
31	F	175/177 (99%)	162 (93%)	10 (6%)	3 (2%)	9	34
32	G	174/176 (99%)	159 (91%)	13 (8%)	2 (1%)	14	44
33	I	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	22	55
34	H	147/149 (99%)	129 (88%)	15 (10%)	3 (2%)	7	30
35	J	140/142 (99%)	134 (96%)	5 (4%)	1 (1%)	22	55
36	K	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	51
37	L	141/143 (99%)	128 (91%)	11 (8%)	2 (1%)	11	37
38	M	134/136 (98%)	119 (89%)	13 (10%)	2 (2%)	10	36
39	N	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
40	O	114/116 (98%)	103 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	P	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
42	Q	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
43	R	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	15	46
44	S	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	17	49
45	T	91/93 (98%)	80 (88%)	11 (12%)	0	100	100
46	U	100/102 (98%)	88 (88%)	10 (10%)	2 (2%)	7	30
47	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
48	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
49	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
50	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9	34
51	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
52	0	54/56 (96%)	48 (89%)	5 (9%)	1 (2%)	8	31
53	1	48/50 (96%)	46 (96%)	1 (2%)	1 (2%)	7	30
54	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
55	3	62/64 (97%)	55 (89%)	6 (10%)	1 (2%)	9	34
56	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
57	6	64/66 (97%)	55 (86%)	8 (12%)	1 (2%)	9	34
All	All	6336/6438 (98%)	5763 (91%)	482 (8%)	91 (1%)	15	37

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
2	b	73	ARG
5	e	93	VAL
6	f	94	HIS
6	f	98	GLU
9	i	57	VAL
10	j	34	ALA
10	j	42	LEU
10	j	57	VAL
10	j	92	LEU
11	k	92	ARG
12	l	75	GLU
14	n	34	ASN
14	n	57	SER

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Mol	Chain	Res	Type
17	q	49	ASN
17	q	51	GLU
18	r	11	ARG
18	r	17	VAL
19	s	82	HIS
19	s	86	LYS
25	z	191	VAL
25	z	487	PHE
28	C	121	ALA
30	E	83	VAL
31	F	173	ASP
32	G	118	ALA
33	I	64	ARG
34	H	9	VAL
35	J	81	ILE
36	K	35	VAL
37	L	36	LYS
38	M	58	LYS
44	S	64	ALA
46	U	6	ARG
46	U	88	ASP
52	0	2	VAL
55	3	31	ILE
2	b	17	HIS
2	b	153	MET
5	e	89	THR
6	f	92	THR
9	i	120	ALA
9	i	125	GLN
12	l	101	LEU
19	s	80	ARG
25	z	328	ALA
25	z	490	GLU
32	G	108	PHE
34	H	41	LYS
57	6	40	CYS
2	b	74	ALA
3	c	61	LYS
4	d	45	PRO
4	d	191	SER
4	d	192	ALA
9	i	107	ALA

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Mol	Chain	Res	Type
13	m	4	ALA
13	m	65	GLU
16	p	44	SER
21	u	24	LYS
25	z	301	GLU
28	C	204	LEU
31	F	149	ARG
2	b	15	PHE
4	d	29	THR
5	e	122	VAL
7	g	50	ALA
7	g	149	ALA
14	n	2	LYS
15	o	87	ARG
17	q	72	TRP
19	s	4	LEU
25	z	85	ASP
50	Y	22	LEU
13	m	6	ILE
15	o	45	HIS
15	o	75	ALA
21	u	19	LYS
21	u	34	ARG
31	F	20	ASN
37	L	29	LYS
5	e	23	THR
12	l	2	THR
19	s	3	SER
34	H	3	VAL
25	z	600	GLY
38	M	69	PRO
4	d	166	LYS
5	e	24	VAL
43	R	52	PRO
53	1	4	ILE

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 PDB entries followed by that with respect to all EM entries.

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	
2	b	180/180 (100%)	179 (99%)	1 (1%)	86	94
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	170 (99%)	2 (1%)	71	85
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	86 (99%)	1 (1%)	73	86
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	102 (98%)	2 (2%)	57	78
9	i	105/105 (100%)	104 (99%)	1 (1%)	76	88
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	88 (99%)	1 (1%)	73	86
12	l	103/103 (100%)	102 (99%)	1 (1%)	76	88
13	m	92/92 (100%)	91 (99%)	1 (1%)	73	86
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	74/74 (100%)	73 (99%)	1 (1%)	67	83
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	74/74 (100%)	74 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	43 (98%)	1 (2%)	50	74
25	z	501/501 (100%)	498 (99%)	3 (1%)	86	94
28	C	216/216 (100%)	215 (100%)	1 (0%)	88	94
29	D	164/164 (100%)	163 (99%)	1 (1%)	86	94
30	E	165/165 (100%)	165 (100%)	0	100	100
31	F	148/148 (100%)	147 (99%)	1 (1%)	84	92
32	G	137/137 (100%)	136 (99%)	1 (1%)	84	92
33	I	109/109 (100%)	109 (100%)	0	100	100
34	H	114/114 (100%)	114 (100%)	0	100	100
35	J	116/116 (100%)	116 (100%)	0	100	100
36	K	103/103 (100%)	102 (99%)	1 (1%)	76	88
37	L	102/102 (100%)	101 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	M	109/109 (100%)	109 (100%)	0	100	100
39	N	100/100 (100%)	98 (98%)	2 (2%)	55	77
40	O	86/86 (100%)	86 (100%)	0	100	100
41	P	99/99 (100%)	99 (100%)	0	100	100
42	Q	89/89 (100%)	89 (100%)	0	100	100
43	R	84/84 (100%)	84 (100%)	0	100	100
44	S	93/93 (100%)	93 (100%)	0	100	100
45	T	80/80 (100%)	79 (99%)	1 (1%)	69	84
46	U	83/83 (100%)	81 (98%)	2 (2%)	49	74
47	V	78/78 (100%)	78 (100%)	0	100	100
48	W	57/57 (100%)	57 (100%)	0	100	100
49	X	67/67 (100%)	67 (100%)	0	100	100
50	Y	55/55 (100%)	54 (98%)	1 (2%)	59	79
51	Z	48/48 (100%)	48 (100%)	0	100	100
52	0	47/47 (100%)	47 (100%)	0	100	100
53	1	45/45 (100%)	45 (100%)	0	100	100
54	2	38/38 (100%)	38 (100%)	0	100	100
55	3	51/51 (100%)	51 (100%)	0	100	100
56	4	34/34 (100%)	34 (100%)	0	100	100
57	6	59/59 (100%)	59 (100%)	0	100	100
All	All	5233/5256 (100%)	5206 (100%)	27 (0%)	89	94

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	107	ARG
4	d	43	ARG
4	d	201	GLU
6	f	54	LEU
8	h	15	ASN
8	h	79	ARG
9	i	18	VAL
11	k	39	ASN
12	l	30	ARG
13	m	43	LYS

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Mol	Chain	Res	Type
17	q	19	SER
21	u	17	ARG
25	z	26	ASP
25	z	27	ARG
25	z	344	ARG
28	C	187	CYS
29	D	128	ARG
31	F	103	ILE
32	G	72	ASN
36	K	43	ILE
37	L	91	ASP
39	N	2	ARG
39	N	118	ARG
45	T	85	VAL
46	U	40	LEU
46	U	73	ASN
50	Y	58	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	23	ASN
2	b	38	HIS
3	c	175	HIS
4	d	39	GLN
4	d	99	ASN
4	d	163	GLN
7	g	27	ASN
7	g	129	ASN
9	i	80	HIS
9	i	109	GLN
10	j	35	GLN
11	k	37	GLN
11	k	39	ASN
13	m	13	HIS
16	p	79	ASN
17	q	30	HIS
19	s	68	HIS
19	s	82	HIS
20	t	12	GLN
20	t	60	GLN
25	z	11	HIS

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Mol	Chain	Res	Type
25	z	47	GLN
25	z	61	HIS
25	z	91	GLN
25	z	100	GLN
25	z	420	GLN
25	z	431	HIS
25	z	475	HIS
25	z	491	GLN
25	z	532	GLN
29	D	150	GLN
30	E	41	GLN
30	E	46	GLN
30	E	195	GLN
31	F	26	GLN
32	G	138	GLN
42	Q	43	GLN
44	S	7	HIS
44	S	15	GLN
47	V	78	GLN
52	0	5	ASN
54	2	16	HIS
54	2	26	ASN
56	4	37	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	187 (12%)	0
22	v	76/77 (98%)	8 (10%)	0
23	x	47/48 (97%)	23 (48%)	0
24	y	93/95 (97%)	12 (12%)	0
26	A	2898/2903 (99%)	411 (14%)	8 (0%)
27	B	119/120 (99%)	17 (14%)	0
58	w	2/3 (66%)	0	0
All	All	4770/4785 (99%)	658 (13%)	8 (0%)

All (658) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	7	A
1	a	9	G

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Mol	Chain	Res	Type
1	a	22	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	49	U
1	a	50	A
1	a	51	A
1	a	84	U
1	a	86	G
1	a	87	C
1	a	94	G
1	a	95	C
1	a	96	U
1	a	121	U
1	a	130	A
1	a	131	A
1	a	141	G
1	a	163	C
1	a	164	G
1	a	173	U
1	a	177	G
1	a	182	A
1	a	197	A
1	a	209	U
1	a	210	C
1	a	211	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	252	U
1	a	253	A
1	a	266	G
1	a	267	C
1	a	289	G
1	a	298	A
1	a	328	C
1	a	329	A
1	a	347	G
1	a	348	G
1	a	351	G
1	a	352	C

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Mol	Chain	Res	Type
1	a	354	G
1	a	356	A
1	a	367	U
1	a	372	C
1	a	373	A
1	a	388	G
1	a	406	G
1	a	411	A
1	a	414	A
1	a	429	U
1	a	439	U
1	a	467	U
1	a	481	G
1	a	482	A
1	a	495	A
1	a	497	G
1	a	505	G
1	a	511	C
1	a	518	C
1	a	519	C
1	a	521	G
1	a	524	G
1	a	527	G7M
1	a	528	C
1	a	531	U
1	a	532	A
1	a	546	A
1	a	547	A
1	a	564	C
1	a	572	A
1	a	573	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	596	A
1	a	633	G
1	a	642	A
1	a	653	U
1	a	665	A
1	a	695	A
1	a	723	U
1	a	733	G

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Mol	Chain	Res	Type
1	a	734	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	817	C
1	a	819	A
1	a	832	G
1	a	836	G
1	a	841	C
1	a	843	U
1	a	844	G
1	a	845	A
1	a	878	A
1	a	902	G
1	a	914	A
1	a	926	G
1	a	933	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	968	A
1	a	969	A
1	a	971	G
1	a	972	C
1	a	975	A
1	a	976	G
1	a	977	A
1	a	992	U
1	a	993	G
1	a	1004	A
1	a	1020	G
1	a	1028	C
1	a	1030	U
1	a	1033	G
1	a	1034	G
1	a	1043	G
1	a	1050	G
1	a	1065	U
1	a	1085	U

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Mol	Chain	Res	Type
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1139	G
1	a	1140	C
1	a	1158	C
1	a	1159	U
1	a	1160	G
1	a	1168	U
1	a	1169	A
1	a	1182	G
1	a	1196	A
1	a	1197	A
1	a	1206	G
1	a	1213	A
1	a	1214	C
1	a	1227	A
1	a	1228	C
1	a	1236	A
1	a	1238	A
1	a	1256	A
1	a	1258	G
1	a	1260	G
1	a	1278	G
1	a	1280	A
1	a	1286	U
1	a	1287	A
1	a	1300	G
1	a	1301	U
1	a	1302	C
1	a	1317	C
1	a	1320	C
1	a	1346	A
1	a	1353	G
1	a	1363	A
1	a	1364	U
1	a	1370	G
1	a	1378	C
1	a	1406	U

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Mol	Chain	Res	Type
1	a	1419	G
1	a	1441	A
1	a	1487	G
1	a	1492	A
1	a	1503	A
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1538	C
1	a	1539	C
1	a	1540	U
22	v	9	G
22	v	13	C
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	54	5MU
22	v	56	C
22	v	76	A
23	x	88	A
23	x	90	G
23	x	91	A
23	x	96	C
23	x	97	A
23	x	98	U
23	x	109	C
23	x	110	G
23	x	113	C
23	x	114	C
23	x	115	A
23	x	116	U
23	x	117	C
23	x	123	C
23	x	124	A
23	x	125	G
23	x	126	G

