



## Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 10:58 am BST

PDB ID : 8RCL  
EMDB ID : EMD-19054  
Title : Escherichia coli paused disome complex (Non-rotated disome interface class 1)  
Authors : Fluegel, T.; Schacherl, M.  
Deposited on : 2023-12-06  
Resolution : 3.49 Å (reported)  
Based on initial model : 7N1P

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

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

A user guide is available at

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

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

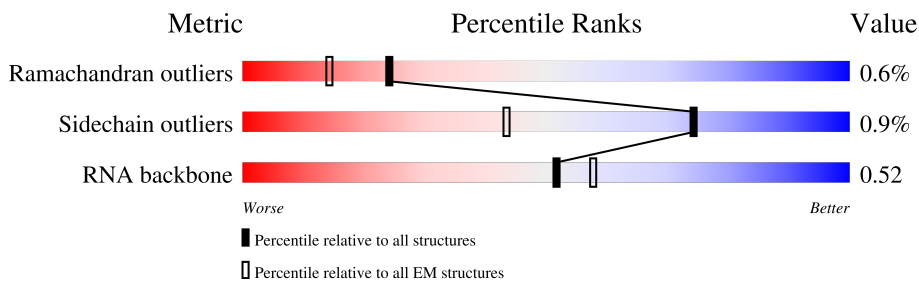
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.49 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.




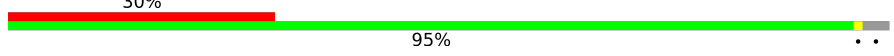
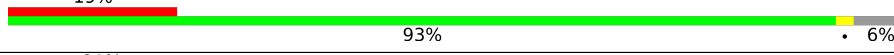
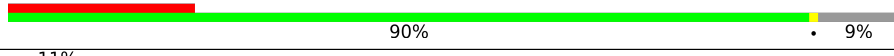
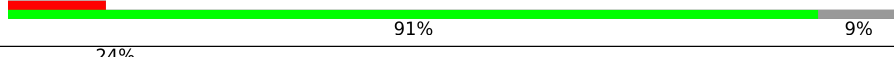
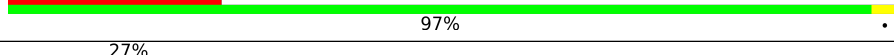
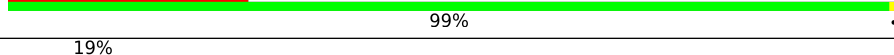
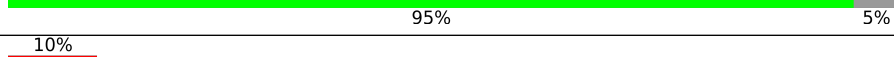
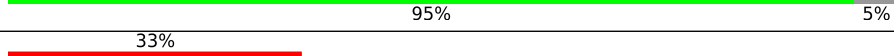
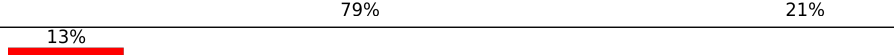
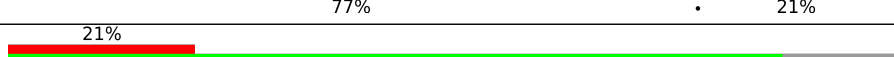
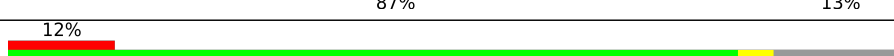

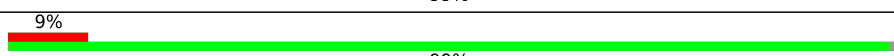
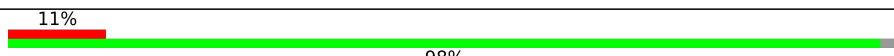
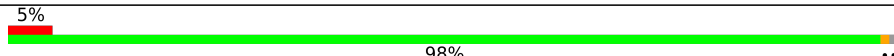
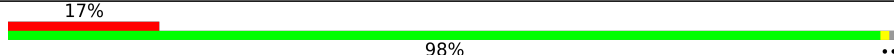
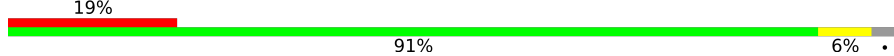

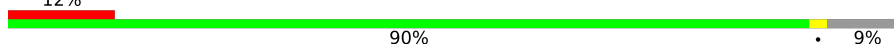
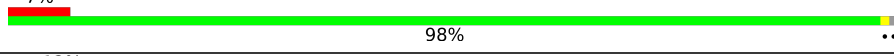
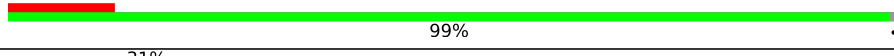
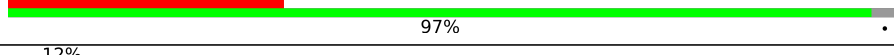
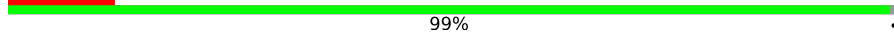

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	12	78	
2	32	59	
3	4	70	
4	62	65	
5	71	2904	
5	72	2904	
6	82	120	
7	A1	1542	

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Mol	Chain	Length	Quality of chain
7	A2	1542	
8	B	241	
8	B2	241	
9	C1	233	
9	C2	233	
10	D1	206	
10	D2	206	
11	E1	167	
11	E2	167	
12	F1	135	
12	F2	135	
13	G1	179	
13	G2	179	
14	H1	130	
14	H2	130	
15	I1	130	
15	I2	130	
16	J1	103	
16	J2	103	
17	K1	129	
17	K2	129	
18	L1	124	
18	L2	124	
19	M1	118	
19	M2	118	

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Mol	Chain	Length	Quality of chain
20	N1	101	15% 97%
20	N2	101	5% 99%
21	O1	89	20% 99%
21	O2	89	11% 98%
22	P1	82	9% 99%
23	Q1	84	14% 95% 5%
23	Q2	84	13% 94% 5%
24	R1	75	35% 96%
24	R2	75	25% 93% 5%
25	S1	92	30% 89% 10%
25	S2	92	8% 90% 10%
26	T1	87	11% 92% 7%
27	U1	71	44% 96%
27	U2	71	28% 96%
28	V2	64	64% 31% 67%
29	W	76	5% 59% 32% 9%
30	W1	76	7% 29% 17% 53%
31	X2	77	45% 58% 35% 6%
32	Y1	76	16% 38% 8% 53%
33	Y2	76	93% 64% 32%
34	Z1	557	98%
35	a2	234	51% 57% 43%
36	b2	273	8% 99%
37	e2	179	18% 98%
38	g2	55	24% 95% 5%

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Mol	Chain	Length	Quality of chain
39	h2	136	<p>21% 100%</p>
40	i2	149	<p>28% 97%</p>
41	l2	46	<p>9% 98%</p>
42	o2	144	<p>35% 65%</p>
43	p	10	<p>90% 70% 20% 10%</p>
44	r2	117	<p>24% 99%</p>
45	z2	85	<p>15% 89% 11%</p>

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 188653 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 protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	12	77	625	388	129	106	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	32	58	449	281	87	79	2	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	67	529	328	100	95	6	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	62	64	504	323	105	74	2	0	0

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	71	30	644	288	119	207	30	0	0
5	72	2904	62355	27824	11468	20159	2904	0	0

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	82	120	2569	1144	468	837	120	0	0

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	A1	1542	33092	14767	6064	10719	1542	0	0
7	A2	1537	32990	14721	6049	10683	1537	0	0

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	B	233	1815	1145	325	337	8	0	0
8	B2	227	1776	1123	318	327	8	0	0

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C1	213	1665	1054	312	295	4	0	0
9	C2	212	1658	1049	311	294	4	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D1	205	1643	1026	315	298	4	0	0
10	D2	205	1643	1026	315	298	4	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E1	158	1166	725	220	215	6	0	0
11	E2	158	1166	725	220	215	6	0	0

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F1	106	Total	C	N	O	S	0	0
			862	545	156	154	7		
12	F2	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G1	155	Total	C	N	O	S	0	0
			1228	767	237	220	4		
13	G2	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H1	129	Total	C	N	O	S	0	0
			979	616	173	184	6		
14	H2	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		
15	I2	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J1	102	Total	C	N	O	S	0	0
			817	509	157	150	1		
16	J2	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.



Mol	Chain	Residues	Atoms					AltConf	Trace
17	K1	115	Total	C	N	O	S	0	0
			857	528	168	158	3		
17	K2	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L1	123	Total	C	N	O	S	0	0
			955	590	196	165	4		
18	L2	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M1	115	Total	C	N	O	S	0	0
			891	552	179	157	3		
19	M2	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		
20	N2	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		
21	O2	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P1	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q1	80	Total	C	N	O	S	0	0
			648	411	121	113	3		
23	Q2	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R1	74	Total	C	N	O	S	0	0
			624	395	122	105	2		
24	R2	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S1	83	Total	C	N	O	S	0	0
			663	424	126	111	2		
25	S2	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U1	70	Total	C	N	O	S	0	0
			590	366	125	98	1		
27	U2	70	Total	C	N	O	S	0	0
			584	363	122	98	1		

- Molecule 28 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V2	64	Total	C	N	O	P	0	0
			1382	619	267	432	64		

- Molecule 29 is a RNA chain called tRNA-Trp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
29	W	76	1630	730	286	536	76	2	0	0

- Molecule 30 is a RNA chain called tRNA-Phe (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
30	W1	36	781	352	143	248	36	2	0	0

- Molecule 31 is a RNA chain called tRNA-Arg (E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
31	X2	77	1654	740	297	538	77	2	0	0

- Molecule 32 is a RNA chain called tRNA-Val (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
32	Y1	36	778	348	142	252	36	0	0

- Molecule 33 is a RNA chain called tRNA-Ala (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
33	Y2	76	1628	726	293	533	76	0	0

- Molecule 34 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	Z1	9	75	49	10	16	0	0

- Molecule 35 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	a2	134	1026	645	186	193	2	0	0

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	b2	271	2082	1288	423	364	7	0	0

- Molecule 37 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	e2	178	1420	905	251	258	6	0	0

- Molecule 38 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	g2	52	427	275	78	74	0	0

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	h2	136	1085	692	209	178	6	1	0

- Molecule 40 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	i2	149	1111	699	197	214	1	0	0

- Molecule 41 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	l2	46	377	228	90	57	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	o2	51	377	231	83	62	1	0	0

- Molecule 43 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	p	10	76	47	18	11	0	0

- Molecule 44 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	r2	116	891	552	178	161	0	0

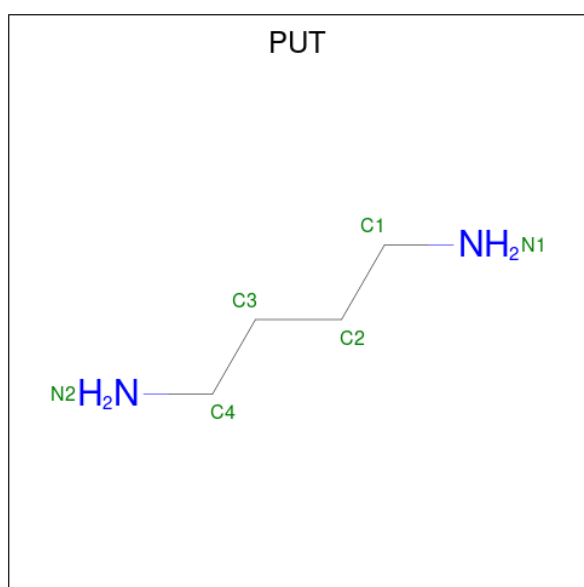
- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	z2	76	582	360	117	104	1	0	0

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

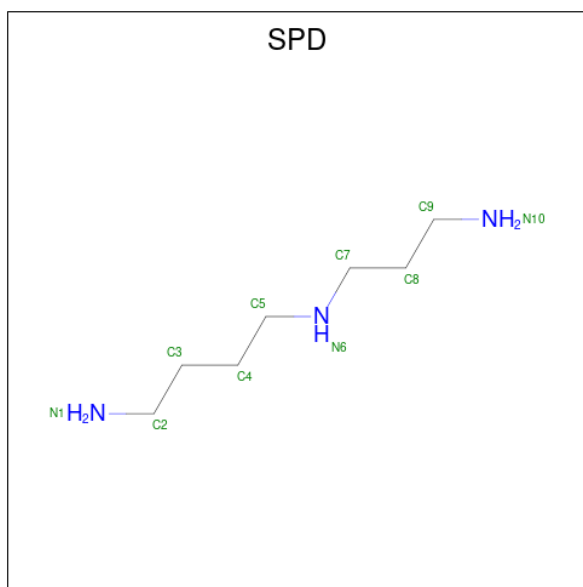
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
46	4	1	1	1	0
46	B	1	1	1	0

- Molecule 47 is 1,4-DIAMINOBTUTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
47	72	1	Total	C	N	0
			6	4	2	
47	72	1	Total	C	N	0
			6	4	2	

- Molecule 48 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
48	72	1	Total	C	N	0
			10	7	3	

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

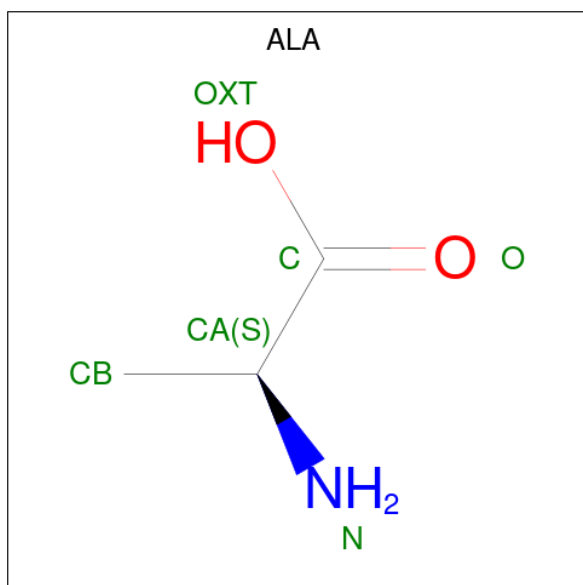
Mol	Chain	Residues	Atoms		AltConf
49	72	189	Total	Mg	0
			189	189	
49	82	1	Total	Mg	0
			1	1	
49	A1	59	Total	Mg	0
			59	59	
49	A2	42	Total	Mg	0
			42	42	
49	V2	1	Total	Mg	0
			1	1	
49	W	1	Total	Mg	0
			1	1	
49	Y2	1	Total	Mg	0
			1	1	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
49	b2	1	Total	Mg	0
			1	1	
49	o2	1	Total	Mg	0
			1	1	

- Molecule 50 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).

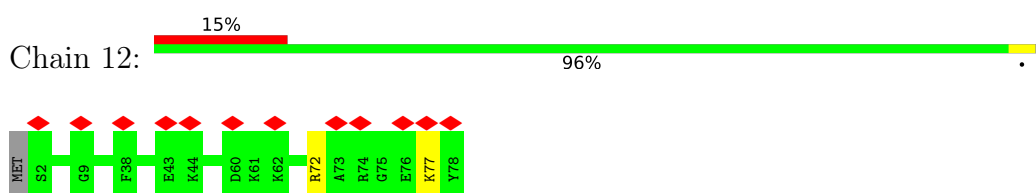


Mol	Chain	Residues	Atoms				AltConf
50	Y2	1	Total	C	N	O	0
			5	3	1	1	

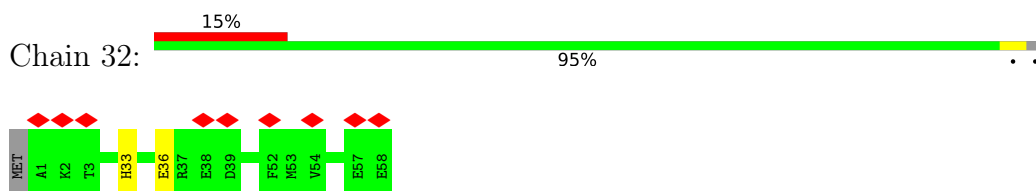
### 3 Residue-property plots [i](#)

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.

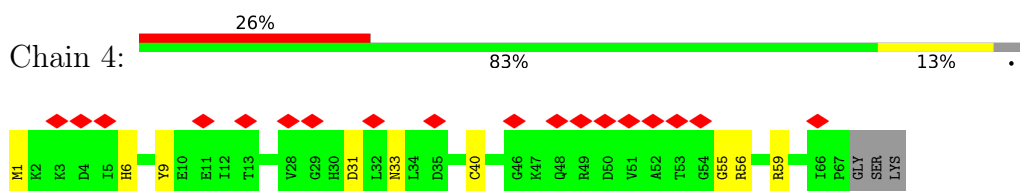
- Molecule 1: 50S ribosomal protein L28



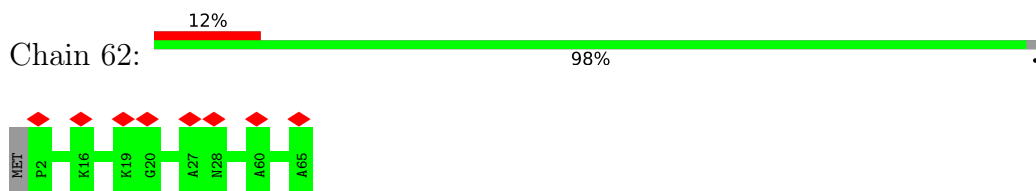
- Molecule 2: 50S ribosomal protein L30



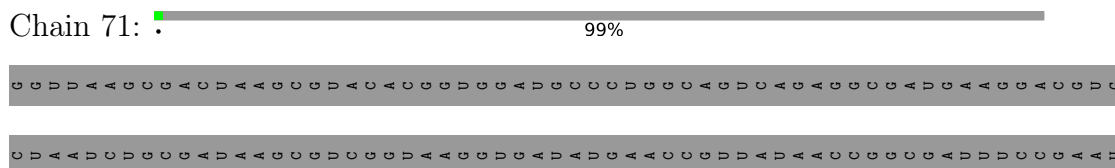
- Molecule 3: Large ribosomal subunit protein bL31



- Molecule 4: 50S ribosomal protein L35

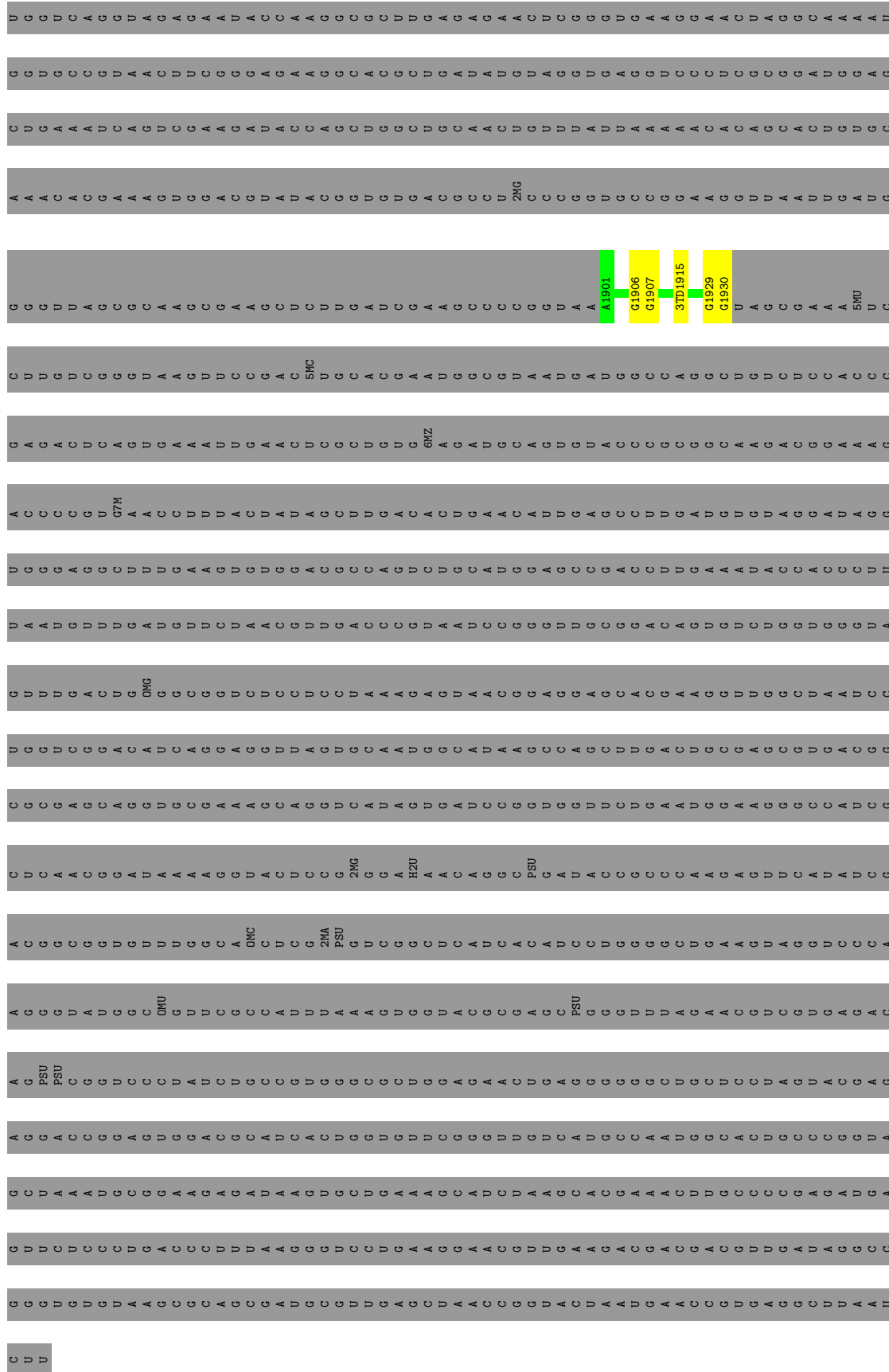


- Molecule 5: 23S ribosomal RNA



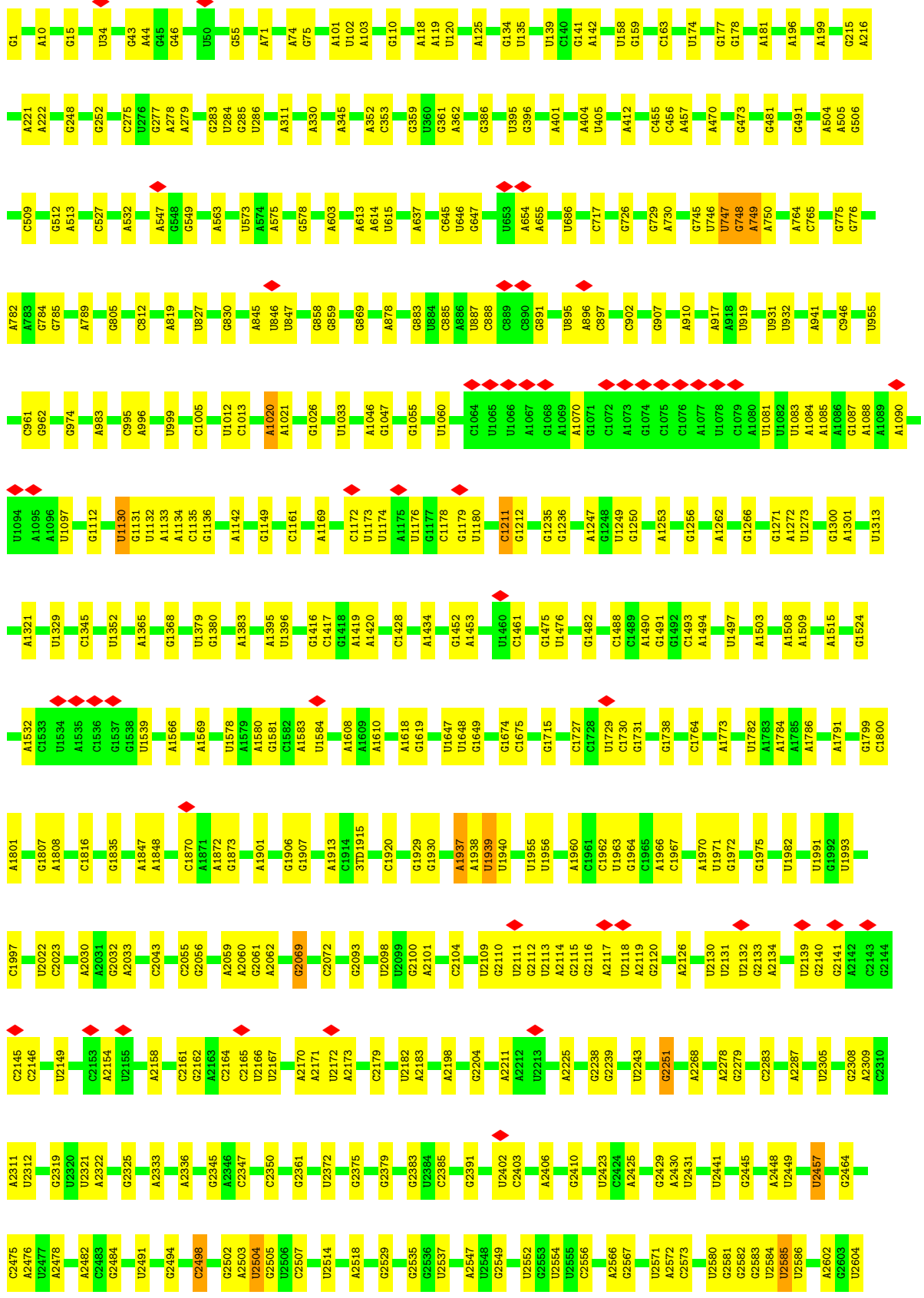
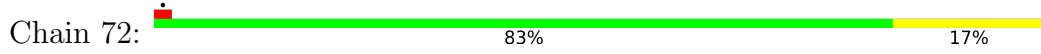


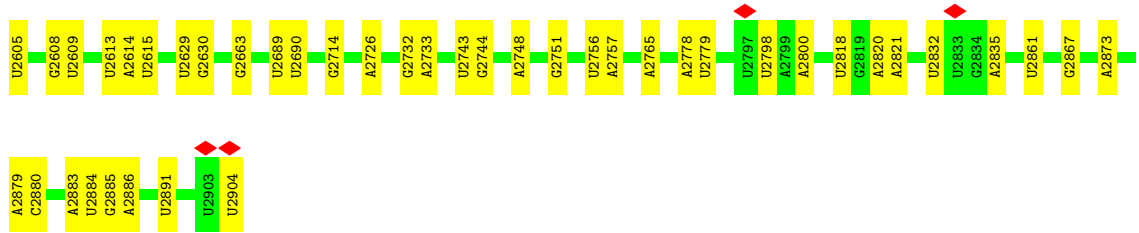
G G G G A A C C C C A A G U G U G U U U C C G A A C U U V A A C U U V A A C U U G A A A C C A U A A G G U U A A G C C  
A A C C G G G G A A C C G U G A A A A A C C A U A C C A A G U A A C C C C G A A G A A A C C A A A G G U U C C C C C  
A G U A G C C G G C G A A G A A G C G G A A A C C G G A A G C C C A A G C C C U G A A A C C A A A G U G G A A G G A A  
G G U C U G G A A A A A G C G A G A A A C C G G G A A A C C A A G G U G A  
G A C C U C G A A G A A G A A G G G C C G G A G G A A C C A A C C G U G G U A C C C U G A A U G A A A A A A A A A A A A  
C A A G G C U A A A A A A C C U U C C C U G A C U U G A A A A A C C G A A U A  
G A A C C C G G C A A G G C G A G G G G A  
A C G C U U A G G C C G U G U G A A A A C C C A U U A  
C A A G G U U A A A C C G A A A A A G G G A A C C G A A A A G G U G A  
A G G G U A A G A A C C C G A A A A A A A C C G A U C U A  
A A C U G G A A G A A C C C A A A A C C A  
A A A G G C C A A U C A A C C A A C C G G G A A C A  
G U G A A U U C A A U C C G G A A U C C G G A  
C C C A A U G C A A A C C A A U G G A  
C G U C C G U C G A A G U G A A G G A  
A G U G G A A A A C C A A U G G G A  
U U U A A A A G A A A A A C C U U A  
U A A A C A U G C A A C C A A G G A A C C U G C C G A A G C A  
U G U A A A G C C A A G G A  
C A U A A A A C C A  
A A C G U U A  
G G A A A C C A A G G U U A A U C C U U G C C A  
G U U G G C C G G A A C G A G G U U C C U U C C A  
G A A A A C A A G G C U U G G A A C G A G G A  
C U U C C A A G A A A A A C C U U A A G G A  
6RZ  
G G



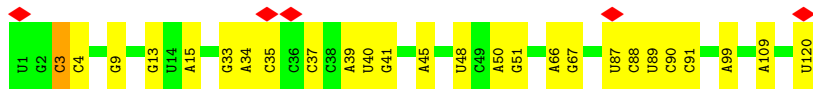
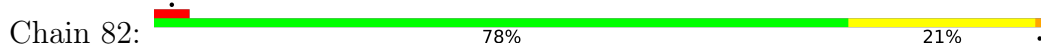
• Molecule 5: 23S ribosomal RNA



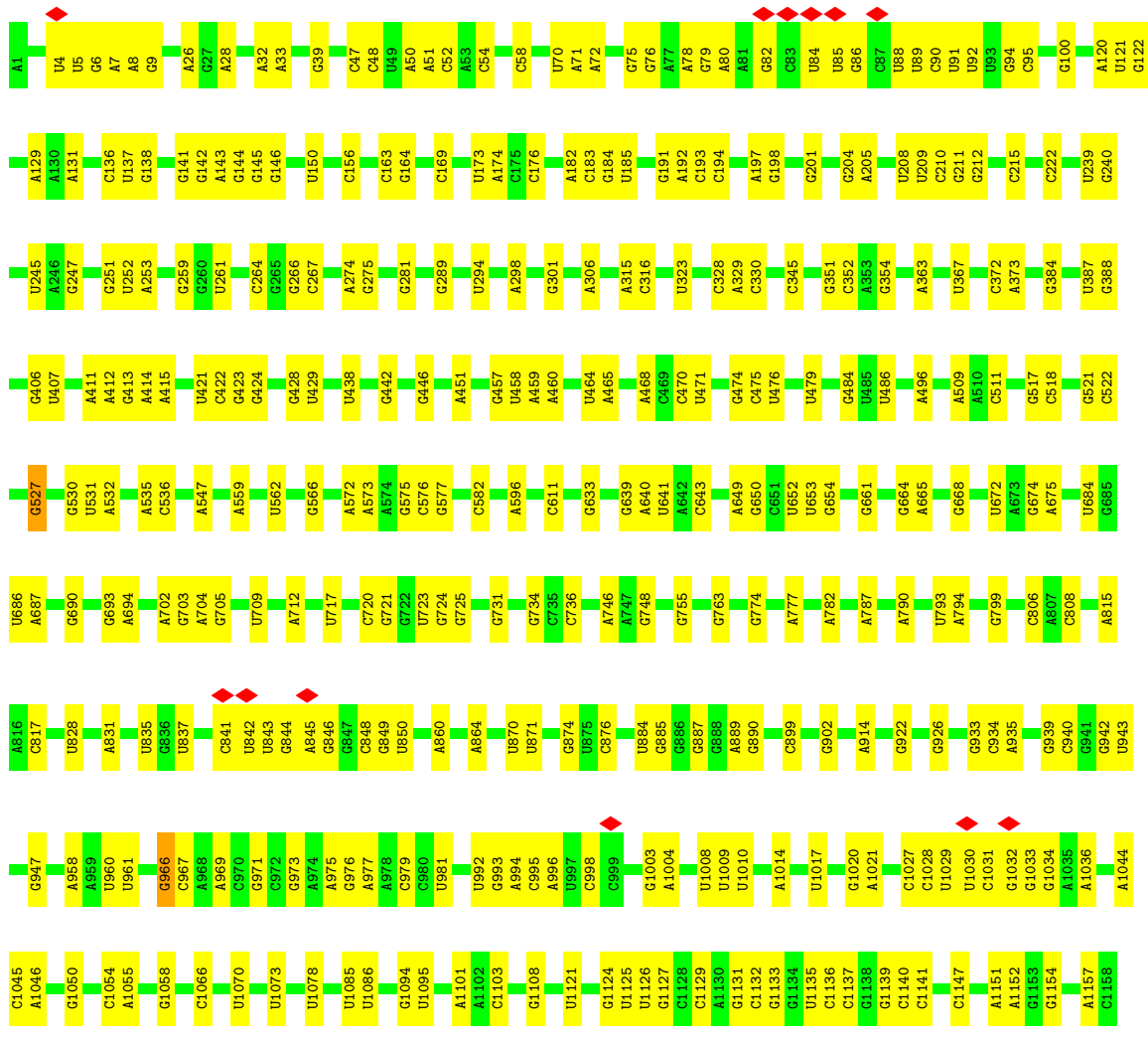




• Molecule 6: 5S ribosomal RNA

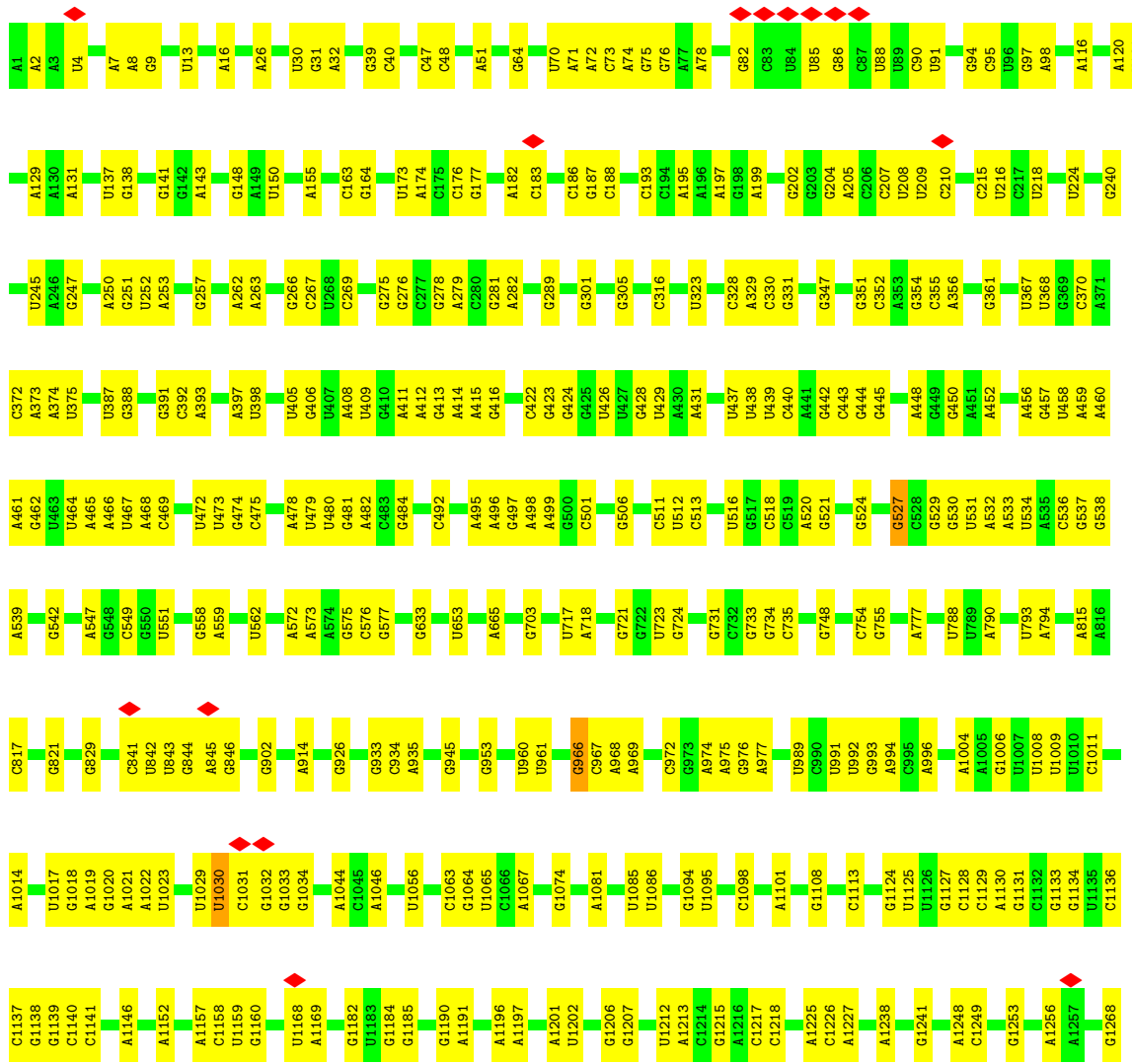
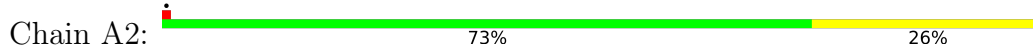