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Mol	Chain	Res	Type
23	x	127	U
23	x	128	C
23	x	129	U
23	x	130	G
23	x	133	C
23	x	134	C
24	y	8	G
24	y	9	U
24	y	17	G
24	y	18	G
24	y	20	G
24	y	45	U
24	y	47(E)	G
24	y	47(G)	C
24	y	47(H)	A
24	y	47(I)	G
24	y	47(J)	C
24	y	49	G
26	A	10	A
26	A	14	A
26	A	34	U
26	A	63	A
26	A	71	A
26	A	74	A
26	A	75	G
26	A	91	A
26	A	101	A
26	A	102	U
26	A	103	A
26	A	118	A
26	A	119	A
26	A	120	U
26	A	131	A
26	A	138	U
26	A	139	U
26	A	142	A
26	A	163	C
26	A	196	A
26	A	197	A
26	A	199	A
26	A	204	A
26	A	215	G

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Mol	Chain	Res	Type
26	A	216	A
26	A	221	A
26	A	222	A
26	A	228	C
26	A	230	G
26	A	232	G
26	A	248	G
26	A	255	A
26	A	277	G
26	A	278	A
26	A	285	G
26	A	294	A
26	A	295	G
26	A	297	G
26	A	300	A
26	A	311	A
26	A	329	G
26	A	330	A
26	A	346	A
26	A	362	A
26	A	383	C
26	A	385	C
26	A	386	G
26	A	387	U
26	A	396	G
26	A	404	A
26	A	405	U
26	A	411	G
26	A	412	A
26	A	429	A
26	A	435	C
26	A	455	C
26	A	480	A
26	A	481	G
26	A	490	C
26	A	491	G
26	A	504	A
26	A	505	A
26	A	509	C
26	A	510	C
26	A	529	A
26	A	530	G

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Mol	Chain	Res	Type
26	A	531	C
26	A	532	A
26	A	547	A
26	A	549	G
26	A	563	A
26	A	568	U
26	A	573	U
26	A	575	A
26	A	586	A
26	A	588	U
26	A	603	A
26	A	613	A
26	A	614	A
26	A	615	U
26	A	616	A
26	A	622	G
26	A	637	A
26	A	645	C
26	A	646	U
26	A	647	G
26	A	653	U
26	A	655	A
26	A	678	C
26	A	685	A
26	A	686	U
26	A	717	C
26	A	730	A
26	A	747	5MU
26	A	748	G
26	A	764	A
26	A	765	C
26	A	775	G
26	A	776	G
26	A	782	A
26	A	783	A
26	A	784	G
26	A	785	G
26	A	792	A
26	A	805	G
26	A	811	U
26	A	812	C
26	A	845	A

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Mol	Chain	Res	Type
26	A	846	U
26	A	859	G
26	A	869	G
26	A	883	G
26	A	885	C
26	A	886	A
26	A	887	U
26	A	888	C
26	A	891	G
26	A	893	C
26	A	910	A
26	A	914	G
26	A	932	U
26	A	941	A
26	A	945	A
26	A	946	C
26	A	961	C
26	A	965	C
26	A	974	G
26	A	983	A
26	A	989	G
26	A	996	A
26	A	1006	C
26	A	1009	A
26	A	1012	U
26	A	1013	C
26	A	1022	G
26	A	1025	G
26	A	1026	G
26	A	1033	U
26	A	1040	A
26	A	1045	C
26	A	1046	A
26	A	1047	G
26	A	1054	A
26	A	1057	A
26	A	1060	U
26	A	1061	U
26	A	1062	G
26	A	1064	C
26	A	1065	U
26	A	1066	U

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Mol	Chain	Res	Type
26	A	1067	A
26	A	1068	G
26	A	1070	A
26	A	1073	A
26	A	1076	C
26	A	1077	A
26	A	1078	U
26	A	1079	C
26	A	1082	U
26	A	1084	A
26	A	1088	A
26	A	1101	U
26	A	1108	U
26	A	1110	G
26	A	1112	G
26	A	1132	U
26	A	1133	A
26	A	1134	A
26	A	1135	C
26	A	1141	U
26	A	1142	A
26	A	1143	A
26	A	1155	A
26	A	1171	G
26	A	1175	A
26	A	1178	C
26	A	1179	G
26	A	1180	U
26	A	1181	U
26	A	1206	G
26	A	1210	G
26	A	1211	C
26	A	1241	A
26	A	1253	A
26	A	1255	U
26	A	1256	G
26	A	1271	G
26	A	1272	A
26	A	1273	U
26	A	1300	G
26	A	1301	A
26	A	1311	G

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Mol	Chain	Res	Type
26	A	1325	U
26	A	1329	U
26	A	1332	G
26	A	1345	C
26	A	1359	A
26	A	1365	A
26	A	1368	G
26	A	1379	U
26	A	1383	A
26	A	1392	A
26	A	1395	A
26	A	1416	G
26	A	1417	C
26	A	1420	A
26	A	1428	C
26	A	1452	G
26	A	1458	U
26	A	1468	U
26	A	1476	U
26	A	1482	G
26	A	1493	C
26	A	1497	U
26	A	1498	C
26	A	1499	C
26	A	1515	A
26	A	1516	G
26	A	1535	A
26	A	1537	G
26	A	1538	G
26	A	1566	A
26	A	1569	A
26	A	1578	U
26	A	1607	C
26	A	1608	A
26	A	1609	A
26	A	1619	G
26	A	1648	U
26	A	1649	G
26	A	1651	G
26	A	1654	A
26	A	1674	G
26	A	1675	C

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Mol	Chain	Res	Type
26	A	1715	G
26	A	1732	C
26	A	1738	G
26	A	1758	U
26	A	1764	C
26	A	1773	A
26	A	1784	A
26	A	1786	A
26	A	1799	G
26	A	1800	C
26	A	1801	A
26	A	1808	A
26	A	1811	G
26	A	1816	C
26	A	1829	A
26	A	1847	A
26	A	1870	C
26	A	1884	G
26	A	1906	G
26	A	1913	A
26	A	1918	A
26	A	1929	G
26	A	1930	G
26	A	1936	A
26	A	1937	A
26	A	1942	C
26	A	1955	U
26	A	1960	A
26	A	1962	5MC
26	A	1963	U
26	A	1964	G
26	A	1967	C
26	A	1970	A
26	A	1971	U
26	A	1972	G
26	A	1982	U
26	A	1991	U
26	A	1993	U
26	A	2021	C
26	A	2022	U
26	A	2023	C
26	A	2031	A

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Mol	Chain	Res	Type
26	A	2032	G
26	A	2033	A
26	A	2043	C
26	A	2055	C
26	A	2056	G
26	A	2060	A
26	A	2061	G
26	A	2062	A
26	A	2068	U
26	A	2069	G7M
26	A	2070	A
26	A	2080	A
26	A	2093	G
26	A	2105	U
26	A	2107	G
26	A	2110	G
26	A	2111	U
26	A	2112	G
26	A	2113	U
26	A	2116	G
26	A	2118	U
26	A	2119	A
26	A	2120	G
26	A	2125	G
26	A	2127	G
26	A	2128	G
26	A	2129	C
26	A	2131	U
26	A	2132	U
26	A	2133	G
26	A	2134	A
26	A	2145	C
26	A	2146	C
26	A	2147	A
26	A	2149	U
26	A	2157	G
26	A	2158	A
26	A	2159	G
26	A	2160	C
26	A	2162	G
26	A	2164	C
26	A	2168	G

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Mol	Chain	Res	Type
26	A	2172	U
26	A	2173	A
26	A	2174	C
26	A	2177	C
26	A	2178	C
26	A	2179	C
26	A	2198	A
26	A	2204	G
26	A	2211	A
26	A	2225	A
26	A	2238	G
26	A	2239	G
26	A	2250	G
26	A	2251	OMG
26	A	2268	A
26	A	2273	A
26	A	2278	A
26	A	2283	C
26	A	2287	A
26	A	2288	A
26	A	2308	G
26	A	2310	C
26	A	2322	A
26	A	2325	G
26	A	2333	A
26	A	2335	A
26	A	2342	C
26	A	2345	G
26	A	2347	C
26	A	2350	C
26	A	2354	C
26	A	2361	G
26	A	2383	G
26	A	2385	C
26	A	2389	G
26	A	2402	U
26	A	2403	C
26	A	2406	A
26	A	2424	C
26	A	2429	G
26	A	2430	A
26	A	2434	A

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Mol	Chain	Res	Type
26	A	2436	G
26	A	2441	U
26	A	2445	2MG
26	A	2447	G
26	A	2448	A
26	A	2470	G
26	A	2476	A
26	A	2484	G
26	A	2502	G
26	A	2504	PSU
26	A	2505	G
26	A	2506	U
26	A	2513	A
26	A	2518	A
26	A	2520	C
26	A	2529	G
26	A	2547	A
26	A	2566	A
26	A	2567	G
26	A	2573	C
26	A	2602	A
26	A	2609	U
26	A	2613	U
26	A	2615	U
26	A	2629	U
26	A	2630	G
26	A	2689	U
26	A	2690	U
26	A	2714	G
26	A	2716	C
26	A	2726	A
26	A	2733	A
26	A	2739	U
26	A	2744	G
26	A	2748	A
26	A	2750	A
26	A	2755	C
26	A	2757	A
26	A	2765	A
26	A	2778	A
26	A	2791	G
26	A	2794	C

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Mol	Chain	Res	Type
26	A	2797	U
26	A	2798	U
26	A	2818	U
26	A	2821	A
26	A	2848	G
26	A	2849	U
26	A	2850	A
26	A	2873	A
26	A	2884	U
27	B	13	G
27	B	24	G
27	B	25	U
27	B	27	C
27	B	30	C
27	B	35	C
27	B	38	C
27	B	42	C
27	B	43	C
27	B	51	G
27	B	57	A
27	B	67	G
27	B	87	U
27	B	89	U
27	B	90	C
27	B	108	A
27	B	109	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	885	C
26	A	886	A
26	A	890	C
26	A	960	A
26	A	1536	C
26	A	2211	A
26	A	2250	G
26	A	2430	A

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

43 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
26	2MA	A	2503	26	17,25,26	1.04	1 (5%)	17,37,40	0.95	1 (5%)
22	PSU	v	55	22	18,21,22	1.44	3 (16%)	22,30,33	1.87	4 (18%)
26	PSU	A	2605	26	18,21,22	1.34	3 (16%)	22,30,33	1.88	4 (18%)
26	5MU	A	1939	26	19,22,23	1.35	4 (21%)	28,32,35	2.30	6 (21%)
26	PSU	A	2504	26	18,21,22	1.51	3 (16%)	22,30,33	1.85	4 (18%)
24	PSU	y	55	24	18,21,22	1.47	3 (16%)	22,30,33	1.98	4 (18%)
1	MA6	a	1519	1	19,26,27	0.93	1 (5%)	18,38,41	1.76	4 (22%)
26	1MG	A	745	26	18,26,27	0.88	1 (5%)	19,39,42	1.06	2 (10%)
22	5MU	v	54	22	19,22,23	1.48	6 (31%)	28,32,35	2.13	9 (32%)
26	PSU	A	746	26	18,21,22	1.42	3 (16%)	22,30,33	1.85	4 (18%)
22	H2U	v	20	22	18,21,22	1.02	2 (11%)	21,30,33	1.91	2 (9%)
26	2MG	A	1835	26	18,26,27	0.93	1 (5%)	16,38,41	1.22	3 (18%)
26	G7M	A	2069	26	20,26,27	1.54	3 (15%)	17,39,42	1.60	4 (23%)
26	2MG	A	2445	26	18,26,27	1.07	1 (5%)	16,38,41	1.26	3 (18%)
26	OMU	A	2552	26	19,22,23	1.23	2 (10%)	26,31,34	1.93	7 (26%)
24	6IA	y	37	24	22,29,30	0.78	1 (4%)	22,41,44	1.69	3 (13%)
1	2MG	a	1516	1	18,26,27	0.94	1 (5%)	16,38,41	1.22	2 (12%)
26	PSU	A	2580	26	18,21,22	1.40	4 (22%)	22,30,33	1.95	4 (18%)
26	PSU	A	2604	26	18,21,22	1.43	3 (16%)	22,30,33	1.90	4 (18%)
26	PSU	A	1917	26	18,21,22	1.48	5 (27%)	22,30,33	1.95	5 (22%)
24	5MU	y	54	24	19,22,23	1.43	6 (31%)	28,32,35	1.92	7 (25%)
26	OMC	A	2498	26	19,22,23	0.88	0	26,31,34	1.22	3 (11%)
26	H2U	A	2449	26	18,21,22	1.24	3 (16%)	21,30,33	2.25	1 (4%)
26	6MZ	A	2030	26	18,25,26	1.01	1 (5%)	16,36,39	1.91	4 (25%)
26	PSU	A	955	26	18,21,22	1.49	4 (22%)	22,30,33	1.90	3 (13%)
26	OMG	A	2251	22,26	18,26,27	0.99	1 (5%)	19,38,41	1.14	2 (10%)
26	PSU	A	2457	26	18,21,22	1.47	3 (16%)	22,30,33	2.03	4 (18%)
1	G7M	a	527	1	20,26,27	1.55	3 (15%)	17,39,42	1.62	3 (17%)
24	H2U	y	19	24	18,21,22	1.03	2 (11%)	21,30,33	1.76	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	6MZ	A	1618	26	18,25,26	0.96	1 (5%)	16,36,39	2.28	4 (25%)
26	5MU	A	747	26	19,22,23	1.47	5 (26%)	28,32,35	2.03	7 (25%)
26	3TD	A	1915	26	18,22,23	4.03	7 (38%)	22,32,35	1.87	3 (13%)
1	PSU	a	516	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	5 (22%)
1	2MG	a	966	1	18,26,27	1.05	1 (5%)	16,38,41	1.10	2 (12%)
26	5MC	A	1962	26	18,22,23	1.03	2 (11%)	26,32,35	1.70	5 (19%)
1	2MG	a	1207	1	18,26,27	1.03	1 (5%)	16,38,41	1.14	2 (12%)
26	PSU	A	1911	26	18,21,22	1.46	4 (22%)	22,30,33	2.05	4 (18%)
1	UR3	a	1498	1	19,22,23	0.95	1 (5%)	26,32,35	1.81	5 (19%)
1	5MC	a	967	1	18,22,23	0.94	1 (5%)	26,32,35	1.14	2 (7%)
22	4SU	v	8	22	18,21,22	1.73	4 (22%)	26,30,33	2.69	6 (23%)
1	5MC	a	1407	1	18,22,23	0.85	2 (11%)	26,32,35	1.17	3 (11%)
1	4OC	a	1402	1	20,23,24	0.77	0	26,32,35	1.41	4 (15%)
1	MA6	a	1518	1	19,26,27	0.95	1 (5%)	18,38,41	2.09	5 (27%)