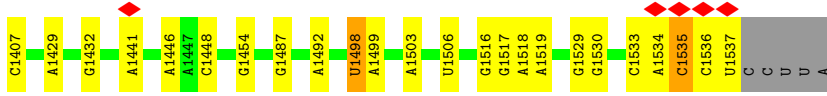
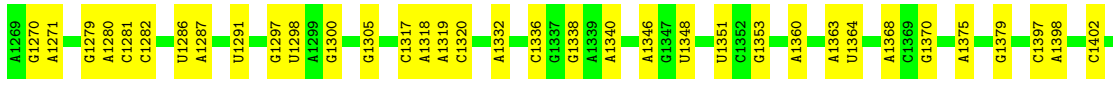
• Molecule 7: 16S ribosomal RNA



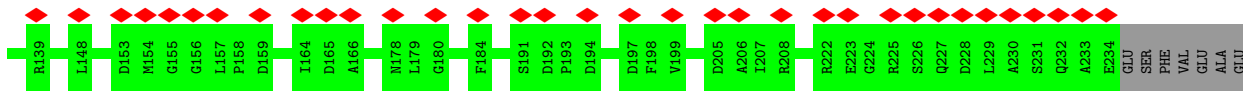
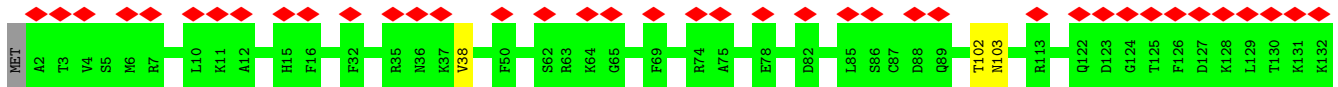


• Molecule 7: 16S ribosomal RNA

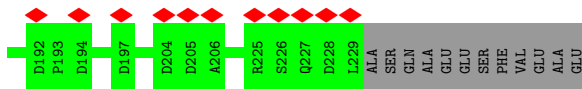
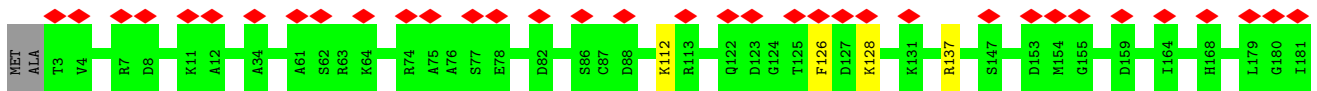




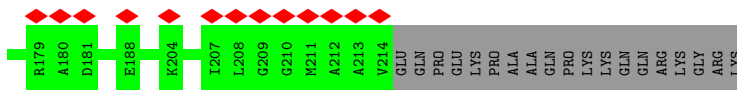
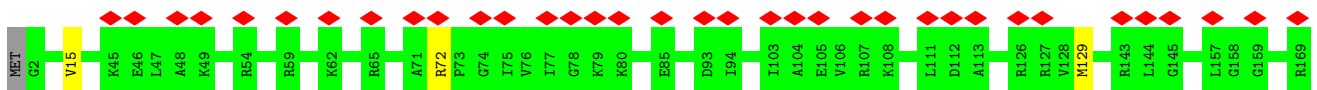
• Molecule 8: Small ribosomal subunit protein uS2



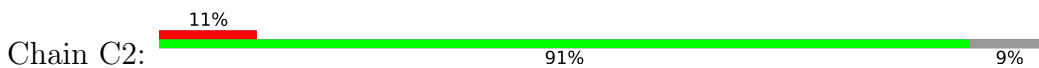
• Molecule 8: Small ribosomal subunit protein uS2



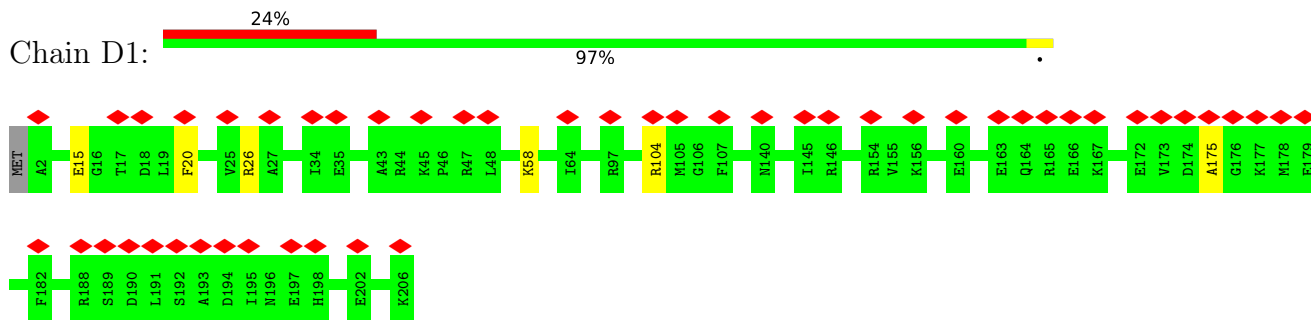
• Molecule 9: Small ribosomal subunit protein uS3



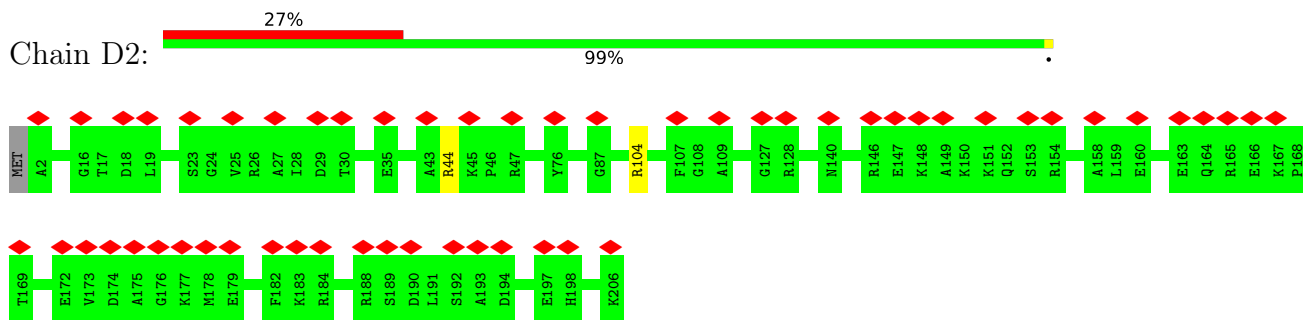
• Molecule 9: Small ribosomal subunit protein uS3



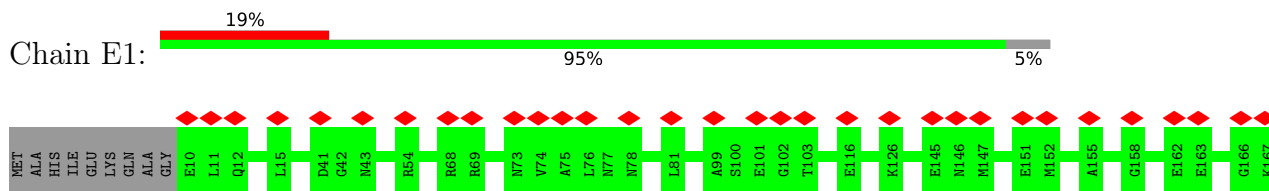
• Molecule 10: Small ribosomal subunit protein uS4



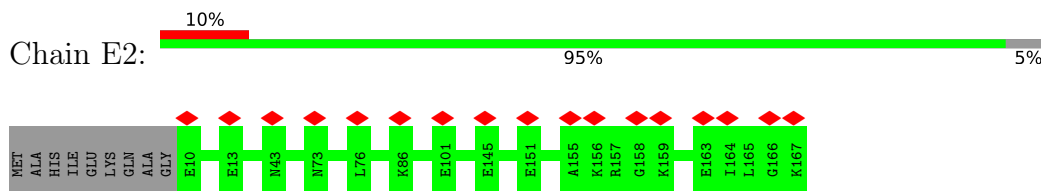
• Molecule 10: Small ribosomal subunit protein uS4



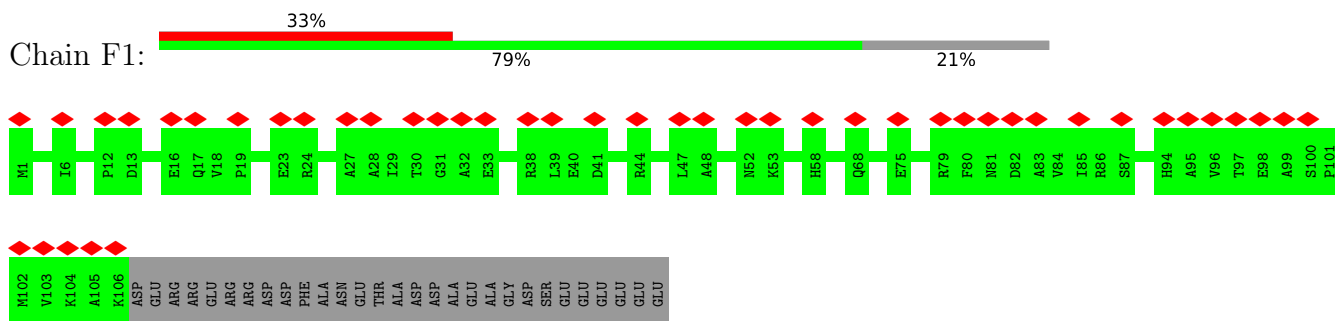
• Molecule 11: Small ribosomal subunit protein uS5



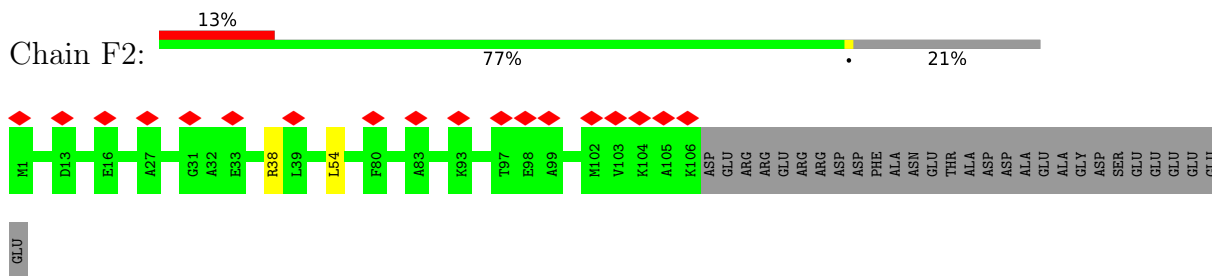
• Molecule 11: Small ribosomal subunit protein uS5



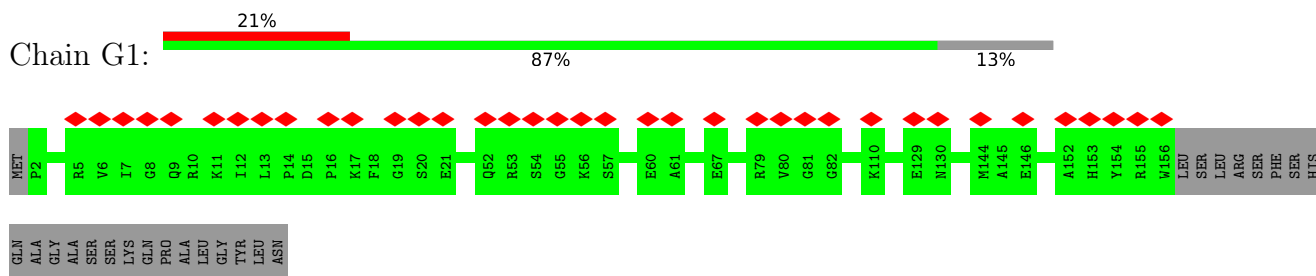
• Molecule 12: 30S ribosomal protein S6



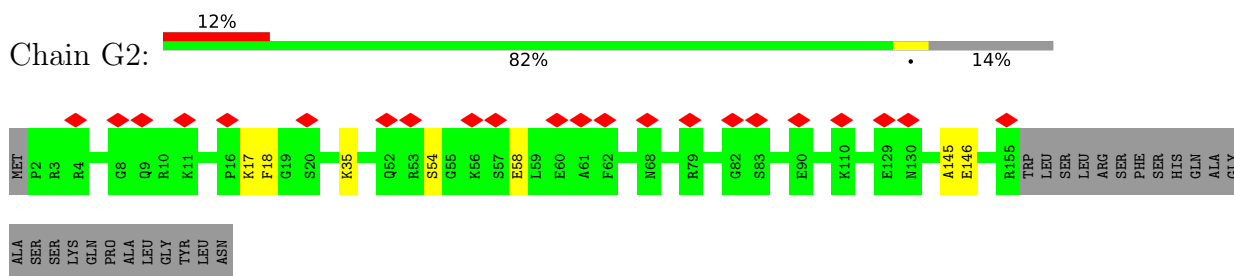
• Molecule 12: 30S ribosomal protein S6



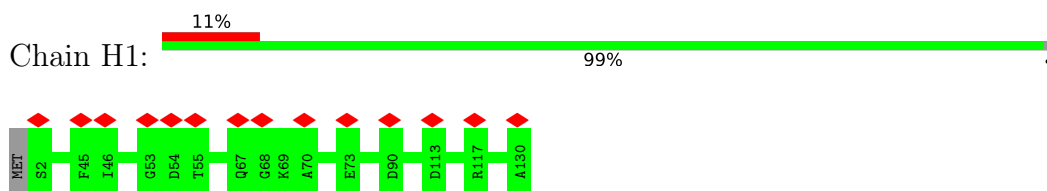
• Molecule 13: 30S ribosomal protein S7



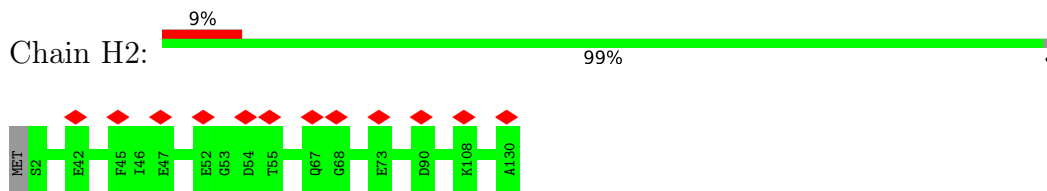
• Molecule 13: 30S ribosomal protein S7



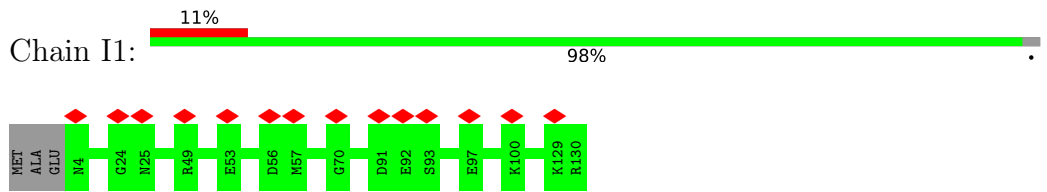
• Molecule 14: Small ribosomal subunit protein uS8



• Molecule 14: Small ribosomal subunit protein uS8

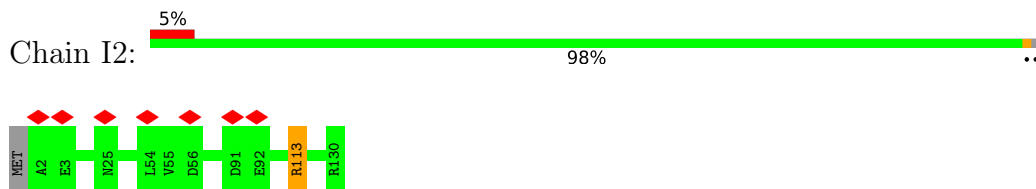


• Molecule 15: Small ribosomal subunit protein uS9

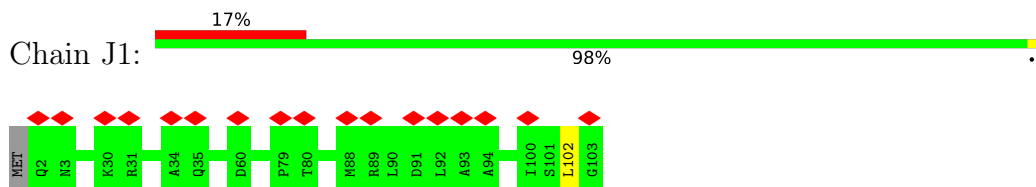




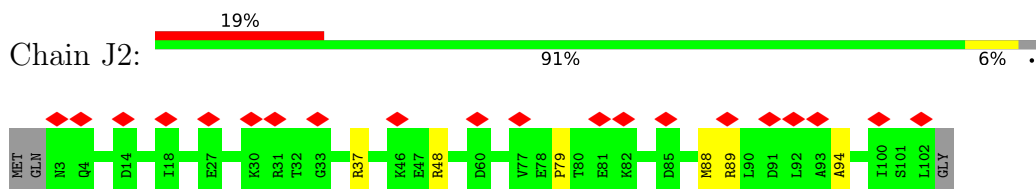
- Molecule 15: Small ribosomal subunit protein uS9