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
26	2MA	A	2503	26	-	1/3/25/26	0/3/3/3
22	PSU	v	55	22	-	2/7/25/26	0/2/2/2
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2504	26	-	2/7/25/26	0/2/2/2
24	PSU	y	55	24	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	3/7/29/30	0/3/3/3
26	1MG	A	745	26	-	0/3/25/26	0/3/3/3
22	5MU	v	54	22	-	3/7/25/26	0/2/2/2
26	PSU	A	746	26	-	2/7/25/26	0/2/2/2
22	H2U	v	20	22	-	1/7/38/39	0/2/2/2
26	G7M	A	2069	26	2/2/5/5	2/3/25/26	0/3/3/3
26	2MG	A	1835	26	-	0/5/27/28	0/3/3/3
26	2MG	A	2445	26	-	2/5/27/28	0/3/3/3
26	OMU	A	2552	26	-	2/9/27/28	0/2/2/2
24	6IA	y	37	24	-	3/9/31/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
26	PSU	A	1917	26	-	3/7/25/26	0/2/2/2
24	5MU	y	54	24	-	0/7/25/26	0/2/2/2
26	OMC	A	2498	26	-	0/9/27/28	0/2/2/2
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
26	6MZ	A	2030	26	-	3/5/27/28	0/3/3/3
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
26	OMG	A	2251	22,26	-	1/5/27/28	0/3/3/3
26	PSU	A	2457	26	-	2/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	1/3/25/26	0/3/3/3
24	H2U	y	19	24	-	4/7/38/39	0/2/2/2
26	6MZ	A	1618	26	-	2/5/27/28	0/3/3/3
26	5MU	A	747	26	-	0/7/25/26	0/2/2/2
26	3TD	A	1915	26	-	4/7/25/26	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	2MG	a	966	1	-	2/5/27/28	0/3/3/3
26	5MC	A	1962	26	-	5/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
26	PSU	A	1911	26	-	2/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	4/9/29/30	0/2/2/2
1	MA6	a	1518	1	-	2/7/29/30	0/3/3/3

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1915	3TD	C6-C5	11.98	1.49	1.35
26	A	1915	3TD	C2-N1	8.84	1.48	1.37
26	A	1915	3TD	C6-N1	5.60	1.45	1.36
22	v	8	4SU	C4-S4	-4.56	1.59	1.68
26	A	2069	G7M	C5-C4	4.25	1.47	1.39
1	a	527	G7M	C5-C4	4.22	1.47	1.39
24	y	55	PSU	C6-C5	3.95	1.39	1.35
26	A	1911	PSU	C6-C5	3.55	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2504	PSU	C6-C5	3.43	1.39	1.35
26	A	1915	3TD	C2-N3	3.26	1.45	1.38
22	v	55	PSU	C6-C5	3.23	1.39	1.35
1	a	966	2MG	C6-N1	-3.22	1.33	1.37
22	v	54	5MU	C2-N1	3.21	1.43	1.38
26	A	2457	PSU	C4-N3	-3.20	1.32	1.38
22	v	8	4SU	C5-C4	-3.16	1.38	1.42
22	v	55	PSU	C4-N3	-3.11	1.33	1.38
26	A	747	5MU	C4-N3	-3.03	1.33	1.38
26	A	2445	2MG	C6-N1	-3.02	1.33	1.37
1	a	527	G7M	C6-N1	-3.01	1.33	1.37
26	A	746	PSU	C6-C5	2.99	1.38	1.35
26	A	1618	6MZ	C5-C4	2.98	1.48	1.40
26	A	2504	PSU	C4-N3	-2.98	1.33	1.38
1	a	1207	2MG	C6-N1	-2.97	1.33	1.37
26	A	2604	PSU	C4-N3	-2.96	1.33	1.38
26	A	1939	5MU	C6-N1	-2.96	1.33	1.38
26	A	2580	PSU	C4-N3	-2.96	1.33	1.38
26	A	746	PSU	C4-N3	-2.95	1.33	1.38
26	A	2069	G7M	C6-N1	-2.94	1.33	1.37
26	A	955	PSU	C4-N3	-2.93	1.33	1.38
26	A	955	PSU	C6-C5	2.91	1.38	1.35
26	A	2251	OMG	C6-N1	-2.91	1.33	1.37
26	A	2449	H2U	C2-N3	-2.91	1.32	1.38
26	A	1939	5MU	C4-N3	-2.90	1.33	1.38
26	A	2605	PSU	C6-C5	2.88	1.38	1.35
26	A	2030	6MZ	C5-C4	2.88	1.48	1.40
26	A	2457	PSU	C6-C5	2.87	1.38	1.35
22	v	20	H2U	C2-N3	-2.86	1.32	1.38
26	A	1917	PSU	C4-N3	-2.85	1.33	1.38
26	A	1915	3TD	O2-C2	-2.83	1.17	1.23
26	A	2605	PSU	C4-N3	-2.83	1.33	1.38
26	A	2449	H2U	C2-N1	-2.83	1.31	1.35
26	A	1911	PSU	C4-N3	-2.82	1.33	1.38
26	A	2604	PSU	C6-C5	2.80	1.38	1.35
24	y	54	5MU	C6-C5	2.80	1.39	1.34
1	a	1518	MA6	C5-C4	2.80	1.48	1.40
26	A	1915	3TD	O4-C4	-2.78	1.17	1.23
24	y	54	5MU	C4-N3	-2.78	1.33	1.38
26	A	1962	5MC	C6-C5	2.78	1.39	1.34
26	A	1917	PSU	C6-C5	2.74	1.38	1.35
24	y	19	H2U	C2-N3	-2.74	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1835	2MG	C6-N1	-2.74	1.33	1.37
22	v	54	5MU	C4-N3	-2.73	1.33	1.38
1	a	527	G7M	O2'-C2'	-2.71	1.36	1.43
26	A	747	5MU	C6-C5	2.67	1.39	1.34
26	A	2449	H2U	C4-N3	-2.66	1.33	1.37
1	a	1519	MA6	C5-C4	2.63	1.47	1.40
26	A	2580	PSU	C6-C5	2.63	1.38	1.35
1	a	1516	2MG	C6-N1	-2.61	1.34	1.37
1	a	967	5MC	C6-N1	-2.59	1.33	1.38
22	v	8	4SU	C4-N3	-2.57	1.34	1.37
24	y	19	H2U	C4-N3	-2.57	1.33	1.37
22	v	20	H2U	C4-N3	-2.56	1.33	1.37
1	a	516	PSU	C4-N3	-2.56	1.34	1.38
22	v	55	PSU	C2-N3	-2.54	1.33	1.37
22	v	54	5MU	C6-C5	2.53	1.38	1.34
26	A	2552	OMU	C4-N3	-2.53	1.34	1.38
26	A	2069	G7M	O2'-C2'	-2.51	1.37	1.43
1	a	516	PSU	C6-C5	2.48	1.38	1.35
26	A	1915	3TD	C4-N3	2.46	1.45	1.40
24	y	54	5MU	C2-N1	2.45	1.42	1.38
26	A	1917	PSU	C2-N1	-2.44	1.33	1.36
26	A	1939	5MU	C2-N3	-2.44	1.33	1.38
24	y	55	PSU	C4-N3	-2.42	1.34	1.38
26	A	2604	PSU	C2-N3	-2.38	1.33	1.37
26	A	747	5MU	C2-N3	-2.34	1.33	1.38
26	A	2504	PSU	C2-N3	-2.34	1.33	1.37
26	A	747	5MU	C2-N1	2.34	1.42	1.38
26	A	2503	2MA	C2-N3	2.32	1.36	1.31
26	A	747	5MU	C6-N1	-2.30	1.34	1.38
26	A	2457	PSU	C2-N3	-2.27	1.33	1.37
26	A	955	PSU	C2-N3	-2.24	1.33	1.37
26	A	1917	PSU	C2-N3	-2.21	1.33	1.37
26	A	745	1MG	C5-C4	2.20	1.48	1.43
22	v	8	4SU	C2-N1	2.19	1.42	1.38
24	y	37	6IA	C5-C4	2.18	1.46	1.40
24	y	54	5MU	C6-N1	-2.16	1.34	1.38
26	A	2552	OMU	C2-N3	-2.16	1.34	1.38
26	A	2580	PSU	O4'-C1'	-2.15	1.40	1.43
24	y	54	5MU	C4-C5	2.13	1.48	1.44
22	v	54	5MU	C4-C5	2.12	1.48	1.44
1	a	1407	5MC	C6-C5	2.12	1.38	1.34
24	y	55	PSU	C2-N1	-2.09	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2605	PSU	C2-N3	-2.09	1.33	1.37
26	A	2580	PSU	C2-N3	-2.09	1.33	1.37
26	A	1917	PSU	C4-C5	2.07	1.50	1.44
26	A	1911	PSU	C2-N3	-2.06	1.34	1.37
26	A	746	PSU	C2-N3	-2.06	1.34	1.37
26	A	1962	5MC	C6-N1	-2.06	1.34	1.38
22	v	54	5MU	C6-N1	-2.06	1.34	1.38
24	y	54	5MU	C2-N3	-2.04	1.34	1.38
22	v	54	5MU	C2-N3	-2.04	1.34	1.38
26	A	1911	PSU	C2-N1	-2.04	1.34	1.36
1	a	1407	5MC	C6-N1	-2.02	1.34	1.38
26	A	1939	5MU	C6-C5	2.02	1.37	1.34
26	A	955	PSU	C2-N1	-2.01	1.34	1.36
1	a	1498	UR3	C2-N1	2.00	1.41	1.38