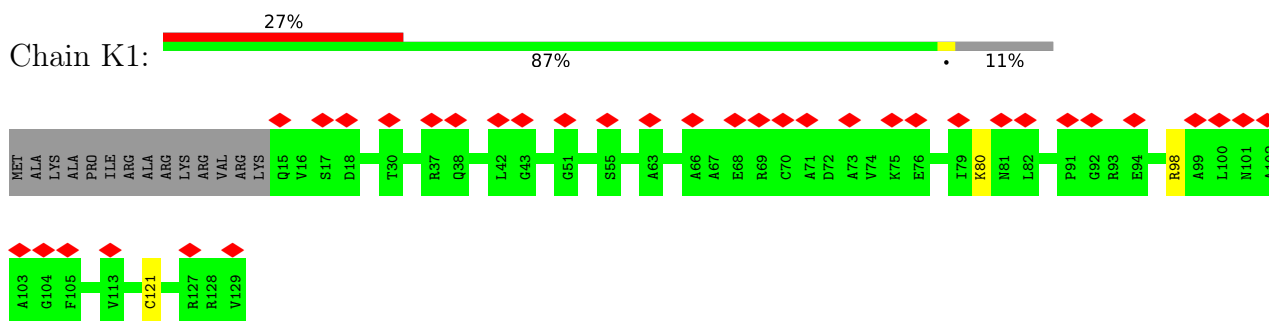
- Molecule 16: 30S ribosomal protein S10



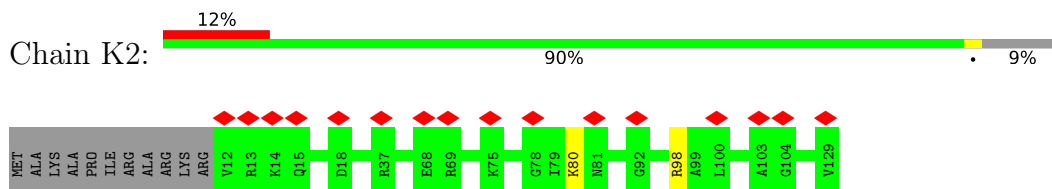
- Molecule 16: 30S ribosomal protein S10



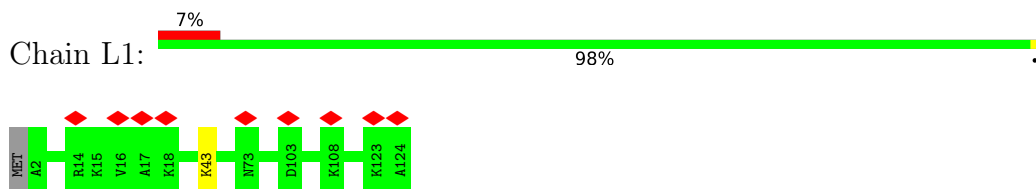
- Molecule 17: Small ribosomal subunit protein uS11



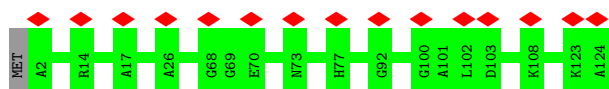
- Molecule 17: Small ribosomal subunit protein uS11



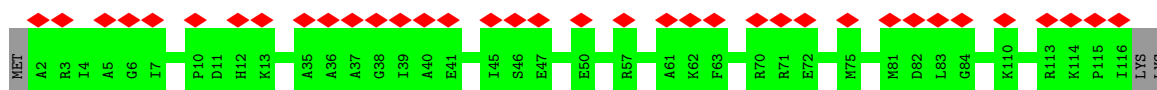
- Molecule 18: Small ribosomal subunit protein uS12



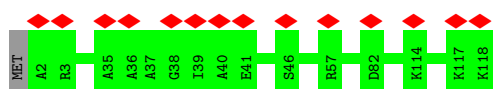
- Molecule 18: Small ribosomal subunit protein uS12



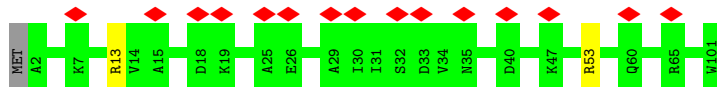
- Molecule 19: Small ribosomal subunit protein uS13



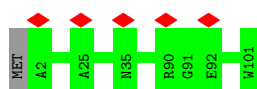
- Molecule 19: Small ribosomal subunit protein uS13



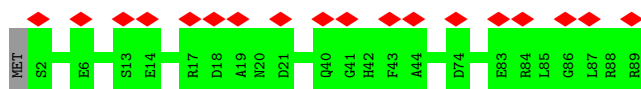
- Molecule 20: Small ribosomal subunit protein uS14



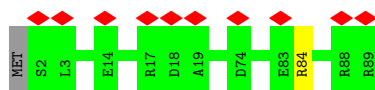
- Molecule 20: Small ribosomal subunit protein uS14



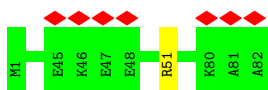
- Molecule 21: 30S ribosomal protein S15



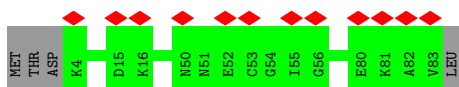
- Molecule 21: 30S ribosomal protein S15



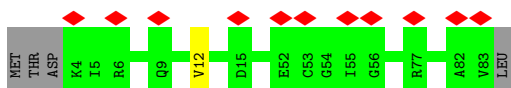
- Molecule 22: 30S ribosomal protein S16



- Molecule 23: Small ribosomal subunit protein uS17



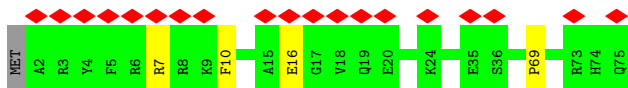
- Molecule 23: Small ribosomal subunit protein uS17



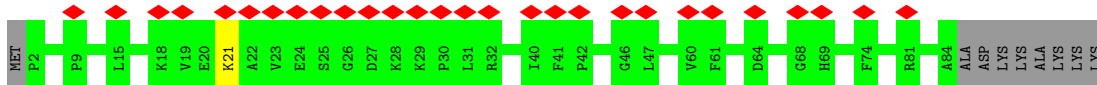
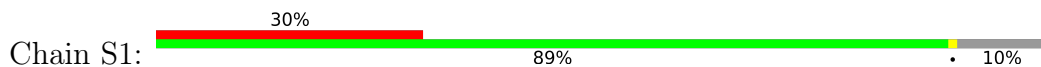
- Molecule 24: Small ribosomal subunit protein bS18



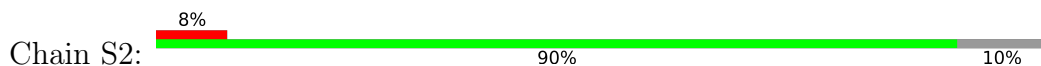
- Molecule 24: Small ribosomal subunit protein bS18

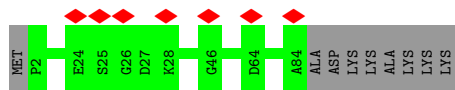


- Molecule 25: Small ribosomal subunit protein uS19

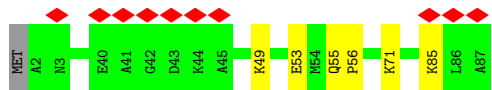
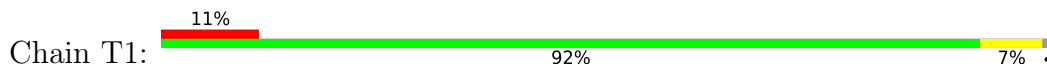


- Molecule 25: Small ribosomal subunit protein uS19

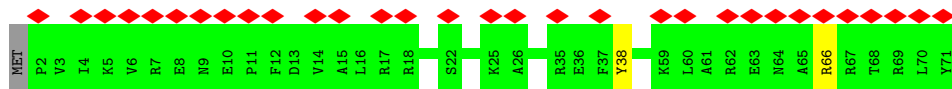




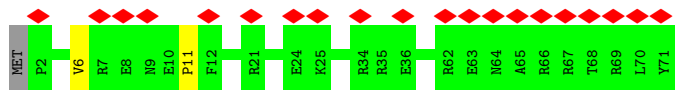
- Molecule 26: Small ribosomal subunit protein bS20



- Molecule 27: 30S ribosomal protein S21



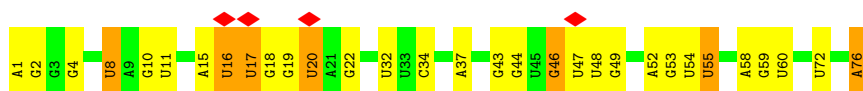
- Molecule 27: 30S ribosomal protein S21



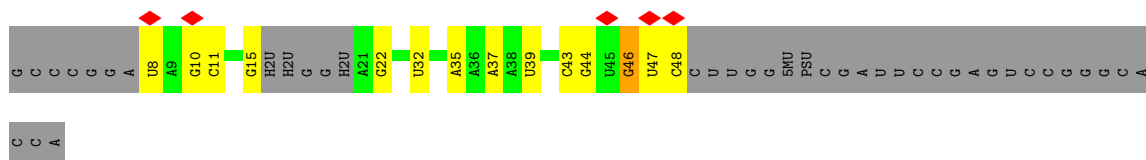
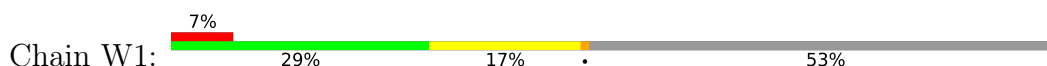
- Molecule 28: messenger RNA



- Molecule 29: tRNA-Trp (P-site)



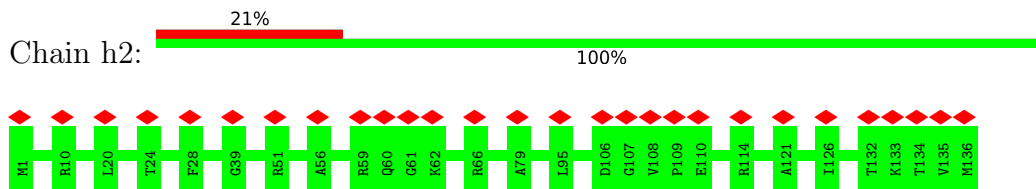
- Molecule 30: tRNA-Phe (P-site)



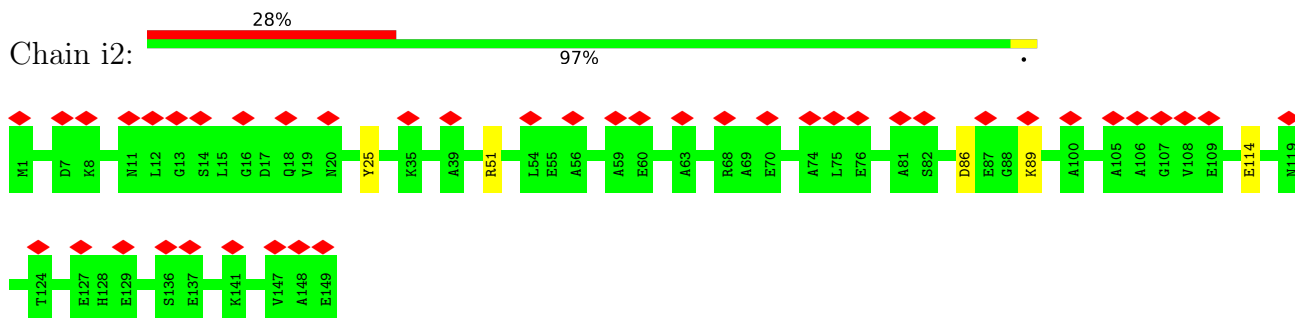




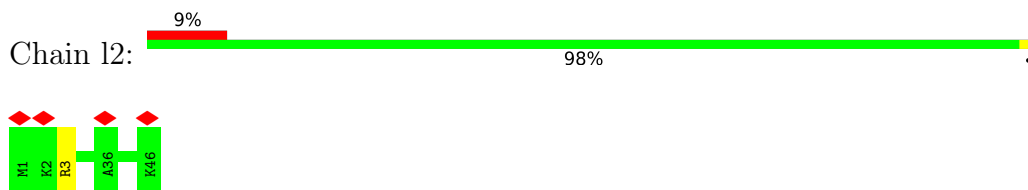
- Molecule 39: 50S ribosomal protein L16



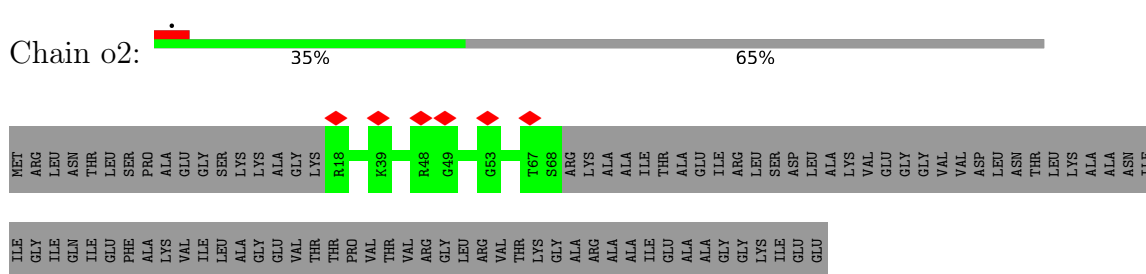
- Molecule 40: 50S ribosomal protein L9



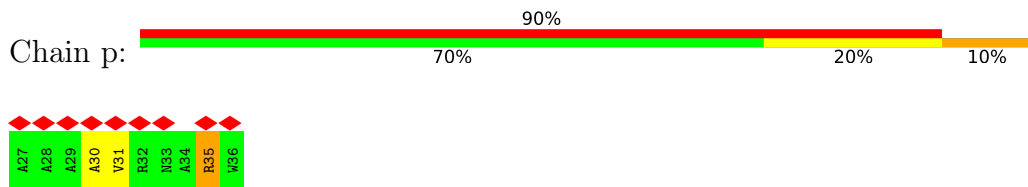
- Molecule 41: 50S ribosomal protein L34



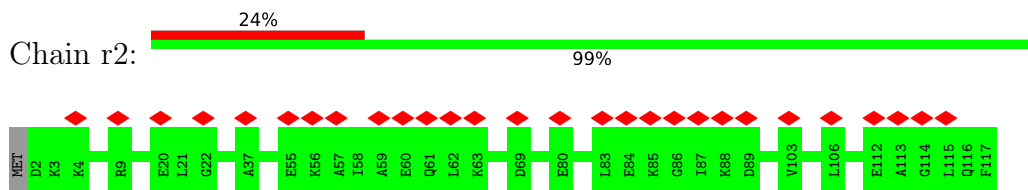
- Molecule 42: 50S ribosomal protein L15



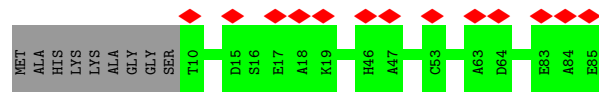
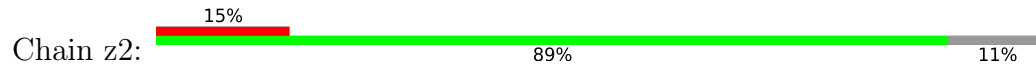
- Molecule 43: Nascent chain



- Molecule 44: 50S ribosomal protein L18



• Molecule 45: 50S ribosomal protein L27





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39441	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	24.615	Depositor
Minimum map value	-5.965	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.974	Depositor
Recommended contour level	5.5	Depositor
Map size ( $\text{\AA}$ )	744.12, 744.12, 744.12	wwPDB
Map dimensions	468, 468, 468	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.59, 1.59, 1.59	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, 2MA, 4SU, ZN, SPD, UR3, 4OC, 7MG, 3TD, OMC, G7M, MG, 5MC, 3AU, OMU, 5MU, MIA, OMG, PSU, 1MG, PUT, RSP, MA6, CM0, H2U, 2MG