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2449	H2U	C4-N3-C2	-9.42	117.98	125.79
22	v	20	H2U	C4-N3-C2	-7.55	119.53	125.79
22	v	8	4SU	C4-N3-C2	-7.47	120.09	127.34
22	v	8	4SU	C5-C4-S4	-6.78	115.74	124.47
26	A	2457	PSU	N1-C2-N3	6.66	122.68	115.13
22	v	8	4SU	C5-C4-N3	6.40	120.62	114.69
26	A	1618	6MZ	C2-N1-C6	6.29	121.98	116.59
24	y	19	H2U	C4-N3-C2	-6.19	120.66	125.79
26	A	955	PSU	N1-C2-N3	6.12	122.06	115.13
26	A	1911	PSU	N1-C2-N3	6.08	122.02	115.13
26	A	2580	PSU	N1-C2-N3	6.06	122.00	115.13
26	A	1915	3TD	N1-C2-N3	6.04	120.90	116.14
26	A	746	PSU	N1-C2-N3	5.92	121.83	115.13
26	A	1939	5MU	C4-N3-C2	-5.83	119.81	127.35
24	y	55	PSU	N1-C2-N3	5.81	121.72	115.13
26	A	2604	PSU	N1-C2-N3	5.75	121.64	115.13
26	A	2504	PSU	N1-C2-N3	5.69	121.58	115.13
1	a	516	PSU	N1-C2-N3	5.66	121.55	115.13
24	y	37	6IA	C2-N1-C6	5.62	121.41	116.59
26	A	1917	PSU	N1-C2-N3	5.57	121.44	115.13
26	A	2605	PSU	N1-C2-N3	5.56	121.43	115.13
22	v	55	PSU	N1-C2-N3	5.53	121.40	115.13
1	a	1498	UR3	C4-N3-C2	-5.40	119.48	124.56
26	A	747	5MU	N3-C2-N1	5.34	121.98	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1939	5MU	C5-C4-N3	5.11	119.67	115.31
26	A	2030	6MZ	C4-C5-N7	-5.06	104.12	109.40
24	y	54	5MU	N3-C2-N1	4.86	121.34	114.89
26	A	747	5MU	C4-N3-C2	-4.83	121.10	127.35
26	A	1939	5MU	N3-C2-N1	4.77	121.22	114.89
26	A	1939	5MU	C5-C6-N1	-4.70	118.51	123.34
1	a	1519	MA6	C4-C5-N7	-4.61	104.59	109.40
22	v	54	5MU	N3-C2-N1	4.60	121.00	114.89
24	y	54	5MU	C4-N3-C2	-4.56	121.44	127.35
26	A	1618	6MZ	C9-N6-C6	-4.50	118.99	122.87
1	a	1518	MA6	C4-C5-N7	-4.47	104.74	109.40
26	A	2552	OMU	C1'-N1-C2	4.45	125.63	117.57
1	a	1402	4OC	O2-C2-N3	-4.42	115.15	122.33
22	v	54	5MU	C4-N3-C2	-4.40	121.66	127.35
26	A	1939	5MU	O4-C4-C5	-4.39	119.81	124.90
1	a	1498	UR3	C1'-N1-C2	4.33	124.30	116.99
26	A	2552	OMU	N3-C2-N1	4.28	120.57	114.89
22	v	54	5MU	C5-C4-N3	4.21	118.90	115.31
26	A	1962	5MC	C5-C4-N3	-4.20	117.14	121.67
26	A	1915	3TD	C4-N3-C2	-4.17	120.08	124.61
26	A	2457	PSU	C4-N3-C2	-4.16	120.34	126.34
26	A	1911	PSU	C4-N3-C2	-4.14	120.37	126.34
22	v	54	5MU	C1'-N1-C2	4.08	124.96	117.57
26	A	746	PSU	C4-N3-C2	-4.08	120.46	126.34
26	A	2605	PSU	C4-N3-C2	-4.02	120.54	126.34
24	y	55	PSU	O2-C2-N1	-4.00	118.38	122.79
26	A	2552	OMU	C4-N3-C2	-3.99	121.31	126.58
26	A	1962	5MC	N4-C4-N3	3.94	125.66	118.48
26	A	2580	PSU	C4-N3-C2	-3.88	120.75	126.34
26	A	1917	PSU	C6-C5-C4	-3.82	115.53	118.20
26	A	747	5MU	C5-C4-N3	3.80	118.56	115.31
26	A	955	PSU	C4-N3-C2	-3.79	120.88	126.34
22	v	54	5MU	O4-C4-C5	-3.78	120.52	124.90
24	y	54	5MU	C5-C4-N3	3.77	118.53	115.31
1	a	516	PSU	C4-N3-C2	-3.75	120.93	126.34
22	v	8	4SU	N3-C2-N1	3.72	119.83	114.89
26	A	1911	PSU	O2-C2-N1	-3.72	118.70	122.79
22	v	55	PSU	C4-N3-C2	-3.68	121.03	126.34
1	a	1518	MA6	N3-C2-N1	-3.63	123.00	128.68
26	A	2604	PSU	C4-N3-C2	-3.62	121.12	126.34
1	a	1518	MA6	N1-C6-N6	-3.62	113.25	117.06
24	y	54	5MU	O4-C4-C5	-3.60	120.72	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2498	OMC	O2-C2-N3	-3.59	116.49	122.33
26	A	2069	G7M	O3'-C3'-C4'	3.58	121.39	111.05
26	A	1917	PSU	O2-C2-N1	-3.57	118.86	122.79
26	A	747	5MU	O4-C4-C5	-3.56	120.78	124.90
1	a	516	PSU	O2-C2-N1	-3.55	118.89	122.79
26	A	2030	6MZ	C9-N6-C6	-3.53	119.83	122.87
26	A	1939	5MU	O2-C2-N1	-3.53	118.10	122.79
22	v	8	4SU	S4-C4-N3	3.48	123.64	120.21
26	A	2504	PSU	C4-N3-C2	-3.45	121.37	126.34
24	y	37	6IA	N3-C2-N1	-3.44	123.31	128.68
1	a	1518	MA6	C10-N6-C9	-3.39	105.19	116.12
26	A	955	PSU	O2-C2-N1	-3.39	119.06	122.79
24	y	55	PSU	C4-N3-C2	-3.35	121.51	126.34
1	a	1519	MA6	C10-N6-C6	-3.29	109.54	119.51
26	A	2552	OMU	C5-C4-N3	3.29	119.76	114.84
26	A	747	5MU	C5-C6-N1	-3.24	120.01	123.34
26	A	2457	PSU	O2-C2-N1	-3.24	119.22	122.79
22	v	55	PSU	C6-C5-C4	-3.24	115.94	118.20
1	a	1498	UR3	C6-N1-C2	-3.23	118.89	121.79
24	y	55	PSU	C6-C5-C4	-3.23	115.94	118.20
1	a	527	G7M	O3'-C3'-C4'	3.22	120.36	111.05
1	a	1519	MA6	C10-N6-C9	-3.21	105.78	116.12
1	a	1518	MA6	C9-N6-C6	-3.21	109.80	119.51
22	v	54	5MU	O2-C2-N3	-3.19	115.55	121.50
22	v	54	5MU	C1'-N1-C6	-3.19	115.82	121.12
1	a	1498	UR3	O2-C2-N3	-3.16	116.89	121.34
24	y	54	5MU	C5-C6-N1	-3.15	120.09	123.34
1	a	527	G7M	O3'-C3'-C2'	3.13	121.94	111.82
26	A	1618	6MZ	C4-C5-N7	-3.12	106.15	109.40
1	a	1407	5MC	O2-C2-N3	-3.08	117.33	122.33
26	A	1618	6MZ	N3-C2-N1	-3.05	123.91	128.68
26	A	2504	PSU	O2-C2-N1	-3.05	119.44	122.79
24	y	37	6IA	C12-N6-C6	-3.03	117.79	122.89
26	A	2552	OMU	O4-C4-C5	-2.97	119.93	125.16
26	A	2605	PSU	O2-C2-N1	-2.96	119.53	122.79
1	a	1519	MA6	N3-C2-N1	-2.96	124.05	128.68
26	A	2580	PSU	O2-C2-N1	-2.92	119.57	122.79
26	A	1962	5MC	C5-C4-N4	-2.92	117.11	121.48
26	A	2504	PSU	C6-C5-C4	-2.91	116.16	118.20
26	A	1917	PSU	C4-N3-C2	-2.90	122.16	126.34
26	A	2604	PSU	O2-C2-N1	-2.87	119.63	122.79
26	A	1911	PSU	C6-C5-C4	-2.84	116.21	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	967	5MC	C1'-N1-C6	-2.83	116.41	121.12
26	A	746	PSU	O2-C2-N1	-2.81	119.70	122.79
22	v	8	4SU	C1'-N1-C2	2.78	122.60	117.57
26	A	2069	G7M	C3'-C2'-C1'	2.76	105.14	100.98
1	a	967	5MC	CM5-C5-C6	-2.76	119.16	122.85
26	A	1962	5MC	C6-N1-C2	-2.75	117.07	120.87
24	y	19	H2U	O2-C2-N1	2.72	126.52	123.11
26	A	2069	G7M	O3'-C3'-C2'	2.65	120.40	111.82
1	a	1407	5MC	C5-C4-N3	-2.63	118.84	121.67
26	A	747	5MU	O2-C2-N3	-2.60	116.65	121.50
26	A	1915	3TD	O4-C4-N3	-2.57	115.59	120.30
26	A	1835	2MG	C5-C6-N1	2.57	118.49	113.95
26	A	2604	PSU	C6-C5-C4	-2.57	116.40	118.20
26	A	2580	PSU	O4'-C1'-C2'	2.56	108.75	105.14
26	A	2445	2MG	CM2-N2-C2	-2.53	118.28	123.86
26	A	2498	OMC	CM2-O2'-C2'	-2.50	107.95	114.52
26	A	2605	PSU	C6-C5-C4	-2.50	116.45	118.20
26	A	2030	6MZ	C1'-N9-C4	2.43	130.92	126.64
26	A	746	PSU	C5-C6-N1	-2.42	118.47	122.11
26	A	2445	2MG	C5-C6-N1	2.38	118.16	113.95
26	A	745	1MG	C8-N7-C5	2.38	107.52	102.99
1	a	1516	2MG	C5-C6-N1	2.36	118.13	113.95
26	A	2498	OMC	O2-C2-N1	2.35	123.75	118.89
1	a	527	G7M	C3'-C2'-C1'	2.34	104.50	100.98
1	a	1207	2MG	C5-C6-N1	2.34	118.08	113.95
26	A	2251	OMG	C5-C6-N1	2.32	118.06	113.95
26	A	2552	OMU	O2-C2-N3	-2.32	117.19	121.50
26	A	2069	G7M	C5'-C4'-C3'	2.30	123.81	115.18
1	a	1498	UR3	C3U-N3-C4	2.30	121.18	117.89
1	a	1516	2MG	C8-N7-C5	2.29	107.36	102.99
1	a	516	PSU	O4'-C1'-C2'	2.29	108.38	105.14
26	A	1835	2MG	C8-N7-C5	2.28	107.33	102.99
26	A	2445	2MG	C8-N7-C5	2.27	107.32	102.99
26	A	2552	OMU	C1'-N1-C6	-2.26	115.90	120.84
26	A	745	1MG	C5-C6-N1	2.25	117.28	113.90
26	A	2503	2MA	C5-C6-N1	2.25	117.90	114.02
1	a	1402	4OC	O2-C2-N1	2.24	123.51	118.89
1	a	1402	4OC	C6-C5-C4	2.23	119.69	116.96
1	a	966	2MG	C5-C6-N1	2.23	117.89	113.95
1	a	966	2MG	C8-N7-C5	2.22	107.22	102.99
22	v	55	PSU	O2-C2-N3	-2.21	117.65	121.82
1	a	1402	4OC	C1'-N1-C2	2.20	123.33	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1835	2MG	CM2-N2-C2	-2.19	119.02	123.86
1	a	516	PSU	C6-C5-C4	-2.17	116.68	118.20
26	A	2457	PSU	C5-C6-N1	-2.16	118.88	122.11
22	v	54	5MU	C5-C6-N1	-2.14	121.14	123.34
24	y	54	5MU	O2-C2-N3	-2.13	117.54	121.50
1	a	1207	2MG	C8-N7-C5	2.12	107.02	102.99
22	v	54	5MU	C6-N1-C2	-2.10	119.17	121.30
26	A	2030	6MZ	C2-N1-C6	2.08	118.37	116.59
26	A	1962	5MC	O4'-C1'-N1	2.07	113.10	108.36
1	a	1407	5MC	C5-C6-N1	-2.06	121.22	123.34
24	y	54	5MU	C1'-N1-C2	2.05	121.27	117.57
26	A	747	5MU	C1'-N1-C2	2.04	121.26	117.57
26	A	2251	OMG	C8-N7-C5	2.03	106.86	102.99
22	v	20	H2U	O2-C2-N1	2.02	125.64	123.11
24	y	19	H2U	O2-C2-N3	-2.01	117.75	121.50
26	A	1917	PSU	O4-C4-N3	-2.00	116.28	120.12

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3'
1	a	527	G7M	C4'
26	A	2069	G7M	C3'
26	A	2069	G7M	C4'

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	966	2MG	N1-C2-N2-CM2
1	a	966	2MG	N3-C2-N2-CM2
1	a	1402	4OC	O4'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C2
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	N1-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C10
22	v	54	5MU	C3'-C4'-C5'-O5'
22	v	54	5MU	O4'-C4'-C5'-O5'
22	v	55	PSU	O4'-C1'-C5-C4
22	v	55	PSU	O4'-C1'-C5-C6
24	y	19	H2U	O4'-C1'-N1-C2
24	y	19	H2U	O4'-C1'-N1-C6
24	y	37	6IA	C5-C6-N6-C12

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Mol	Chain	Res	Type	Atoms
26	A	746	PSU	C2'-C1'-C5-C4
26	A	1618	6MZ	O4'-C4'-C5'-O5'
26	A	1618	6MZ	C3'-C4'-C5'-O5'
26	A	1915	3TD	O4'-C1'-C5-C4
26	A	1915	3TD	O4'-C1'-C5-C6
26	A	1915	3TD	C3'-C4'-C5'-O5'
26	A	1915	3TD	O4'-C4'-C5'-O5'
26	A	1917	PSU	C2'-C1'-C5-C4
26	A	1962	5MC	C2'-C1'-N1-C6
26	A	2030	6MZ	N1-C6-N6-C9
26	A	2030	6MZ	C3'-C4'-C5'-O5'
26	A	2445	2MG	O4'-C4'-C5'-O5'
26	A	2445	2MG	C3'-C4'-C5'-O5'
26	A	2503	2MA	O4'-C4'-C5'-O5'
26	A	2552	OMU	O4'-C1'-N1-C2
1	a	1498	UR3	O4'-C1'-N1-C6
26	A	1962	5MC	C2'-C1'-N1-C2
26	A	1917	PSU	O4'-C4'-C5'-O5'
26	A	2504	PSU	O4'-C4'-C5'-O5'
1	a	1402	4OC	C3'-C4'-C5'-O5'
26	A	1917	PSU	C3'-C4'-C5'-O5'
26	A	2069	G7M	O4'-C4'-C5'-O5'
26	A	2069	G7M	C3'-C4'-C5'-O5'
26	A	2457	PSU	O4'-C4'-C5'-O5'
26	A	2504	PSU	C3'-C4'-C5'-O5'
1	a	1519	MA6	N1-C6-N6-C10
26	A	2552	OMU	O4'-C1'-N1-C6
26	A	2030	6MZ	O4'-C4'-C5'-O5'
24	y	37	6IA	N1-C6-N6-C12
24	y	19	H2U	O4'-C4'-C5'-O5'
1	a	1519	MA6	C5-C6-N6-C9
24	y	19	H2U	C3'-C4'-C5'-O5'
26	A	1962	5MC	C4'-C5'-O5'-P
26	A	2251	OMG	C4'-C5'-O5'-P
26	A	2457	PSU	C3'-C4'-C5'-O5'
26	A	1962	5MC	O4'-C1'-N1-C6
26	A	1911	PSU	O4'-C1'-C5-C4
1	a	1402	4OC	C3'-C2'-O2'-CM2
26	A	1962	5MC	O4'-C1'-N1-C2
24	y	37	6IA	C12-C13-C14-C15
1	a	527	G7M	C3'-C4'-C5'-O5'
26	A	746	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
26	A	1911	PSU	O4'-C1'-C5-C6
22	v	54	5MU	C2'-C1'-N1-C2
1	a	1402	4OC	C2'-C1'-N1-C2
22	v	20	H2U	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 153 ligands modelled in this entry, 150 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	FME	v	101	22	8,9,10	0.93	0	7,9,11	1.47	1 (14%)
63	GNP	z	701	60	29,34,34	1.50	4 (13%)	33,54,54	2.08	10 (30%)
62	SEC	y	701	24	2,5,6	0.72	0	0,5,7	-	-

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
61	FME	v	101	22	-	4/7/9/11	-
63	GNP	z	701	60	-	5/14/38/38	0/3/3/3
62	SEC	y	701	24	-	0/0/4/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	701	GNP	PB-N3B	3.83	1.73	1.63
63	z	701	GNP	C5-C6	3.81	1.47	1.41
63	z	701	GNP	PG-N3B	3.51	1.72	1.63
63	z	701	GNP	C5-C4	2.48	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	701	GNP	PB-O3A-PA	-5.05	114.82	132.62
63	z	701	GNP	C2-N3-C4	4.57	120.58	115.36
63	z	701	GNP	C5-C6-N1	-4.15	117.76	123.43
63	z	701	GNP	C2-N1-C6	3.99	122.26	115.93
63	z	701	GNP	C4-C5-C6	-3.27	117.68	120.80
61	v	101	FME	O-C-CA	-3.25	116.26	124.78
63	z	701	GNP	N3-C2-N1	-2.92	123.33	127.22
63	z	701	GNP	C3'-C2'-C1'	2.86	105.28	100.98
63	z	701	GNP	O3G-PG-O1G	-2.37	107.51	113.45
63	z	701	GNP	C4-C5-N7	-2.33	106.97	109.40
63	z	701	GNP	O1G-PG-N3B	-2.07	108.73	111.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

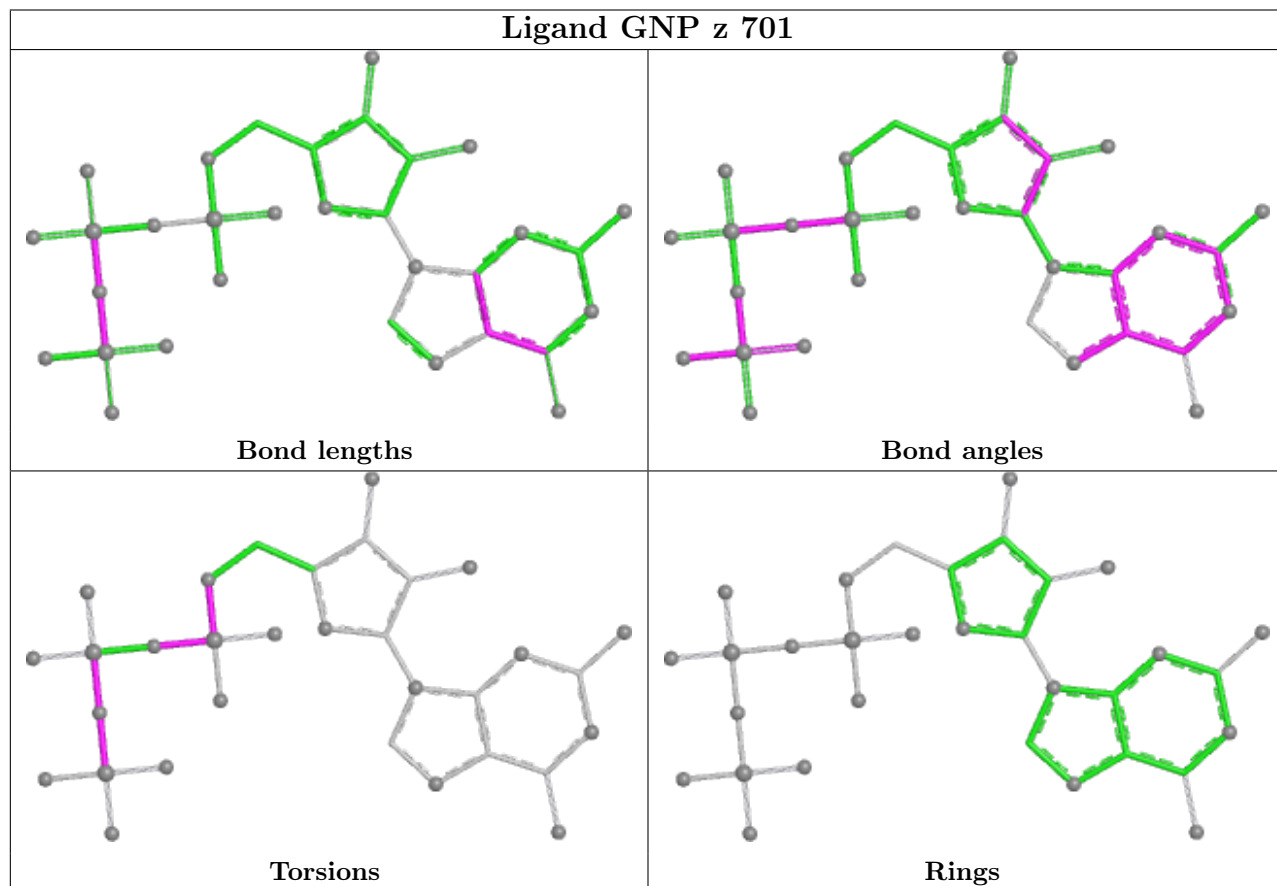
Mol	Chain	Res	Type	Atoms
61	v	101	FME	O1-CN-N-CA
61	v	101	FME	C-CA-CB-CG
63	z	701	GNP	PB-N3B-PG-O1G
63	z	701	GNP	PG-N3B-PB-O1B
63	z	701	GNP	C5'-O5'-PA-O3A
63	z	701	GNP	C5'-O5'-PA-O2A
61	v	101	FME	CB-CA-N-CN
63	z	701	GNP	PB-O3A-PA-O2A
61	v	101	FME	N-CA-CB-CG

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.

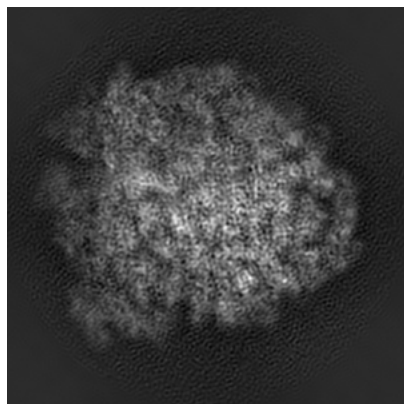
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4124. These allow visual inspection of the internal detail of the map and identification of artifacts.

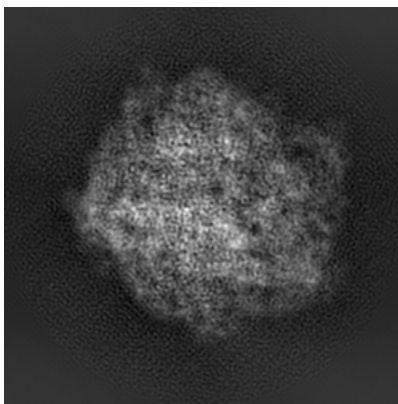
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

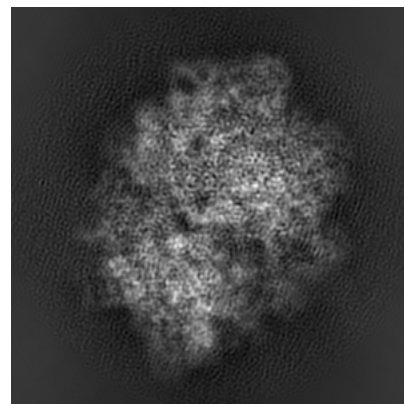
6.1.1 Primary map



X

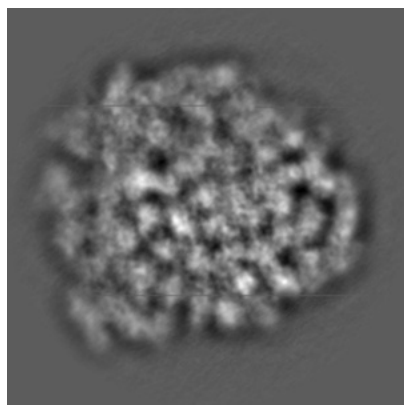


Y

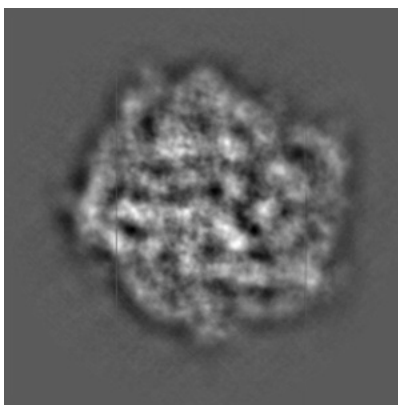


Z

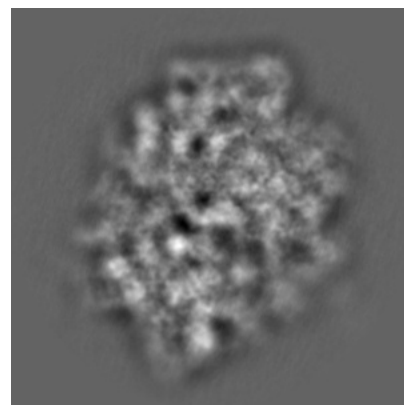
6.1.2 Raw map



X



Y

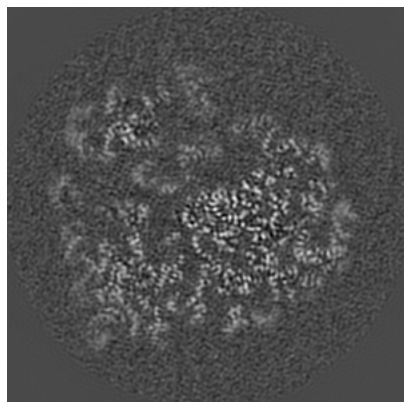


Z

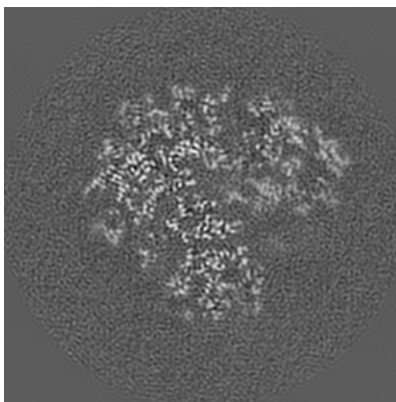
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