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	12	0.24	0/635	0.60	0/848
2	32	0.23	0/453	0.52	0/605
3	4	0.63	0/539	0.63	0/721
4	62	0.24	0/513	0.56	0/676
5	71	0.18	0/696	0.70	0/1081
5	72	0.20	1/69306 (0.0%)	0.70	20/108116 (0.0%)
6	82	0.22	1/2872 (0.0%)	0.75	2/4478 (0.0%)
7	A1	0.25	0/36794	0.77	1/57392 (0.0%)
7	A2	0.25	0/36681	0.75	7/57217 (0.0%)
8	B	0.24	0/1846	0.52	0/2488
8	B2	0.25	0/1807	0.49	0/2435
9	C1	0.25	0/1692	0.54	0/2280
9	C2	0.26	0/1685	0.56	0/2270
10	D1	0.25	0/1665	0.54	0/2227
10	D2	0.25	0/1665	0.55	0/2227
11	E1	0.27	0/1179	0.52	0/1584
11	E2	0.27	0/1179	0.53	0/1584
12	F1	0.24	0/881	0.51	0/1189
12	F2	0.25	0/881	0.50	0/1189
13	G1	0.25	0/1246	0.53	0/1672
13	G2	0.25	0/1230	0.56	0/1649
14	H1	0.26	0/989	0.54	0/1326
14	H2	0.26	0/989	0.54	0/1326
15	I1	0.25	0/1034	0.58	0/1375
15	I2	0.26	0/1048	0.58	0/1394
16	J1	0.28	0/827	0.59	0/1117
16	J2	0.26	0/813	0.63	0/1100
17	K1	0.25	0/873	0.55	0/1180
17	K2	0.26	0/900	0.56	0/1215
18	L1	0.27	0/969	0.61	0/1300
18	L2	0.27	0/969	0.61	0/1300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	M1	0.24	0/900	0.57	0/1204
19	M2	0.24	0/919	0.58	0/1226
20	N1	0.26	0/817	0.57	0/1088
20	N2	0.25	0/817	0.59	0/1088
21	O1	0.24	0/722	0.57	0/964
21	O2	0.24	0/722	0.59	0/964
22	P1	0.26	0/659	0.60	0/884
23	Q1	0.27	0/657	0.58	0/881
23	Q2	0.25	0/657	0.56	0/881
24	R1	0.25	0/635	0.57	0/849
24	R2	0.25	0/637	0.59	0/851
25	S1	0.25	0/680	0.51	0/915
25	S2	0.26	0/680	0.53	0/915
26	T1	0.25	0/676	0.52	0/895
27	U1	0.26	0/598	0.62	0/792
27	U2	0.25	0/592	0.58	0/785
28	V2	0.31	0/1552	0.88	3/2419 (0.1%)
29	W	0.41	1/1604 (0.1%)	0.81	1/2496 (0.0%)
30	W1	0.18	0/747	0.73	0/1161
31	X2	0.49	3/1628 (0.2%)	0.81	1/2526 (0.0%)
32	Y1	0.20	0/786	0.75	0/1216
33	Y2	0.38	1/1725 (0.1%)	0.82	2/2687 (0.1%)
34	Z1	0.27	0/76	0.34	0/101
35	a2	0.24	0/1033	0.47	0/1387
36	b2	0.26	0/2121	0.59	0/2852
37	e2	0.25	0/1444	0.52	0/1937
38	g2	0.25	0/434	0.51	0/576
39	h2	0.25	0/1104	0.57	0/1474
40	i2	0.25	0/1122	0.51	0/1515
41	l2	0.24	0/380	0.63	0/498
42	o2	0.27	0/383	0.69	0/501
43	p	0.58	0/77	0.86	0/104
44	r2	0.25	0/901	0.60	0/1209
45	z2	0.26	0/589	0.55	0/779
All	All	0.25	7/203930 (0.0%)	0.70	37/307181 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	D1	0	2
10	D2	0	1
15	I2	0	1
16	J2	0	2
17	K1	0	1
17	K2	0	1
21	O2	0	1
22	P1	0	1
43	p	0	1
All	All	0	13

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	1	A	OP3-P	-10.60	1.48	1.61
5	72	1	G	OP3-P	-10.59	1.48	1.61
31	X2	1	G	OP3-P	-10.57	1.48	1.61
33	Y2	1	G	OP3-P	-10.57	1.48	1.61
31	X2	35	I	C5-C6	7.33	1.54	1.39
31	X2	35	I	N3-C4	7.04	1.50	1.35
6	82	120	U	C1'-N1	5.91	1.57	1.48

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2584	U	P-O3'-C3'	-13.29	103.75	119.70
5	72	2585	U	P-O3'-C3'	-12.31	104.93	119.70
5	72	1939	5MU	P-O3'-C3'	-11.85	105.48	119.70
5	72	747	5MU	P-O3'-C3'	-11.14	106.33	119.70
5	72	749	A	P-O3'-C3'	-10.63	106.94	119.70
33	Y2	52	G	P-O3'-C3'	-9.84	107.89	119.70
5	72	748	G	P-O3'-C3'	-9.64	108.13	119.70
33	Y2	74	C	P-O3'-C3'	-9.24	108.61	119.70
5	72	2585	U	C3'-C2'-C1'	-8.26	94.89	101.50
5	72	2583	G	P-O3'-C3'	-6.59	111.79	119.70
28	V2	32	U	N1-C2-O2	6.29	127.20	122.80
7	A2	1030	U	C2-N1-C1'	6.27	125.22	117.70
5	72	1937	A	P-O3'-C3'	-6.18	112.28	119.70
5	72	1313	U	N1-C2-O2	6.07	127.05	122.80
28	V2	32	U	C2-N1-C1'	6.07	124.98	117.70
5	72	1313	U	C2-N1-C1'	5.99	124.89	117.70
5	72	1211	C	OP2-P-O3'	5.88	118.14	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	V2	32	U	N3-C2-O2	-5.83	118.12	122.20
7	A1	1536	C	OP2-P-O3'	5.76	117.88	105.20
6	82	3	C	OP1-P-O3'	5.75	117.86	105.20
29	W	76	A	OP1-P-OP2	-5.74	110.99	119.60
5	72	1020	A	P-O3'-C3'	5.62	126.44	119.70
7	A2	1030	U	N3-C2-O2	-5.60	118.28	122.20
6	82	3	C	P-O3'-C3'	5.53	126.33	119.70
5	72	1313	U	N3-C2-O2	-5.51	118.34	122.20
7	A2	1030	U	N1-C2-O2	5.49	126.64	122.80
5	72	1675	C	N1-C2-O2	5.36	122.12	118.90
5	72	1675	C	C2-N1-C1'	5.33	124.67	118.80
5	72	1130	U	P-O3'-C3'	5.32	126.08	119.70
5	72	1020	A	OP2-P-O3'	5.30	116.87	105.20
7	A2	1535	C	P-O3'-C3'	5.29	126.05	119.70
5	72	2585	U	C2'-C3'-O3'	-5.15	98.16	109.50
5	72	1938	A	C3'-C2'-C1'	-5.12	97.40	101.50
31	X2	73	C	N1-C2-O2	5.12	121.97	118.90
7	A2	754	C	C2-N1-C1'	5.10	124.41	118.80
7	A2	392	C	N1-C2-O2	5.01	121.91	118.90
7	A2	1030	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	56	ARG	Sidechain
3	4	59	ARG	Sidechain
10	D1	104	ARG	Sidechain
10	D1	15	GLU	Peptide
10	D2	104	ARG	Sidechain
15	I2	113	ARG	Sidechain
16	J2	37	ARG	Sidechain
16	J2	48	ARG	Sidechain
17	K1	98	ARG	Sidechain
17	K2	98	ARG	Sidechain
21	O2	84	ARG	Sidechain
22	P1	51	ARG	Sidechain
43	p	35	ARG	Sidechain

## 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	
1	12	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
2	32	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	35
3	4	65/70 (93%)	54 (83%)	10 (15%)	1 (2%)	8	39
4	62	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	B	231/241 (96%)	193 (84%)	35 (15%)	3 (1%)	10	41
8	B2	225/241 (93%)	189 (84%)	36 (16%)	0	100	100
9	C1	211/233 (91%)	186 (88%)	23 (11%)	2 (1%)	14	49
9	C2	210/233 (90%)	184 (88%)	26 (12%)	0	100	100
10	D1	203/206 (98%)	181 (89%)	21 (10%)	1 (0%)	25	59
10	D2	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
11	E1	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
11	E2	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
12	F1	104/135 (77%)	104 (100%)	0	0	100	100
12	F2	104/135 (77%)	79 (76%)	23 (22%)	2 (2%)	6	34
13	G1	153/179 (86%)	151 (99%)	2 (1%)	0	100	100
13	G2	152/179 (85%)	122 (80%)	24 (16%)	6 (4%)	2	21
14	H1	127/130 (98%)	127 (100%)	0	0	100	100
14	H2	127/130 (98%)	127 (100%)	0	0	100	100
15	I1	125/130 (96%)	103 (82%)	22 (18%)	0	100	100
15	I2	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
16	J1	100/103 (97%)	92 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	J2	98/103 (95%)	86 (88%)	8 (8%)	4 (4%)	2	20
17	K1	113/129 (88%)	97 (86%)	15 (13%)	1 (1%)	14	49
17	K2	116/129 (90%)	100 (86%)	15 (13%)	1 (1%)	14	49
18	L1	121/124 (98%)	114 (94%)	6 (5%)	1 (1%)	16	51
18	L2	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
19	M1	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
19	M2	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
20	N1	98/101 (97%)	85 (87%)	13 (13%)	0	100	100
20	N2	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
21	O1	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	O2	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
22	P1	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
23	Q1	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
23	Q2	78/84 (93%)	75 (96%)	2 (3%)	1 (1%)	10	41
24	R1	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	9	40
24	R2	72/75 (96%)	53 (74%)	18 (25%)	1 (1%)	9	40
25	S1	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
25	S2	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
26	T1	84/87 (97%)	79 (94%)	3 (4%)	2 (2%)	5	30
27	U1	68/71 (96%)	57 (84%)	11 (16%)	0	100	100
27	U2	68/71 (96%)	59 (87%)	7 (10%)	2 (3%)	3	27
34	Z1	7/557 (1%)	7 (100%)	0	0	100	100
35	a2	130/234 (56%)	123 (95%)	7 (5%)	0	100	100
36	b2	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
37	e2	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
38	g2	50/55 (91%)	50 (100%)	0	0	100	100
39	h2	135/136 (99%)	135 (100%)	0	0	100	100
40	i2	147/149 (99%)	116 (79%)	29 (20%)	2 (1%)	9	40
41	l2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
42	o2	49/144 (34%)	45 (92%)	4 (8%)	0	100	100
43	p	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	r2	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
45	z2	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
All	All	6102/7240 (84%)	5611 (92%)	457 (8%)	34 (1%)	24	56

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C1	15	VAL
13	G2	18	PHE
13	G2	35	LYS
13	G2	54	SER
13	G2	146	GLU
23	Q2	12	VAL
10	D1	175	ALA
12	F2	38	ARG
13	G2	17	LYS
13	G2	145	ALA
16	J2	89	ARG
16	J2	94	ALA
40	i2	89	LYS
43	p	30	ALA
8	B	102	THR
8	B	103	ASN
17	K1	80	LYS
17	K2	80	LYS
18	L1	43	LYS
24	R1	21	ILE
26	T1	55	GLN
2	32	33	HIS
9	C1	129	MET
3	4	55	GLY
12	F2	54	LEU
16	J2	88	MET
40	i2	86	ASP
16	J2	79	PRO
8	B	38	VAL
26	T1	56	PRO
27	U2	6	VAL
43	p	31	VAL
27	U2	11	PRO
24	R2	69	PRO



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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
1	12	67/68 (98%)	65 (97%)	2 (3%)	36	63
2	32	48/49 (98%)	47 (98%)	1 (2%)	48	71
3	4	60/62 (97%)	54 (90%)	6 (10%)	6	26
4	62	51/52 (98%)	51 (100%)	0	100	100
8	B	192/199 (96%)	192 (100%)	0	100	100
8	B2	189/199 (95%)	185 (98%)	4 (2%)	48	71
9	C1	173/190 (91%)	172 (99%)	1 (1%)	84	91
9	C2	172/190 (90%)	171 (99%)	1 (1%)	84	91
10	D1	172/173 (99%)	169 (98%)	3 (2%)	56	75
10	D2	172/173 (99%)	171 (99%)	1 (1%)	84	91
11	E1	120/126 (95%)	120 (100%)	0	100	100
11	E2	120/126 (95%)	120 (100%)	0	100	100
12	F1	92/116 (79%)	92 (100%)	0	100	100
12	F2	92/116 (79%)	92 (100%)	0	100	100
13	G1	128/147 (87%)	128 (100%)	0	100	100
13	G2	127/147 (86%)	126 (99%)	1 (1%)	79	88
14	H1	104/105 (99%)	104 (100%)	0	100	100
14	H2	104/105 (99%)	104 (100%)	0	100	100
15	I1	105/107 (98%)	105 (100%)	0	100	100
15	I2	106/107 (99%)	105 (99%)	1 (1%)	75	86
16	J1	89/90 (99%)	88 (99%)	1 (1%)	70	83
16	J2	88/90 (98%)	88 (100%)	0	100	100
17	K1	88/99 (89%)	87 (99%)	1 (1%)	70	83
17	K2	91/99 (92%)	91 (100%)	0	100	100
18	L1	103/104 (99%)	103 (100%)	0	100	100
18	L2	103/104 (99%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	M1	93/96 (97%)	93 (100%)	0	100	100
19	M2	95/96 (99%)	95 (100%)	0	100	100
20	N1	83/84 (99%)	81 (98%)	2 (2%)	44	68
20	N2	83/84 (99%)	83 (100%)	0	100	100
21	O1	76/77 (99%)	76 (100%)	0	100	100
21	O2	76/77 (99%)	76 (100%)	0	100	100
22	P1	65/65 (100%)	65 (100%)	0	100	100
23	Q1	74/78 (95%)	74 (100%)	0	100	100
23	Q2	74/78 (95%)	74 (100%)	0	100	100
24	R1	64/65 (98%)	63 (98%)	1 (2%)	58	76
24	R2	64/65 (98%)	61 (95%)	3 (5%)	22	51
25	S1	72/79 (91%)	71 (99%)	1 (1%)	62	79
25	S2	72/79 (91%)	72 (100%)	0	100	100
26	T1	65/66 (98%)	61 (94%)	4 (6%)	15	42
27	U1	60/61 (98%)	58 (97%)	2 (3%)	33	61
27	U2	59/61 (97%)	59 (100%)	0	100	100
34	Z1	8/461 (2%)	8 (100%)	0	100	100
35	a2	110/181 (61%)	109 (99%)	1 (1%)	75	86
36	b2	216/218 (99%)	216 (100%)	0	100	100
37	e2	149/150 (99%)	147 (99%)	2 (1%)	65	81
38	g2	47/49 (96%)	47 (100%)	0	100	100
39	h2	110/109 (101%)	110 (100%)	0	100	100
40	i2	114/114 (100%)	111 (97%)	3 (3%)	41	66
41	l2	38/38 (100%)	37 (97%)	1 (3%)	41	66
42	o2	35/103 (34%)	35 (100%)	0	100	100
43	p	5/5 (100%)	4 (80%)	1 (20%)	1	6
44	r2	86/87 (99%)	86 (100%)	0	100	100
45	z2	58/63 (92%)	58 (100%)	0	100	100
All	All	5107/5932 (86%)	5063 (99%)	44 (1%)	74	86

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12	72	ARG
1	12	77	LYS
2	32	36	GLU
3	4	1	MET
3	4	6	HIS
3	4	9	TYR
3	4	31	ASP
3	4	33	ASN
3	4	40	CYS
8	B2	112	LYS
8	B2	126	PHE
8	B2	128	LYS
8	B2	137	ARG
9	C1	72	ARG
9	C2	49	LYS
10	D1	20	PHE
10	D1	26	ARG
10	D1	58	LYS
10	D2	44	ARG
13	G2	58	GLU
15	I2	113	ARG
16	J1	102	LEU
17	K1	121	CYS
20	N1	13	ARG
20	N1	53	ARG
24	R1	8	ARG
24	R2	7	ARG
24	R2	10	PHE
24	R2	16	GLU
25	S1	21	LYS
26	T1	49	LYS
26	T1	53	GLU
26	T1	71	LYS
26	T1	85	LYS
27	U1	38	TYR
27	U1	66	ARG
35	a2	30	LEU
37	e2	3	LYS
37	e2	178	ARG
40	i2	25	TYR
40	i2	51	ARG
40	i2	114	GLU
41	l2	3	ARG

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Mol	Chain	Res	Type
43	p	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	4	6	HIS
3	4	33	ASN
3	4	41	HIS
3	4	61	ASN
8	B	94	HIS
8	B	203	ASN
8	B2	89	GLN
8	B2	177	ASN
9	C2	190	HIS
10	D1	59	GLN
10	D2	85	ASN
16	J2	35	GLN
18	L2	29	GLN
45	z2	50	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	63/64 (98%)	42 (66%)	8 (12%)
29	W	74/76 (97%)	26 (35%)	4 (5%)
30	W1	33/76 (43%)	8 (24%)	2 (6%)
31	X2	73/77 (94%)	26 (35%)	5 (6%)
32	Y1	32/76 (42%)	4 (12%)	2 (6%)
33	Y2	75/76 (98%)	23 (30%)	2 (2%)
5	71	28/2904 (0%)	4 (14%)	0
5	72	2899/2904 (99%)	460 (15%)	33 (1%)
6	82	119/120 (99%)	21 (17%)	4 (3%)
7	A1	1538/1542 (99%)	449 (29%)	36 (2%)
7	A2	1533/1542 (99%)	397 (25%)	33 (2%)
All	All	6467/9457 (68%)	1460 (22%)	129 (1%)