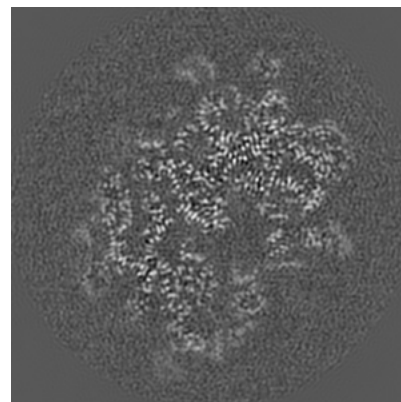
6.2.1 Primary map



X Index: 136

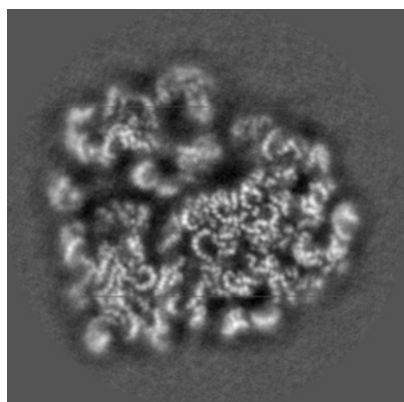


Y Index: 136

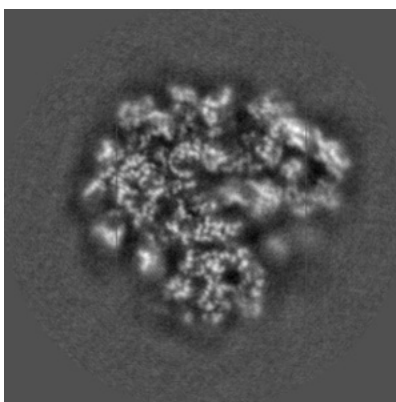


Z Index: 136

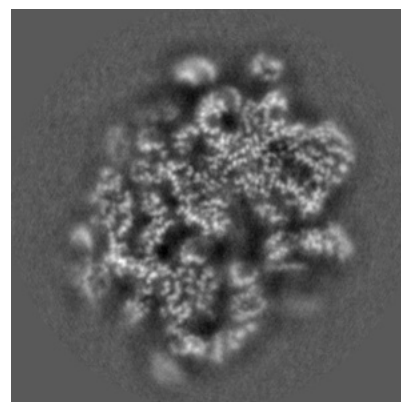
6.2.2 Raw map



X Index: 136



Y Index: 136

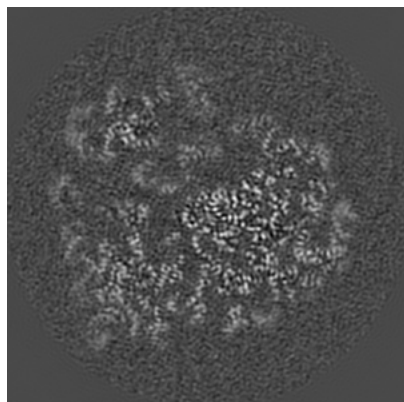


Z Index: 136

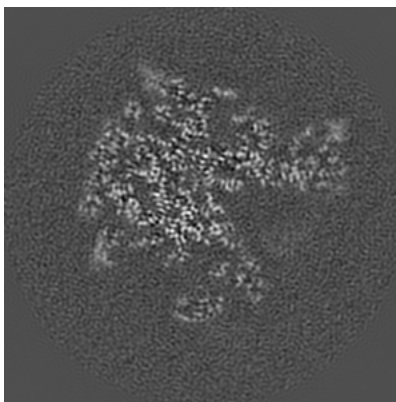
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

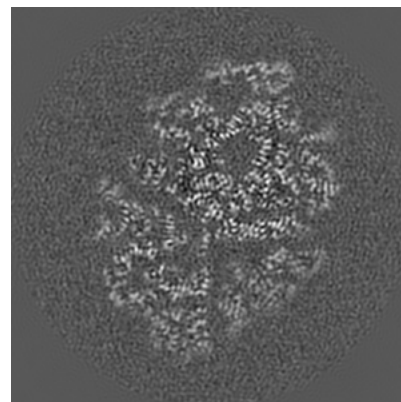
6.3.1 Primary map



X Index: 136

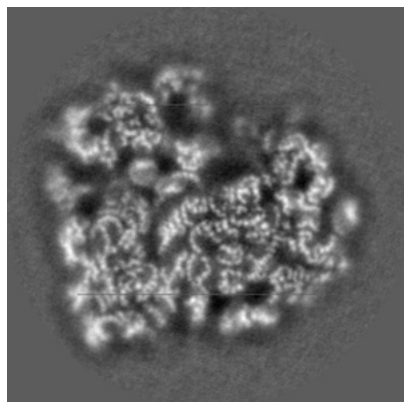


Y Index: 148

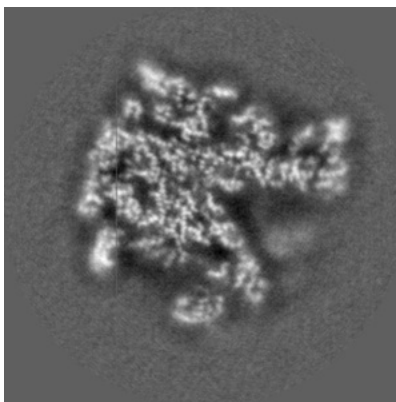


Z Index: 119

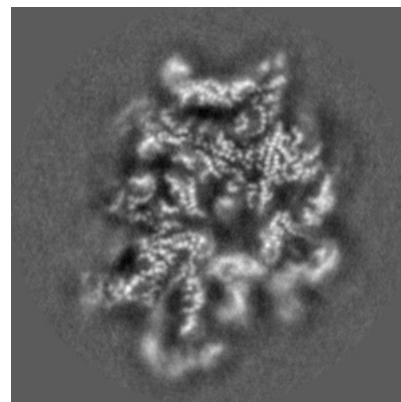
6.3.2 Raw map



X Index: 132



Y Index: 148

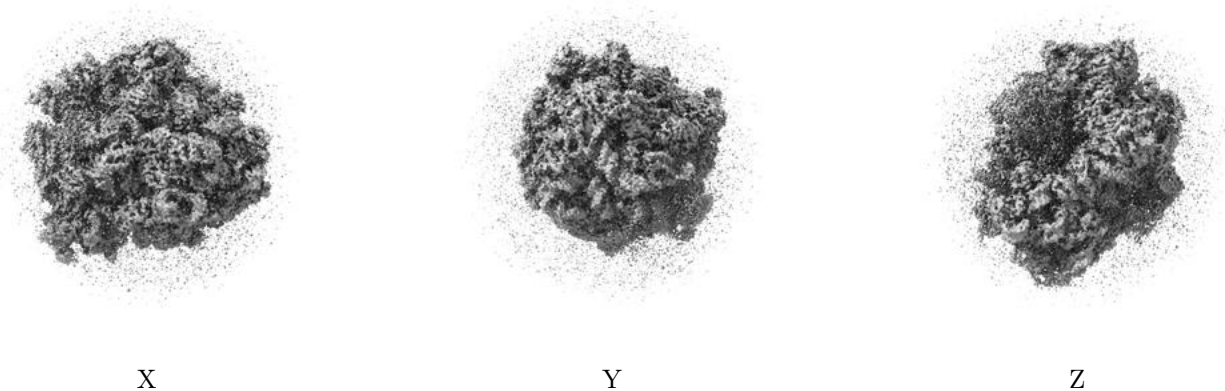


Z Index: 151

The images above show the largest variance slices of the map in three orthogonal directions.

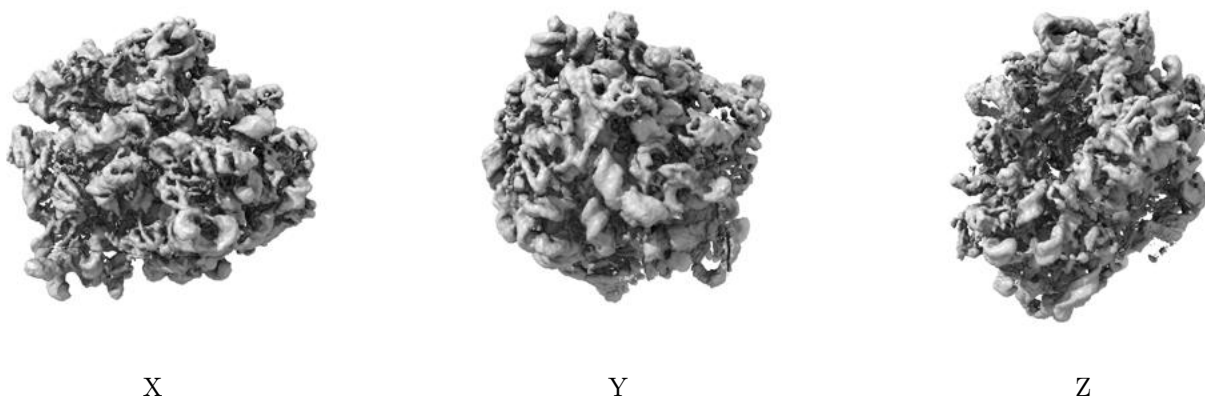
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.56. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

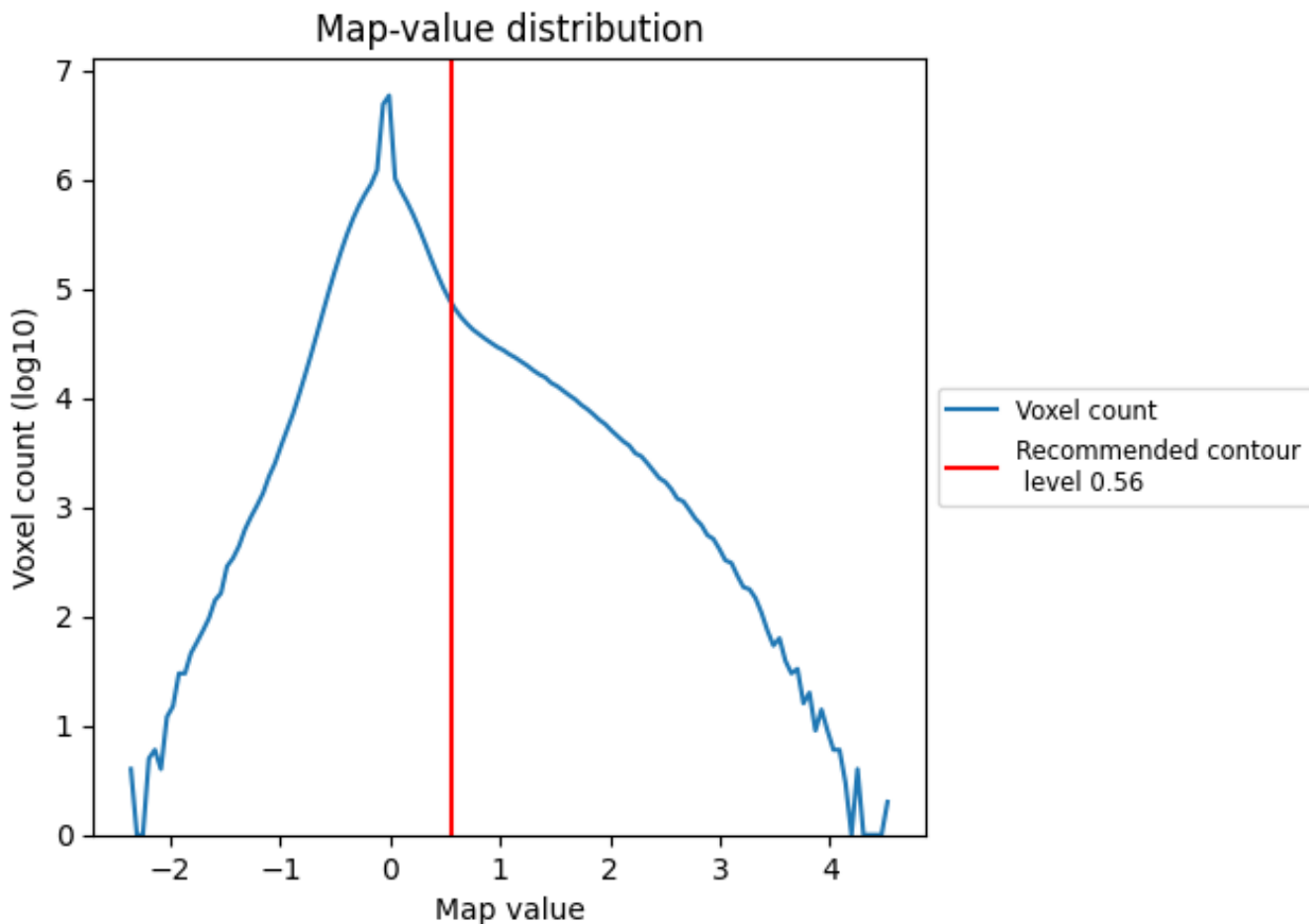
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

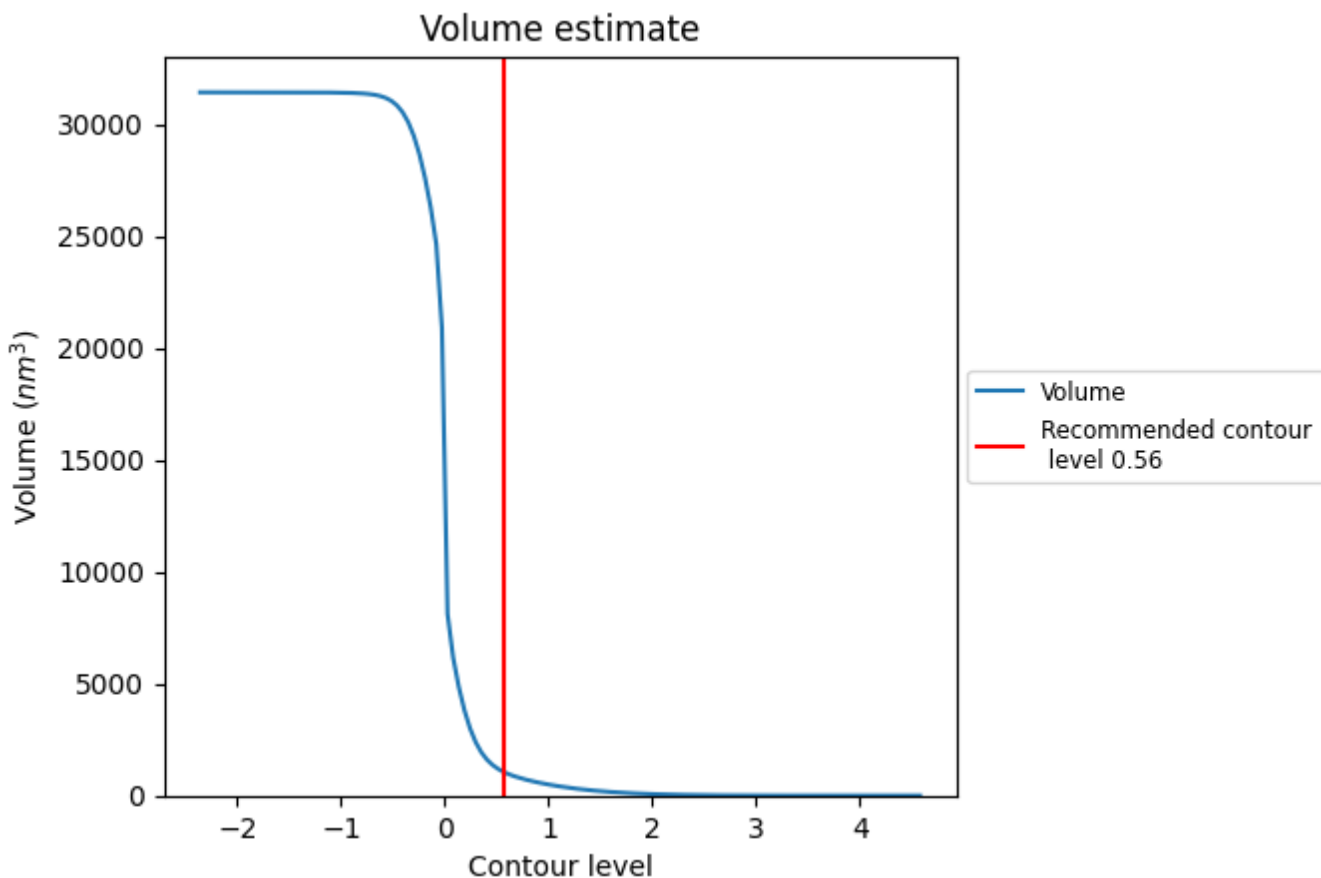
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

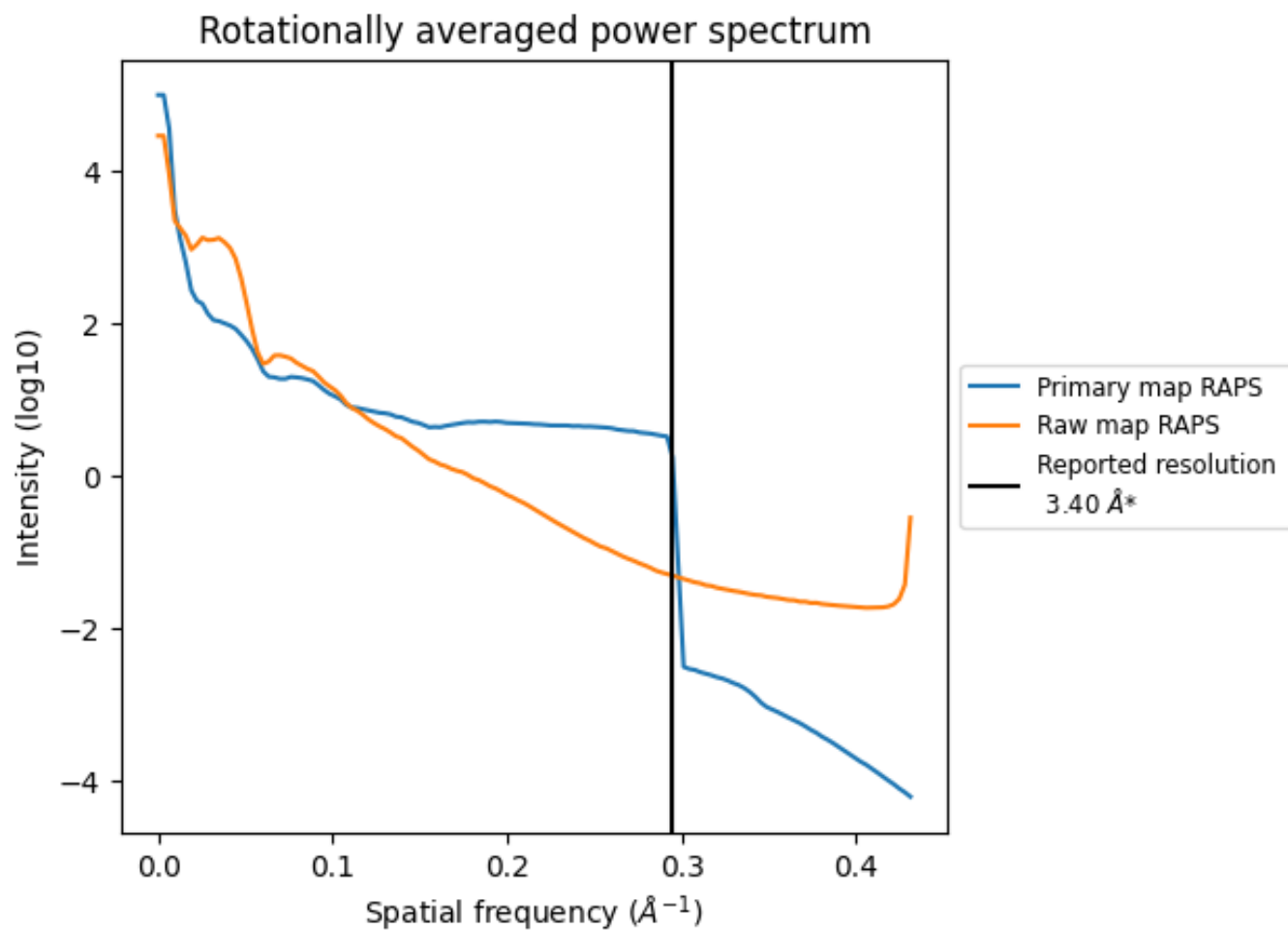
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1071 nm³; this corresponds to an approximate mass of 968 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