All (1460) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	71	1906	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	71	1907	G
5	71	1929	G
5	71	1930	G
5	72	10	A
5	72	15	G
5	72	34	U
5	72	44	A
5	72	46	G
5	72	55	G
5	72	71	A
5	72	74	A
5	72	75	G
5	72	101	A
5	72	102	U
5	72	103	A
5	72	110	G
5	72	118	A
5	72	119	A
5	72	120	U
5	72	125	A
5	72	135	U
5	72	139	U
5	72	141	G
5	72	142	A
5	72	159	G
5	72	163	C
5	72	174	U
5	72	177	G
5	72	178	G
5	72	181	A
5	72	196	A
5	72	199	A
5	72	215	G
5	72	216	A
5	72	221	A
5	72	222	A
5	72	248	G
5	72	252	G
5	72	275	C
5	72	277	G
5	72	278	A
5	72	279	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	283	G
5	72	284	U
5	72	285	G
5	72	286	U
5	72	311	A
5	72	330	A
5	72	345	A
5	72	353	C
5	72	359	G
5	72	361	G
5	72	362	A
5	72	386	G
5	72	395	U
5	72	396	G
5	72	401	A
5	72	405	U
5	72	412	A
5	72	455	C
5	72	456	C
5	72	457	A
5	72	470	A
5	72	473	G
5	72	481	G
5	72	491	G
5	72	505	A
5	72	506	G
5	72	509	C
5	72	513	A
5	72	527	C
5	72	532	A
5	72	547	A
5	72	549	G
5	72	563	A
5	72	573	U
5	72	575	A
5	72	578	G
5	72	603	A
5	72	613	A
5	72	614	A
5	72	615	U
5	72	637	A
5	72	645	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	646	U
5	72	647	G
5	72	654	A
5	72	655	A
5	72	686	U
5	72	717	C
5	72	726	G
5	72	729	G
5	72	730	A
5	72	747	5MU
5	72	748	G
5	72	749	A
5	72	750	A
5	72	764	A
5	72	765	C
5	72	775	G
5	72	776	G
5	72	782	A
5	72	784	G
5	72	785	G
5	72	789	A
5	72	805	G
5	72	812	C
5	72	819	A
5	72	827	U
5	72	830	G
5	72	845	A
5	72	846	U
5	72	847	U
5	72	858	G
5	72	859	G
5	72	869	G
5	72	878	A
5	72	883	G
5	72	885	C
5	72	887	U
5	72	888	C
5	72	891	G
5	72	895	U
5	72	896	A
5	72	897	C
5	72	902	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	907	G
5	72	910	A
5	72	917	A
5	72	919	U
5	72	931	U
5	72	932	U
5	72	941	A
5	72	946	C
5	72	961	C
5	72	962	G
5	72	974	G
5	72	983	A
5	72	995	C
5	72	996	A
5	72	999	U
5	72	1005	C
5	72	1012	U
5	72	1013	C
5	72	1021	A
5	72	1026	G
5	72	1033	U
5	72	1046	A
5	72	1047	G
5	72	1055	G
5	72	1060	U
5	72	1070	A
5	72	1081	U
5	72	1083	U
5	72	1084	A
5	72	1085	A
5	72	1087	G
5	72	1088	A
5	72	1090	A
5	72	1097	U
5	72	1112	G
5	72	1130	U
5	72	1131	G
5	72	1132	U
5	72	1133	A
5	72	1134	A
5	72	1135	C
5	72	1136	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	1142	A
5	72	1149	G
5	72	1161	C
5	72	1169	A
5	72	1172	C
5	72	1173	U
5	72	1174	U
5	72	1176	U
5	72	1178	C
5	72	1179	G
5	72	1180	U
5	72	1212	G
5	72	1235	G
5	72	1236	G
5	72	1247	A
5	72	1249	U
5	72	1250	G
5	72	1253	A
5	72	1256	G
5	72	1262	A
5	72	1271	G
5	72	1272	A
5	72	1273	U
5	72	1300	G
5	72	1301	A
5	72	1321	A
5	72	1329	U
5	72	1345	C
5	72	1352	U
5	72	1365	A
5	72	1368	G
5	72	1379	U
5	72	1380	G
5	72	1383	A
5	72	1395	A
5	72	1396	U
5	72	1416	G
5	72	1417	C
5	72	1419	A
5	72	1420	A
5	72	1428	C
5	72	1434	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	1452	G
5	72	1453	A
5	72	1461	C
5	72	1476	U
5	72	1482	G
5	72	1488	C
5	72	1490	A
5	72	1491	G
5	72	1493	C
5	72	1494	A
5	72	1497	U
5	72	1503	A
5	72	1508	A
5	72	1509	A
5	72	1515	A
5	72	1524	G
5	72	1532	A
5	72	1539	U
5	72	1566	A
5	72	1569	A
5	72	1578	U
5	72	1581	G
5	72	1583	A
5	72	1584	U
5	72	1608	A
5	72	1610	A
5	72	1619	G
5	72	1647	U
5	72	1648	U
5	72	1649	G
5	72	1674	G
5	72	1715	G
5	72	1727	C
5	72	1729	U
5	72	1730	C
5	72	1731	G
5	72	1738	G
5	72	1764	C
5	72	1773	A
5	72	1782	U
5	72	1784	A
5	72	1786	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	1791	A
5	72	1799	G
5	72	1800	C
5	72	1801	A
5	72	1807	G
5	72	1808	A
5	72	1816	C
5	72	1848	A
5	72	1870	C
5	72	1872	A
5	72	1873	G
5	72	1901	A
5	72	1906	G
5	72	1907	G
5	72	1913	A
5	72	1920	C
5	72	1929	G
5	72	1930	G
5	72	1937	A
5	72	1939	5MU
5	72	1940	U
5	72	1955	U
5	72	1956	U
5	72	1960	A
5	72	1963	U
5	72	1964	G
5	72	1966	A
5	72	1967	C
5	72	1970	A
5	72	1971	U
5	72	1972	G
5	72	1975	G
5	72	1982	U
5	72	1991	U
5	72	1993	U
5	72	1997	C
5	72	2022	U
5	72	2023	C
5	72	2032	G
5	72	2033	A
5	72	2043	C
5	72	2055	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	2056	G
5	72	2059	A
5	72	2060	A
5	72	2061	G
5	72	2062	A
5	72	2069	G7M
5	72	2072	C
5	72	2093	G
5	72	2098	U
5	72	2100	G
5	72	2101	A
5	72	2104	C
5	72	2109	U
5	72	2110	G
5	72	2111	U
5	72	2112	G
5	72	2113	U
5	72	2114	A
5	72	2115	G
5	72	2116	G
5	72	2117	A
5	72	2118	U
5	72	2119	A
5	72	2120	G
5	72	2126	A
5	72	2130	U
5	72	2131	U
5	72	2132	U
5	72	2133	G
5	72	2134	A
5	72	2139	U
5	72	2140	G
5	72	2141	G
5	72	2145	C
5	72	2146	C
5	72	2149	U
5	72	2154	A
5	72	2158	A
5	72	2161	C
5	72	2162	G
5	72	2164	C
5	72	2165	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	2166	U
5	72	2167	U
5	72	2170	A
5	72	2171	A
5	72	2172	U
5	72	2173	A
5	72	2179	C
5	72	2182	U
5	72	2183	A
5	72	2198	A
5	72	2204	G
5	72	2211	A
5	72	2225	A
5	72	2238	G
5	72	2239	G
5	72	2243	U
5	72	2251	OMG
5	72	2268	A
5	72	2278	A
5	72	2279	G
5	72	2283	C
5	72	2287	A
5	72	2305	U
5	72	2308	G
5	72	2309	A
5	72	2311	A
5	72	2312	U
5	72	2319	G
5	72	2321	U
5	72	2322	A
5	72	2325	G
5	72	2333	A
5	72	2336	A
5	72	2345	G
5	72	2347	C
5	72	2350	C
5	72	2361	G
5	72	2372	U
5	72	2375	G
5	72	2379	G
5	72	2383	G
5	72	2385	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	2391	G
5	72	2402	U
5	72	2403	C
5	72	2406	A
5	72	2410	G
5	72	2423	U
5	72	2425	A
5	72	2429	G
5	72	2430	A
5	72	2431	U
5	72	2441	U
5	72	2448	A
5	72	2457	PSU
5	72	2464	G
5	72	2475	C
5	72	2476	A
5	72	2478	A
5	72	2482	A
5	72	2484	G
5	72	2491	U
5	72	2494	G
5	72	2498	OMC
5	72	2502	G
5	72	2504	PSU
5	72	2505	G
5	72	2507	C
5	72	2514	U
5	72	2518	A
5	72	2529	G
5	72	2535	G
5	72	2537	U
5	72	2547	A
5	72	2549	G
5	72	2554	U
5	72	2556	C
5	72	2566	A
5	72	2567	G
5	72	2571	U
5	72	2572	A
5	72	2573	C
5	72	2581	G
5	72	2582	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	2585	U
5	72	2586	U
5	72	2602	A
5	72	2608	G
5	72	2609	U
5	72	2613	U
5	72	2614	A
5	72	2615	U
5	72	2629	U
5	72	2630	G
5	72	2663	G
5	72	2689	U
5	72	2690	U
5	72	2714	G
5	72	2726	A
5	72	2732	G
5	72	2733	A
5	72	2743	U
5	72	2744	G
5	72	2748	A
5	72	2751	G
5	72	2757	A
5	72	2765	A
5	72	2778	A
5	72	2779	U
5	72	2798	U
5	72	2800	A
5	72	2818	U
5	72	2820	A
5	72	2821	A
5	72	2832	U
5	72	2835	A
5	72	2861	U
5	72	2867	G
5	72	2873	A
5	72	2879	A
5	72	2880	C
5	72	2883	A
5	72	2884	U
5	72	2885	G
5	72	2886	A
5	72	2891	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	2904	U
6	82	4	C
6	82	9	G
6	82	13	G
6	82	33	G
6	82	34	A
6	82	35	C
6	82	37	C
6	82	40	U
6	82	41	G
6	82	45	A
6	82	48	U
6	82	50	A
6	82	51	G
6	82	66	A
6	82	67	G
6	82	87	U
6	82	89	U
6	82	90	C
6	82	91	C
6	82	99	A
6	82	109	A
7	A1	4	U
7	A1	5	U
7	A1	6	G
7	A1	7	A
7	A1	8	A
7	A1	9	G
7	A1	26	A
7	A1	28	A
7	A1	32	A
7	A1	33	A
7	A1	39	G
7	A1	47	C
7	A1	48	C
7	A1	50	A
7	A1	51	A
7	A1	52	C
7	A1	54	C
7	A1	58	C
7	A1	70	U
7	A1	71	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	72	A
7	A1	75	G
7	A1	76	G
7	A1	78	A
7	A1	79	G
7	A1	80	A
7	A1	82	G
7	A1	84	U
7	A1	85	U
7	A1	86	G
7	A1	88	U
7	A1	89	U
7	A1	90	C
7	A1	91	U
7	A1	92	U
7	A1	94	G
7	A1	95	C
7	A1	100	G
7	A1	120	A
7	A1	121	U
7	A1	122	G
7	A1	129	A
7	A1	131	A
7	A1	136	C
7	A1	137	U
7	A1	138	G
7	A1	141	G
7	A1	142	G
7	A1	143	A
7	A1	144	G
7	A1	145	G
7	A1	146	G
7	A1	150	U
7	A1	156	C
7	A1	163	C
7	A1	164	G
7	A1	169	C
7	A1	173	U
7	A1	174	A
7	A1	176	C
7	A1	182	A
7	A1	183	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	184	G
7	A1	185	U
7	A1	191	G
7	A1	192	A
7	A1	193	C
7	A1	194	C
7	A1	197	A
7	A1	198	G
7	A1	201	G
7	A1	204	G
7	A1	205	A
7	A1	208	U
7	A1	209	U
7	A1	210	C
7	A1	211	G
7	A1	212	G
7	A1	215	C
7	A1	222	C
7	A1	239	U
7	A1	240	G
7	A1	245	U
7	A1	247	G
7	A1	251	G
7	A1	252	U
7	A1	253	A
7	A1	259	G
7	A1	261	U
7	A1	264	C
7	A1	266	G
7	A1	267	C
7	A1	275	G
7	A1	281	G
7	A1	289	G
7	A1	294	U
7	A1	298	A
7	A1	301	G
7	A1	306	A
7	A1	315	A
7	A1	316	C
7	A1	323	U
7	A1	328	C
7	A1	329	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	330	C
7	A1	345	C
7	A1	351	G
7	A1	352	C
7	A1	354	G
7	A1	363	A
7	A1	367	U
7	A1	372	C
7	A1	373	A
7	A1	384	G
7	A1	387	U
7	A1	388	G
7	A1	406	G
7	A1	407	U
7	A1	411	A
7	A1	412	A
7	A1	413	G
7	A1	414	A
7	A1	415	A
7	A1	421	U
7	A1	422	C
7	A1	423	G
7	A1	424	G
7	A1	428	G
7	A1	429	U
7	A1	438	U
7	A1	442	G
7	A1	446	G
7	A1	451	A
7	A1	457	G
7	A1	458	U
7	A1	459	A
7	A1	460	A
7	A1	464	U
7	A1	465	A
7	A1	468	A
7	A1	470	C
7	A1	471	U
7	A1	474	G
7	A1	475	C
7	A1	476	U
7	A1	479	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	484	G
7	A1	486	U
7	A1	496	A
7	A1	509	A
7	A1	511	C
7	A1	517	G
7	A1	518	C
7	A1	521	G
7	A1	522	C
7	A1	527	G7M
7	A1	530	G
7	A1	531	U
7	A1	532	A
7	A1	536	C
7	A1	547	A
7	A1	559	A
7	A1	562	U
7	A1	566	G
7	A1	572	A
7	A1	573	A
7	A1	575	G
7	A1	576	C
7	A1	577	G
7	A1	582	C
7	A1	596	A
7	A1	611	C
7	A1	633	G
7	A1	639	G
7	A1	640	A
7	A1	641	U
7	A1	643	C
7	A1	649	A
7	A1	650	G
7	A1	652	U
7	A1	653	U
7	A1	654	G
7	A1	661	G
7	A1	664	G
7	A1	665	A
7	A1	668	G
7	A1	672	U
7	A1	674	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	675	A
7	A1	684	U
7	A1	686	U
7	A1	687	A
7	A1	690	G
7	A1	693	G
7	A1	694	A
7	A1	702	A
7	A1	703	G
7	A1	704	A
7	A1	705	G
7	A1	709	U
7	A1	712	A
7	A1	717	U
7	A1	720	C
7	A1	721	G
7	A1	723	U
7	A1	724	G
7	A1	725	G
7	A1	731	G
7	A1	734	G
7	A1	736	C
7	A1	746	A
7	A1	748	G
7	A1	755	G
7	A1	763	G
7	A1	774	G
7	A1	777	A
7	A1	782	A
7	A1	787	A
7	A1	790	A
7	A1	793	U
7	A1	794	A
7	A1	799	G
7	A1	806	C
7	A1	808	C
7	A1	815	A
7	A1	817	C
7	A1	828	U
7	A1	831	A
7	A1	835	U
7	A1	837	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	841	C
7	A1	842	U
7	A1	843	U
7	A1	844	G
7	A1	845	A
7	A1	846	G
7	A1	848	C
7	A1	849	G
7	A1	850	U
7	A1	860	A
7	A1	864	A
7	A1	870	U
7	A1	871	U
7	A1	874	G
7	A1	876	C
7	A1	884	U
7	A1	885	G
7	A1	887	G
7	A1	889	A
7	A1	890	G
7	A1	899	C
7	A1	902	G
7	A1	914	A
7	A1	922	G
7	A1	926	G
7	A1	933	G
7	A1	934	C
7	A1	935	A
7	A1	939	G
7	A1	940	C
7	A1	942	G
7	A1	943	U
7	A1	947	G
7	A1	958	A
7	A1	960	U
7	A1	961	U
7	A1	966	2MG
7	A1	969	A
7	A1	971	G
7	A1	973	G
7	A1	975	A
7	A1	976	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	977	A
7	A1	979	C
7	A1	981	U
7	A1	992	U
7	A1	993	G
7	A1	994	A
7	A1	995	C
7	A1	996	A
7	A1	998	C
7	A1	1003	G
7	A1	1004	A
7	A1	1008	U
7	A1	1009	U
7	A1	1010	U
7	A1	1014	A
7	A1	1017	U
7	A1	1020	G
7	A1	1021	A
7	A1	1027	C
7	A1	1028	C
7	A1	1029	U
7	A1	1030	U
7	A1	1031	C
7	A1	1032	G
7	A1	1033	G
7	A1	1034	G
7	A1	1036	A
7	A1	1044	A
7	A1	1045	C
7	A1	1046	A
7	A1	1050	G
7	A1	1054	C
7	A1	1055	A
7	A1	1058	G
7	A1	1066	C
7	A1	1070	U
7	A1	1073	U
7	A1	1078	U
7	A1	1085	U
7	A1	1086	U
7	A1	1094	G
7	A1	1095	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	1101	A
7	A1	1103	C
7	A1	1108	G
7	A1	1121	U
7	A1	1124	G
7	A1	1125	U
7	A1	1126	U
7	A1	1127	G
7	A1	1129	C
7	A1	1131	G
7	A1	1132	C
7	A1	1133	G
7	A1	1135	U
7	A1	1136	C
7	A1	1137	C
7	A1	1139	G
7	A1	1140	C
7	A1	1141	C
7	A1	1147	C
7	A1	1151	A
7	A1	1152	A
7	A1	1154	G
7	A1	1157	A
7	A1	1159	U
7	A1	1161	C
7	A1	1162	C
7	A1	1168	U
7	A1	1169	A
7	A1	1170	A
7	A1	1174	G
7	A1	1182	G
7	A1	1183	U
7	A1	1191	A
7	A1	1196	A
7	A1	1197	A
7	A1	1201	A
7	A1	1202	U
7	A1	1206	G
7	A1	1211	U
7	A1	1212	U
7	A1	1213	A
7	A1	1214	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	1215	G
7	A1	1221	G
7	A1	1224	U
7	A1	1225	A
7	A1	1226	C
7	A1	1227	A
7	A1	1228	C
7	A1	1235	U
7	A1	1236	A
7	A1	1239	A
7	A1	1240	U
7	A1	1241	G
7	A1	1243	C
7	A1	1250	A
7	A1	1253	G
7	A1	1256	A
7	A1	1260	G
7	A1	1270	G
7	A1	1272	G
7	A1	1279	G
7	A1	1280	A
7	A1	1281	C
7	A1	1287	A
7	A1	1298	U
7	A1	1300	G
7	A1	1301	U
7	A1	1302	C
7	A1	1308	U
7	A1	1309	G
7	A1	1310	G
7	A1	1317	C
7	A1	1320	C
7	A1	1328	C
7	A1	1331	G
7	A1	1335	U
7	A1	1336	C
7	A1	1338	G
7	A1	1345	U
7	A1	1346	A
7	A1	1347	G
7	A1	1348	U
7	A1	1352	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	1356	G
7	A1	1363	A
7	A1	1364	U
7	A1	1365	G
7	A1	1368	A
7	A1	1369	C
7	A1	1379	G
7	A1	1383	C
7	A1	1399	C
7	A1	1418	A
7	A1	1419	G
7	A1	1424	U
7	A1	1425	U
7	A1	1426	G
7	A1	1429	A
7	A1	1430	A
7	A1	1432	G
7	A1	1433	A
7	A1	1439	G
7	A1	1440	U
7	A1	1441	A
7	A1	1442	G
7	A1	1446	A
7	A1	1450	U
7	A1	1451	U
7	A1	1452	C
7	A1	1454	G
7	A1	1455	G
7	A1	1460	C
7	A1	1461	G
7	A1	1462	C
7	A1	1464	U
7	A1	1475	G
7	A1	1476	A
7	A1	1486	G
7	A1	1487	G
7	A1	1492	A
7	A1	1493	A
7	A1	1499	A
7	A1	1503	A
7	A1	1505	G
7	A1	1506	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	1507	A
7	A1	1517	G
7	A1	1529	G
7	A1	1530	G
7	A1	1536	C
7	A1	1537	U
7	A1	1539	C
7	A1	1541	U
7	A1	1542	A
7	A2	2	A
7	A2	4	U
7	A2	7	A
7	A2	8	A
7	A2	9	G
7	A2	16	A
7	A2	26	A
7	A2	30	U
7	A2	31	G
7	A2	32	A
7	A2	39	G
7	A2	40	C
7	A2	47	C
7	A2	48	C
7	A2	51	A
7	A2	64	G
7	A2	70	U
7	A2	71	A
7	A2	72	A
7	A2	73	C
7	A2	74	A
7	A2	75	G
7	A2	76	G
7	A2	78	A
7	A2	82	G
7	A2	85	U
7	A2	86	G
7	A2	88	U
7	A2	90	C
7	A2	91	U
7	A2	94	G
7	A2	95	C
7	A2	97	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A2	98	A
7	A2	116	A
7	A2	120	A
7	A2	121	U
7	A2	129	A
7	A2	131	A
7	A2	137	U
7	A2	138	G
7	A2	141	G
7	A2	143	A
7	A2	148	G
7	A2	150	U
7	A2	155	A
7	A2	163	C
7	A2	164	G
7	A2	173	U
7	A2	174	A
7	A2	176	C
7	A2	177	G
7	A2	182	A
7	A2	183	C
7	A2	186	C
7	A2	187	G
7	A2	188	C
7	A2	193	C
7	A2	195	A
7	A2	197	A
7	A2	199	A
7	A2	202	G
7	A2	204	G
7	A2	205	A
7	A2	207	C
7	A2	208	U
7	A2	209	U
7	A2	210	C
7	A2	215	C
7	A2	216	U
7	A2	218	U
7	A2	224	U
7	A2	240	G
7	A2	245	U
7	A2	247	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A2	250	A
7	A2	251	G
7	A2	252	U
7	A2	253	A
7	A2	257	G
7	A2	262	A
7	A2	263	A
7	A2	266	G
7	A2	267	C
7	A2	269	C
7	A2	275	G
7	A2	276	G
7	A2	278	G
7	A2	279	A
7	A2	281	G
7	A2	282	A
7	A2	289	G
7	A2	301	G
7	A2	305	G
7	A2	316	C
7	A2	323	U
7	A2	328	C
7	A2	329	A
7	A2	330	C
7	A2	331	G
7	A2	347	G
7	A2	351	G
7	A2	352	C
7	A2	354	G
7	A2	355	C
7	A2	356	A
7	A2	361	G
7	A2	367	U
7	A2	368	U
7	A2	370	C
7	A2	372	C
7	A2	373	A
7	A2	374	A
7	A2	375	U
7	A2	387	U
7	A2	388	G
7	A2	391	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A2	393	A
7	A2	397	A
7	A2	398	U
7	A2	405	U
7	A2	406	G
7	A2	408	A
7	A2	409	U
7	A2	411	A
7	A2	412	A
7	A2	413	G
7	A2	414	A
7	A2	415	A
7	A2	416	G
7	A2	422	C
7	A2	423	G
7	A2	424	G
7	A2	426	U
7	A2	428	G
7	A2	429	U
7	A2	431	A
7	A2	437	U
7	A2	439	U
7	A2	440	C
7	A2	442	G
7	A2	443	C
7	A2	444	G
7	A2	445	G
7	A2	448	A
7	A2	450	G
7	A2	452	A
7	A2	456	A
7	A2	457	G
7	A2	458	U
7	A2	459	A
7	A2	460	A
7	A2	461	A
7	A2	462	G
7	A2	464	U
7	A2	465	A
7	A2	466	A
7	A2	467	U
7	A2	468	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A2	469	C
7	A2	472	U
7	A2	473	U
7	A2	474	G
7	A2	475	C
7	A2	478	A
7	A2	479	U
7	A2	480	U
7	A2	481	G
7	A2	482	A
7	A2	484	G
7	A2	492	C
7	A2	495	A
7	A2	496	A
7	A2	497	G
7	A2	498	A
7	A2	499	A
7	A2	501	C
7	A2	506	G
7	A2	511	C
7	A2	512	U
7	A2	513	C
7	A2	516	U
7	A2	518	C
7	A2	520	A
7	A2	521	G
7	A2	524	G
7	A2	527	G7M
7	A2	529	G
7	A2	530	G
7	A2	531	U
7	A2	532	A
7	A2	533	A
7	A2	534	U
7	A2	536	C
7	A2	538	G
7	A2	539	A
7	A2	542	G
7	A2	547	A
7	A2	549	C
7	A2	551	U
7	A2	558	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A2	559	A
7	A2	562	U
7	A2	572	A
7	A2	573	A
7	A2	575	G
7	A2	576	C
7	A2	577	G
7	A2	633	G
7	A2	653	U
7	A2	665	A
7	A2	703	G
7	A2	718	A
7	A2	721	G
7	A2	723	U
7	A2	724	G
7	A2	731	G
7	A2	733	G
7	A2	734	G
7	A2	735	C
7	A2	748	G
7	A2	755	G
7	A2	777	A
7	A2	788	U
7	A2	790	A
7	A2	793	U
7	A2	794	A
7	A2	815	A
7	A2	817	C
7	A2	821	G
7	A2	829	G
7	A2	841	C
7	A2	842	U
7	A2	843	U
7	A2	844	G
7	A2	845	A
7	A2	846	G
7	A2	902	G
7	A2	914	A
7	A2	926	G
7	A2	933	G
7	A2	934	C
7	A2	935	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A2	945	G
7	A2	953	G
7	A2	960	U
7	A2	961	U
7	A2	966	2MG
7	A2	968	A
7	A2	969	A
7	A2	972	C
7	A2	974	A
7	A2	975	A
7	A2	976	G
7	A2	977	A
7	A2	989	U
7	A2	991	U
7	A2	992	U
7	A2	993	G
7	A2	994	A
7	A2	996	A
7	A2	1004	A
7	A2	1006	G
7	A2	1008	U
7	A2	1009	U
7	A2	1011	C
7	A2	1014	A
7	A2	1017	U
7	A2	1018	G
7	A2	1019	A
7	A2	1020	G
7	A2	1021	A
7	A2	1022	A
7	A2	1023	U
7	A2	1029	U
7	A2	1030	U
7	A2	1031	C
7	A2	1032	G
7	A2	1033	G
7	A2	1034	G
7	A2	1044	A
7	A2	1046	A
7	A2	1056	U
7	A2	1063	C
7	A2	1064	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A2	1065	U
7	A2	1067	A
7	A2	1074	G
7	A2	1081	A
7	A2	1085	U
7	A2	1086	U
7	A2	1094	G
7	A2	1095	U
7	A2	1098	C
7	A2	1101	A
7	A2	1108	G
7	A2	1113	C
7	A2	1124	G
7	A2	1125	U
7	A2	1127	G
7	A2	1128	C
7	A2	1129	C
7	A2	1130	A
7	A2	1131	G
7	A2	1133	G
7	A2	1134	G
7	A2	1136	C
7	A2	1137	C
7	A2	1138	G
7	A2	1139	G
7	A2	1140	C
7	A2	1141	C
7	A2	1146	A
7	A2	1152	A
7	A2	1157	A
7	A2	1158	C
7	A2	1159	U
7	A2	1160	G
7	A2	1168	U
7	A2	1169	A
7	A2	1182	G
7	A2	1184	G
7	A2	1185	G
7	A2	1191	A
7	A2	1196	A
7	A2	1197	A
7	A2	1201	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A2	1202	U
7	A2	1206	G
7	A2	1212	U
7	A2	1213	A
7	A2	1215	G
7	A2	1217	C
7	A2	1218	C
7	A2	1225	A
7	A2	1226	C
7	A2	1227	A
7	A2	1238	A
7	A2	1241	G
7	A2	1248	A
7	A2	1249	C
7	A2	1253	G
7	A2	1256	A
7	A2	1268	G
7	A2	1270	G
7	A2	1271	A
7	A2	1279	G
7	A2	1280	A
7	A2	1281	C
7	A2	1282	C
7	A2	1286	U
7	A2	1287	A
7	A2	1291	U
7	A2	1297	G
7	A2	1298	U
7	A2	1300	G
7	A2	1305	G
7	A2	1317	C
7	A2	1318	A
7	A2	1320	C
7	A2	1332	A
7	A2	1336	C
7	A2	1338	G
7	A2	1340	A
7	A2	1346	A
7	A2	1348	U
7	A2	1351	U
7	A2	1353	G
7	A2	1360	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A2	1363	A
7	A2	1364	U
7	A2	1368	A
7	A2	1370	G
7	A2	1375	A
7	A2	1379	G
7	A2	1397	C
7	A2	1398	A
7	A2	1429	A
7	A2	1432	G
7	A2	1441	A
7	A2	1446	A
7	A2	1448	C
7	A2	1454	G
7	A2	1487	G
7	A2	1492	A
7	A2	1498	UR3
7	A2	1499	A
7	A2	1503	A
7	A2	1506	U
7	A2	1517	G
7	A2	1529	G
7	A2	1530	G
7	A2	1533	C
7	A2	1534	A
7	A2	1535	C
7	A2	1536	C
7	A2	1537	U
28	V2	6	A
28	V2	8	A
28	V2	9	A
28	V2	10	G
28	V2	11	G
28	V2	14	G
28	V2	15	G
28	V2	16	U
28	V2	17	G
28	V2	18	A
28	V2	19	G
28	V2	20	C
28	V2	21	U
28	V2	23	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
28	V2	24	G
28	V2	30	A
28	V2	32	U
28	V2	33	A
28	V2	34	A
28	V2	35	A
28	V2	37	A
28	V2	38	A
28	V2	39	A
28	V2	40	A
28	V2	41	G
28	V2	42	G
28	V2	43	U
28	V2	45	U
28	V2	46	C
28	V2	47	G
28	V2	48	C
28	V2	50	C
28	V2	53	G
28	V2	54	G
28	V2	57	A
28	V2	58	A
28	V2	61	U
28	V2	62	C
28	V2	63	G
28	V2	64	A
28	V2	66	A
28	V2	67	A
29	W	2	G
29	W	4	G
29	W	8	4SU
29	W	11	U
29	W	15	A
29	W	16	H2U
29	W	17	H2U
29	W	18	G
29	W	19	G
29	W	20	H2U
29	W	22	G
29	W	34	C
29	W	44	G
29	W	46	G7M