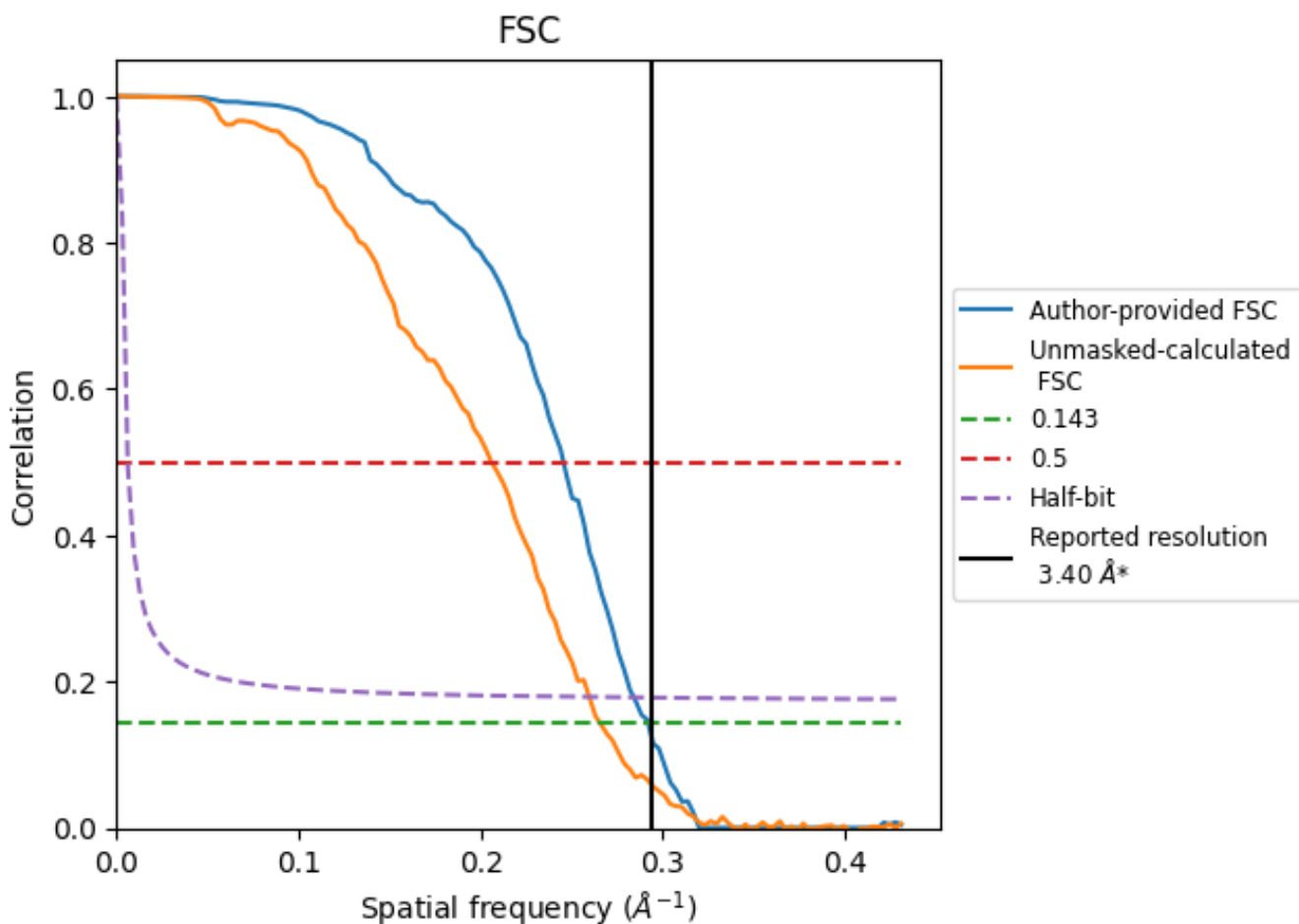


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

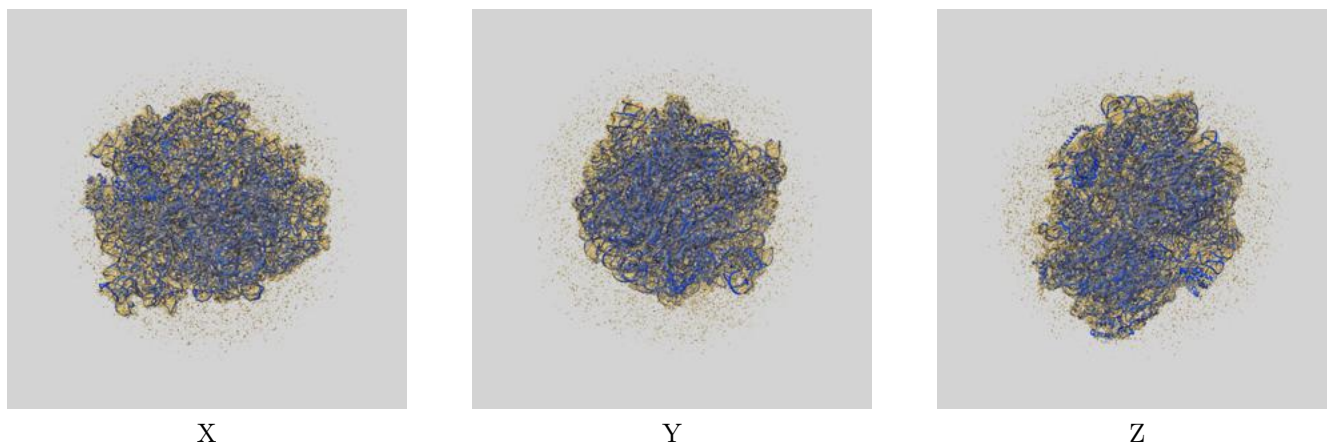
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	4.07	3.52
Unmasked-calculated*	3.76	4.85	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

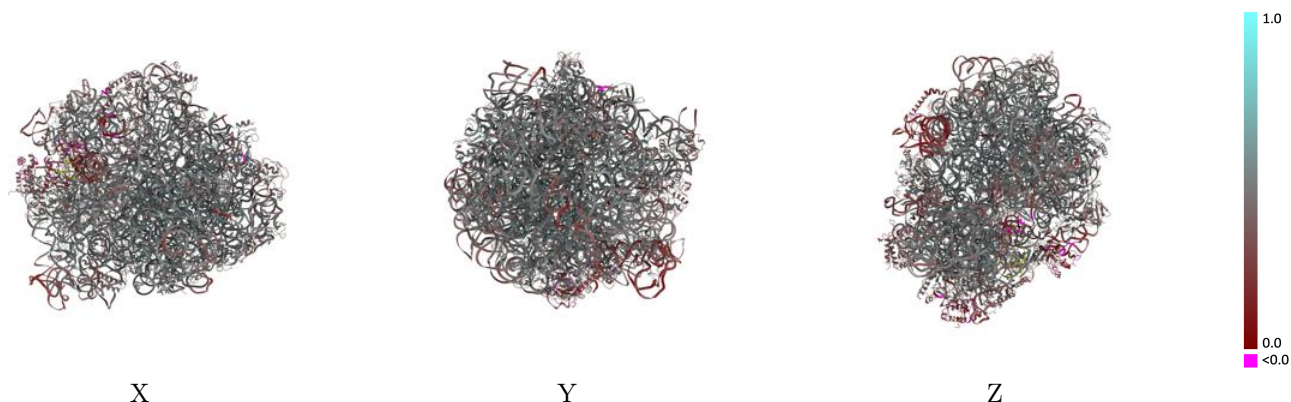
This section contains information regarding the fit between EMDB map EMD-4124 and PDB model 5LZD. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



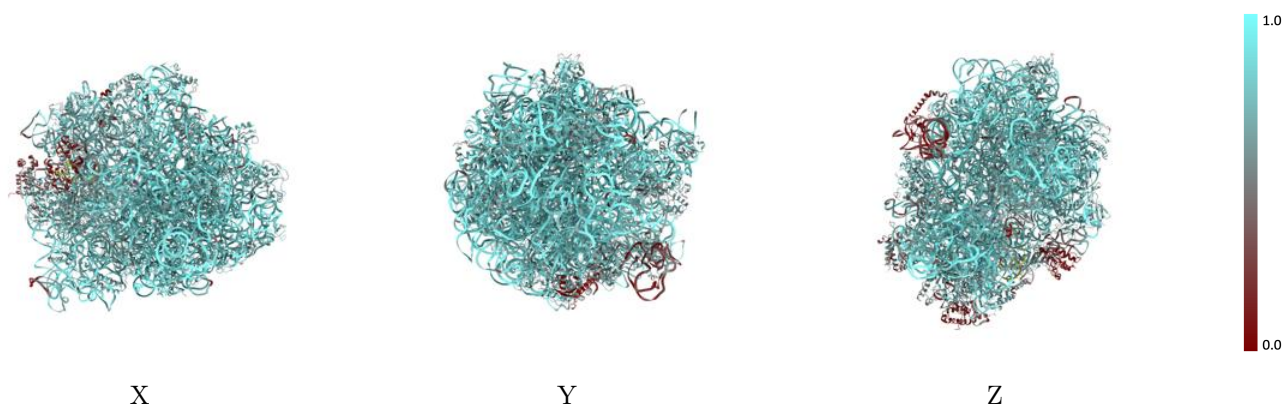
The images above show the 3D surface view of the map at the recommended contour level 0.56 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



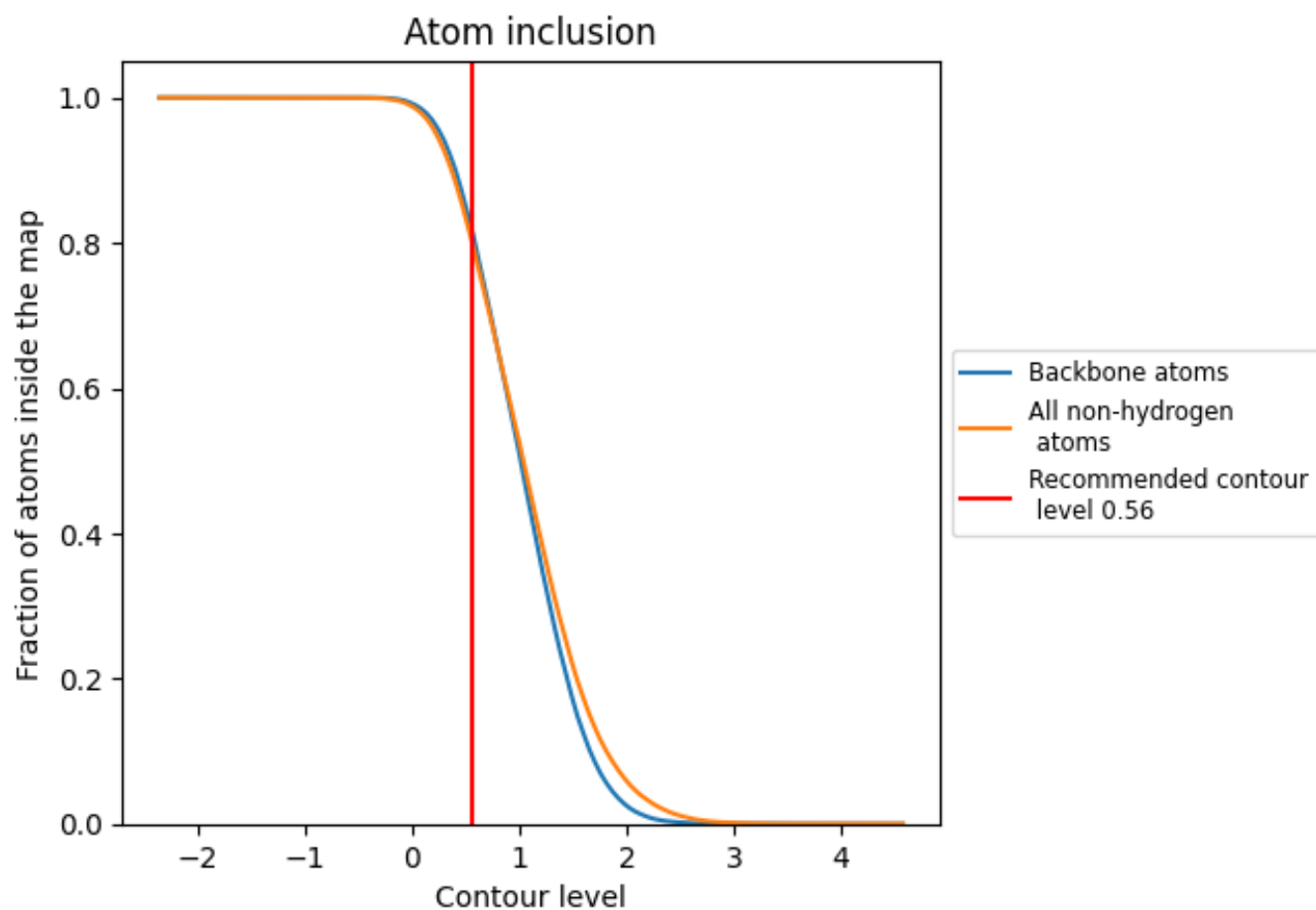
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.56).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

















































The table lists the average atom inclusion at the recommended contour level (0.56) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8004	 0.4520
0	 0.7383	 0.4790
1	 0.6318	 0.4410
2	 0.8282	 0.5080
3	 0.8126	 0.5170
4	 0.7338	 0.4780
6	 0.5673	 0.3210
A	 0.8724	 0.4700
B	 0.8802	 0.4430
C	 0.7918	 0.5040
D	 0.7562	 0.4840
E	 0.6961	 0.4490
F	 0.6485	 0.3980
G	 0.6777	 0.4170
H	 0.2464	 0.2600
I	 0.0656	 0.1740
J	 0.7664	 0.4790
K	 0.7254	 0.4820
L	 0.7421	 0.4720
M	 0.7610	 0.4770
N	 0.7671	 0.4840
O	 0.6999	 0.4230
P	 0.7320	 0.4700
Q	 0.7819	 0.4930
R	 0.7290	 0.4540
S	 0.7213	 0.4790
T	 0.7054	 0.4470
U	 0.6562	 0.4040
V	 0.6870	 0.4470
W	 0.7746	 0.4960
X	 0.7770	 0.4830
Y	 0.6519	 0.3800
Z	 0.7483	 0.4740
a	 0.8847	 0.4690
b	 0.4958	 0.3490



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Chain	Atom inclusion	Q-score
c	 0.7207	 0.4520
d	 0.6484	 0.4210
e	 0.7172	 0.4690
f	 0.7164	 0.4220
g	 0.6419	 0.3950
h	 0.7344	 0.4670
i	 0.6721	 0.4030
j	 0.6234	 0.4000
k	 0.7258	 0.4330
l	 0.7709	 0.4830
m	 0.6948	 0.4050
n	 0.7212	 0.4430
o	 0.7319	 0.4590
p	 0.6986	 0.4330
q	 0.7204	 0.4470
r	 0.7099	 0.4470
s	 0.6766	 0.4110
t	 0.6708	 0.4160
u	 0.5912	 0.3340
v	 0.8300	 0.4470
w	 0.3548	 0.2470
x	 0.4215	 0.2630
y	 0.7601	 0.3610
z	 0.5401	 0.3770