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	W	47	U
29	W	48	U
29	W	49	G
29	W	52	A
29	W	53	G
29	W	54	5MU
29	W	55	PSU
29	W	58	A
29	W	59	G
29	W	60	U
29	W	72	U
29	W	76	A
30	W1	11	C
30	W1	15	G
30	W1	22	G
30	W1	35	A
30	W1	44	G
30	W1	46	G7M
30	W1	47	U
30	W1	48	C
31	X2	2	C
31	X2	3	A
31	X2	8	4SU
31	X2	9	A
31	X2	13	C
31	X2	15	G
31	X2	16	C
31	X2	18	G
31	X2	20	A
31	X2	21	H2U
31	X2	22	A
31	X2	34	U
31	X2	35	I
31	X2	36	C
31	X2	39	A
31	X2	47	G7M
31	X2	49	C
31	X2	55	5MU
31	X2	60	A
31	X2	66	C
31	X2	71	U
31	X2	72	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	X2	73	C
31	X2	74	A
31	X2	76	C
31	X2	77	A
32	Y1	10	G
32	Y1	11	C
32	Y1	46	7MG
32	Y1	48	C
33	Y2	15	G
33	Y2	16	C
33	Y2	17	H2U
33	Y2	18	G
33	Y2	19	G
33	Y2	20	G
33	Y2	21	A
33	Y2	22	G
33	Y2	34	G
33	Y2	36	C
33	Y2	39	G
33	Y2	45	G
33	Y2	46	G7M
33	Y2	48	C
33	Y2	49	A
33	Y2	54	5MU
33	Y2	56	C
33	Y2	64	C
33	Y2	72	C
33	Y2	73	A
33	Y2	74	C
33	Y2	75	C
33	Y2	76	A

All (129) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	43	G
5	72	134	G
5	72	158	U
5	72	277	G
5	72	285	G
5	72	352	A
5	72	404	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	72	504	A
5	72	512	G
5	72	613	A
5	72	747	5MU
5	72	748	G
5	72	749	A
5	72	784	G
5	72	827	U
5	72	1020	A
5	72	1046	A
5	72	1130	U
5	72	1211	C
5	72	1266	G
5	72	1416	G
5	72	1475	G
5	72	1490	A
5	72	1580	A
5	72	1847	A
5	72	1940	U
5	72	2061	G
5	72	2118	U
5	72	2172	U
5	72	2430	A
5	72	2581	G
5	72	2585	U
5	72	2756	U
6	82	3	C
6	82	15	A
6	82	39	A
6	82	88	C
7	A1	5	U
7	A1	7	A
7	A1	51	A
7	A1	70	U
7	A1	129	A
7	A1	173	U
7	A1	197	A
7	A1	209	U
7	A1	251	G
7	A1	274	A
7	A1	372	C
7	A1	412	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	A1	421	U
7	A1	428	G
7	A1	438	U
7	A1	535	A
7	A1	559	A
7	A1	575	G
7	A1	653	U
7	A1	686	U
7	A1	870	U
7	A1	884	U
7	A1	992	U
7	A1	993	G
7	A1	1054	C
7	A1	1085	U
7	A1	1182	G
7	A1	1190	G
7	A1	1201	A
7	A1	1302	C
7	A1	1335	U
7	A1	1432	G
7	A1	1440	U
7	A1	1452	C
7	A1	1463	U
7	A1	1536	C
7	A2	7	A
7	A2	13	U
7	A2	30	U
7	A2	70	U
7	A2	183	C
7	A2	208	U
7	A2	209	U
7	A2	251	G
7	A2	367	U
7	A2	411	A
7	A2	428	G
7	A2	438	U
7	A2	532	A
7	A2	537	G
7	A2	717	U
7	A2	845	A
7	A2	992	U
7	A2	993	G

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Mol	Chain	Res	Type
7	A2	1085	U
7	A2	1101	A
7	A2	1129	C
7	A2	1136	C
7	A2	1140	C
7	A2	1168	U
7	A2	1190	G
7	A2	1201	A
7	A2	1256	A
7	A2	1281	C
7	A2	1297	G
7	A2	1319	A
7	A2	1533	C
7	A2	1534	A
7	A2	1535	C
28	V2	8	A
28	V2	23	C
28	V2	31	U
28	V2	36	A
28	V2	37	A
28	V2	39	A
28	V2	46	C
28	V2	53	G
29	W	10	G
29	W	18	G
29	W	19	G
29	W	43	G
30	W1	10	G
30	W1	43	C
31	X2	15	G
31	X2	22	A
31	X2	47	G7M
31	X2	49	C
31	X2	73	C
32	Y1	10	G
32	Y1	47	U
33	Y2	17	H2U
33	Y2	63	G

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

73 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
30	PSU	W1	32	30	18,21,22	4.65	8 (44%)	22,30,33	1.82	5 (22%)
7	UR3	A2	1498	7	19,22,23	2.73	8 (42%)	26,32,35	1.29	2 (7%)
5	5MU	72	747	5	19,22,23	0.34	0	28,32,35	0.58	0
32	6MZ	Y1	37	32	18,25,26	2.06	3 (16%)	16,36,39	2.35	4 (25%)
7	2MG	A2	966	7	18,26,27	2.85	7 (38%)	16,38,41	1.35	3 (18%)
33	PSU	Y2	55	33	18,21,22	0.88	1 (5%)	22,30,33	0.64	0
31	H2U	X2	21	31	18,21,22	3.07	5 (27%)	21,30,33	2.04	5 (23%)
31	G7M	X2	47	31	20,26,27	2.81	7 (35%)	17,39,42	1.21	1 (5%)
32	7MG	Y1	46	32	22,26,27	3.89	10 (45%)	29,39,42	2.07	9 (31%)
5	PSU	72	2604	5	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
7	UR3	A1	1498	7	19,22,23	2.75	8 (42%)	26,32,35	1.29	3 (11%)
7	2MG	A2	1207	7	18,26,27	2.86	7 (38%)	16,38,41	1.37	3 (18%)
5	OMG	72	2251	5,29	18,26,27	2.82	7 (38%)	19,38,41	1.55	4 (21%)
30	MIA	W1	37	30	24,31,32	2.34	3 (12%)	26,44,47	2.67	7 (26%)
5	PSU	72	955	5	18,21,22	4.67	8 (44%)	22,30,33	1.87	5 (22%)
5	PSU	72	2580	5	18,21,22	4.65	8 (44%)	22,30,33	1.85	6 (27%)
33	G7M	Y2	46	33	20,26,27	2.81	8 (40%)	17,39,42	1.09	1 (5%)
5	2MG	72	2445	5	18,26,27	2.82	7 (38%)	16,38,41	1.41	4 (25%)
5	1MG	72	745	5	18,26,27	2.75	6 (33%)	19,39,42	1.43	3 (15%)
5	3TD	71	1915	5	19,22,23	4.09	7 (36%)	21,32,35	1.70	2 (9%)
5	PSU	72	2504	5,49	18,21,22	4.67	8 (44%)	22,30,33	1.92	5 (22%)
5	5MC	72	1962	5	18,22,23	4.01	7 (38%)	26,32,35	1.06	2 (7%)
29	H2U	W	16	29	18,21,22	3.05	5 (27%)	21,30,33	1.98	5 (23%)
29	H2U	W	20	29	18,21,22	3.04	5 (27%)	21,30,33	2.02	5 (23%)
30	PSU	W1	39	30	18,21,22	4.64	8 (44%)	22,30,33	1.84	5 (22%)
31	PSU	X2	56	31	18,21,22	0.87	1 (5%)	22,30,33	0.49	0
32	CM0	Y1	34	32	23,26,27	3.73	6 (26%)	27,37,40	1.52	2 (7%)
7	MA6	A2	1518	7	18,26,27	1.07	2 (11%)	19,38,41	3.41	3 (15%)
5	6MZ	72	1618	5	18,25,26	2.03	2 (11%)	16,36,39	2.20	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	3AU	X2	48	31	24,28,29	2.84	7 (29%)	33,40,43	1.29	3 (9%)
30	G7M	W1	46	30	20,26,27	2.81	7 (35%)	17,39,42	1.12	1 (5%)
7	G7M	A2	527	7	20,26,27	2.77	7 (35%)	17,39,42	1.02	1 (5%)
30	4SU	W1	8	30	18,21,22	3.80	7 (38%)	26,30,33	2.21	4 (15%)
7	2MG	A1	1516	7	18,26,27	2.84	7 (38%)	16,38,41	1.36	3 (18%)
5	2MG	72	1835	5	18,26,27	2.80	7 (38%)	16,38,41	1.41	4 (25%)
5	PSU	72	2457	5	18,21,22	4.65	8 (44%)	22,30,33	1.88	5 (22%)
33	H2U	Y2	17	33	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
29	4SU	W	8	29	18,21,22	3.77	7 (38%)	26,30,33	2.26	5 (19%)
29	PSU	W	32	29	18,21,22	4.63	8 (44%)	22,30,33	1.88	5 (22%)
5	PSU	72	746	5	18,21,22	0.99	2 (11%)	22,30,33	0.95	1 (4%)
7	MA6	A1	1519	7	18,26,27	1.08	2 (11%)	19,38,41	3.47	3 (15%)
7	5MC	A2	967	7	18,22,23	4.01	7 (38%)	26,32,35	1.00	2 (7%)
7	5MC	A2	1407	7	18,22,23	4.00	7 (38%)	26,32,35	0.97	2 (7%)
31	H2U	X2	17	31	18,21,22	3.09	5 (27%)	21,30,33	1.95	5 (23%)
7	5MC	A1	1407	7	18,22,23	4.03	7 (38%)	26,32,35	0.99	2 (7%)
5	6MZ	72	2030	5	18,25,26	2.07	3 (16%)	16,36,39	2.31	3 (18%)
5	G7M	72	2069	5	20,26,27	2.77	7 (35%)	17,39,42	1.04	1 (5%)
5	H2U	72	2449	5,49	18,21,22	3.04	5 (27%)	21,30,33	2.03	5 (23%)
5	OMC	72	2498	5,49	19,22,23	3.29	8 (42%)	26,31,34	0.76	0
29	5MU	W	54	29	19,22,23	0.25	0	28,32,35	0.39	0
29	H2U	W	17	29	18,21,22	3.08	5 (27%)	21,30,33	2.01	5 (23%)
31	RSP	X2	33	31	17,21,22	4.13	7 (41%)	22,30,33	0.78	0
31	4SU	X2	8	31	18,21,22	3.79	7 (38%)	26,30,33	2.27	4 (15%)
29	MIA	W	37	29	24,31,32	2.32	3 (12%)	26,44,47	2.53	7 (26%)
5	PSU	72	2605	5	18,21,22	4.64	8 (44%)	22,30,33	1.85	5 (22%)
7	MA6	A2	1519	7	18,26,27	1.08	2 (11%)	19,38,41	3.42	3 (15%)
29	G7M	W	46	29	20,26,27	2.79	7 (35%)	17,39,42	1.12	1 (5%)
5	3TD	72	1915	5	19,22,23	4.03	7 (36%)	21,32,35	1.78	3 (14%)
7	2MG	A2	1516	7	18,26,27	2.81	7 (38%)	16,38,41	1.36	3 (18%)
5	5MU	72	1939	5	19,22,23	0.74	0	28,32,35	1.27	2 (7%)
7	2MG	A1	1207	7	18,26,27	2.84	7 (38%)	16,38,41	1.34	3 (18%)
33	5MU	Y2	54	33	19,22,23	0.24	0	28,32,35	0.24	0
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
29	PSU	W	55	29	18,21,22	0.85	1 (5%)	22,30,33	0.79	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	G7M	A1	527	7	20,26,27	2.79	8 (40%)	17,39,42	1.04	1 (5%)
7	2MG	A1	966	7	18,26,27	2.85	7 (38%)	16,38,41	1.41	3 (18%)
7	5MC	A1	967	7	18,22,23	4.03	7 (38%)	26,32,35	1.01	2 (7%)
5	2MA	72	2503	5	17,25,26	2.63	5 (29%)	17,37,40	1.33	2 (11%)
31	5MU	X2	55	31	19,22,23	0.25	0	28,32,35	0.18	0
31	2MA	X2	38	31	17,25,26	2.68	5 (29%)	17,37,40	1.24	2 (11%)
7	4OC	A2	1402	7	20,23,24	3.24	8 (40%)	26,32,35	0.90	1 (3%)
7	4OC	A1	1402	7	20,23,24	3.22	8 (40%)	26,32,35	0.93	1 (3%)
7	MA6	A1	1518	7	18,26,27	1.06	2 (11%)	19,38,41	3.38	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
5	5MU	72	747	5	-	0/7/25/26	0/2/2/2
32	6MZ	Y1	37	32	-	2/5/27/28	0/3/3/3
7	2MG	A2	966	7	-	0/5/27/28	0/3/3/3
33	PSU	Y2	55	33	-	0/7/25/26	0/2/2/2
31	H2U	X2	21	31	-	3/7/38/39	0/2/2/2
31	G7M	X2	47	31	-	3/3/25/26	0/3/3/3
32	7MG	Y1	46	32	-	1/7/37/38	0/3/3/3
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2
7	2MG	A2	1207	7	-	0/5/27/28	0/3/3/3
5	OMG	72	2251	5,29	-	3/5/27/28	0/3/3/3
30	MIA	W1	37	30	-	6/11/33/34	0/3/3/3
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
33	G7M	Y2	46	33	-	2/3/25/26	0/3/3/3
5	2MG	72	2445	5	-	0/5/27/28	0/3/3/3
5	1MG	72	745	5	-	0/3/25/26	0/3/3/3
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
5	PSU	72	2504	5,49	-	1/7/25/26	0/2/2/2
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	H2U	W	20	29	-	1/7/38/39	0/2/2/2
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
31	PSU	X2	56	31	-	2/7/25/26	0/2/2/2
32	CM0	Y1	34	32	-	2/12/30/31	0/2/2/2
7	MA6	A2	1518	7	-	0/7/29/30	0/3/3/3
5	6MZ	72	1618	5	-	4/5/27/28	0/3/3/3
31	3AU	X2	48	31	-	6/16/34/35	0/2/2/2
30	G7M	W1	46	30	-	3/3/25/26	0/3/3/3
7	G7M	A2	527	7	-	3/3/25/26	0/3/3/3
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2
7	2MG	A1	1516	7	-	0/5/27/28	0/3/3/3
5	2MG	72	1835	5	-	0/5/27/28	0/3/3/3
5	PSU	72	2457	5	-	2/7/25/26	0/2/2/2
33	H2U	Y2	17	33	-	7/7/38/39	0/2/2/2
29	4SU	W	8	29	-	2/7/25/26	0/2/2/2
29	PSU	W	32	29	-	0/7/25/26	0/2/2/2
5	PSU	72	746	5	-	1/7/25/26	0/2/2/2
7	MA6	A1	1519	7	-	6/7/29/30	0/3/3/3
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2
31	H2U	X2	17	31	-	6/7/38/39	0/2/2/2
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
5	6MZ	72	2030	5	-	3/5/27/28	0/3/3/3
5	G7M	72	2069	5	-	2/3/25/26	0/3/3/3
5	H2U	72	2449	5,49	-	1/7/38/39	0/2/2/2
5	OMC	72	2498	5,49	-	2/9/27/28	0/2/2/2
29	5MU	W	54	29	-	3/7/25/26	0/2/2/2
29	H2U	W	17	29	-	1/7/38/39	0/2/2/2
31	RSP	X2	33	31	-	1/7/25/26	0/2/2/2
31	4SU	X2	8	31	-	2/7/25/26	0/2/2/2
29	MIA	W	37	29	-	1/11/33/34	0/3/3/3
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2
7	MA6	A2	1519	7	-	2/7/29/30	0/3/3/3
29	G7M	W	46	29	-	3/3/25/26	0/3/3/3
5	3TD	72	1915	5	-	2/7/25/26	0/2/2/2
7	2MG	A2	1516	7	-	0/5/27/28	0/3/3/3
5	5MU	72	1939	5	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	2MG	A1	1207	7	-	0/5/27/28	0/3/3/3
33	5MU	Y2	54	33	-	2/7/25/26	0/2/2/2
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
29	PSU	W	55	29	-	3/7/25/26	0/2/2/2
7	G7M	A1	527	7	-	1/3/25/26	0/3/3/3
7	2MG	A1	966	7	-	0/5/27/28	0/3/3/3
7	5MC	A1	967	7	-	0/7/25/26	0/2/2/2
5	2MA	72	2503	5	-	0/3/25/26	0/3/3/3
31	5MU	X2	55	31	-	2/7/25/26	0/2/2/2
31	2MA	X2	38	31	-	3/3/25/26	0/3/3/3
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
7	4OC	A1	1402	7	-	2/9/29/30	0/2/2/2
7	MA6	A1	1518	7	-	3/7/29/30	0/3/3/3

All (412) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y1	34	CM0	C6-C5	12.87	1.48	1.34
5	71	1915	3TD	C6-C5	12.74	1.50	1.35
5	72	1915	3TD	C6-C5	12.52	1.49	1.35
5	72	2504	PSU	C6-C5	12.20	1.49	1.35
5	72	955	PSU	C6-C5	12.17	1.49	1.35
5	72	2457	PSU	C6-C5	12.13	1.49	1.35
30	W1	32	PSU	C6-C5	12.13	1.49	1.35
30	W1	39	PSU	C6-C5	12.12	1.49	1.35
29	W	32	PSU	C6-C5	12.10	1.49	1.35
5	72	2605	PSU	C6-C5	12.09	1.49	1.35
5	72	2580	PSU	C6-C5	12.06	1.49	1.35
5	72	2604	PSU	C6-C5	12.06	1.49	1.35
31	X2	33	RSP	C2-N3	11.76	1.48	1.36
32	Y1	46	7MG	C8-N9	9.99	1.51	1.46
7	A1	967	5MC	C6-C5	9.98	1.51	1.34
7	A1	1407	5MC	C6-C5	9.89	1.50	1.34
5	72	1962	5MC	C6-C5	9.89	1.50	1.34
7	A2	967	5MC	C6-C5	9.87	1.50	1.34
7	A2	1407	5MC	C6-C5	9.84	1.50	1.34
5	72	2504	PSU	C2-N1	9.63	1.49	1.36
31	X2	17	H2U	C2-N1	9.62	1.49	1.35
5	72	955	PSU	C2-N1	9.58	1.49	1.36
5	72	2580	PSU	C2-N1	9.56	1.49	1.36
30	W1	32	PSU	C2-N1	9.55	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2604	PSU	C2-N1	9.54	1.49	1.36
30	W1	39	PSU	C2-N1	9.53	1.49	1.36
5	72	2457	PSU	C2-N1	9.53	1.49	1.36
5	72	2605	PSU	C2-N1	9.52	1.49	1.36
29	W	32	PSU	C2-N1	9.49	1.49	1.36
29	W	17	H2U	C2-N1	9.46	1.49	1.35
31	X2	21	H2U	C2-N1	9.44	1.49	1.35
33	Y2	17	H2U	C2-N1	9.42	1.49	1.35
29	W	16	H2U	C2-N1	9.39	1.49	1.35
5	72	2449	H2U	C2-N1	9.36	1.49	1.35
29	W	20	H2U	C2-N1	9.34	1.49	1.35
30	W1	8	4SU	C4-N3	8.98	1.47	1.37
5	71	1915	3TD	C2-N1	8.86	1.48	1.37
29	W	8	4SU	C4-N3	8.85	1.47	1.37
5	72	1915	3TD	C2-N1	8.85	1.48	1.37
31	X2	8	4SU	C4-N3	8.83	1.47	1.37
5	72	2504	PSU	C2-N3	8.24	1.51	1.37
5	72	955	PSU	C2-N3	8.23	1.51	1.37
30	W1	32	PSU	C2-N3	8.21	1.51	1.37
29	W	32	PSU	C2-N3	8.21	1.51	1.37
5	72	2605	PSU	C2-N3	8.20	1.51	1.37
5	72	2580	PSU	C2-N3	8.19	1.51	1.37
5	72	2604	PSU	C2-N3	8.19	1.51	1.37
5	72	2457	PSU	C2-N3	8.19	1.51	1.37
30	W1	39	PSU	C2-N3	8.14	1.51	1.37
31	X2	48	3AU	C2-N1	8.13	1.50	1.38
31	X2	38	2MA	C2-N3	8.09	1.48	1.31
5	72	2503	2MA	C2-N3	7.92	1.48	1.31
32	Y1	46	7MG	C5-N7	7.90	1.44	1.35
30	W1	37	MIA	C2-S10	7.71	1.82	1.75
29	W	37	MIA	C2-S10	7.69	1.82	1.75
5	72	1962	5MC	C4-N3	7.46	1.46	1.34
7	A2	967	5MC	C4-N3	7.45	1.46	1.34
7	A1	967	5MC	C4-N3	7.44	1.46	1.34
5	72	2030	6MZ	C6-N6	7.42	1.47	1.35
32	Y1	34	CM0	C2-N1	7.39	1.50	1.38
7	A1	1407	5MC	C4-N3	7.35	1.46	1.34
32	Y1	37	6MZ	C6-N6	7.34	1.47	1.35
7	A2	1407	5MC	C4-N3	7.30	1.46	1.34
5	72	1618	6MZ	C6-N6	7.22	1.46	1.35
5	72	2251	OMG	C2-N2	7.18	1.51	1.34
7	A2	1402	4OC	C4-N3	7.12	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A1	1498	UR3	C2-N1	7.04	1.48	1.38
5	72	2498	OMC	C2-N3	7.00	1.50	1.36
7	A2	1498	UR3	C2-N1	6.98	1.48	1.38
32	Y1	34	CM0	C2-N3	6.98	1.50	1.38
5	72	2552	OMU	C2-N3	6.97	1.50	1.38
7	A1	1407	5MC	C2-N3	6.96	1.50	1.36
7	A1	1402	4OC	C4-N3	6.95	1.44	1.32
7	A1	967	5MC	C2-N3	6.94	1.50	1.36
7	A2	967	5MC	C2-N3	6.92	1.50	1.36
30	W1	8	4SU	C2-N3	6.91	1.50	1.38
30	W1	37	MIA	C6-N6	6.91	1.47	1.34
5	72	1962	5MC	C2-N3	6.90	1.50	1.36
7	A2	1407	5MC	C2-N3	6.90	1.50	1.36
31	X2	8	4SU	C2-N3	6.86	1.50	1.38
29	W	8	4SU	C2-N3	6.82	1.50	1.38
5	72	745	1MG	C2-N3	6.80	1.47	1.34
29	W	37	MIA	C6-N6	6.80	1.47	1.34
31	X2	33	RSP	C6-C5	6.72	1.50	1.35
31	X2	33	RSP	C4-N4	6.65	1.49	1.33
33	Y2	46	G7M	C2-N2	6.61	1.49	1.34
31	X2	47	G7M	C2-N2	6.59	1.49	1.34
29	W	46	G7M	C2-N2	6.58	1.49	1.34
5	72	2069	G7M	C2-N2	6.58	1.49	1.34
30	W1	46	G7M	C2-N2	6.56	1.49	1.34
7	A2	527	G7M	C2-N2	6.55	1.49	1.34
7	A2	1207	2MG	C2-N2	6.54	1.47	1.33
7	A1	527	G7M	C2-N2	6.53	1.49	1.34
5	72	2552	OMU	C2-N1	6.53	1.48	1.38
29	W	17	H2U	C2-N3	6.52	1.49	1.38
31	X2	17	H2U	C2-N3	6.49	1.49	1.38
33	Y2	17	H2U	C2-N3	6.49	1.49	1.38
7	A1	1516	2MG	C2-N2	6.48	1.47	1.33
31	X2	21	H2U	C2-N3	6.47	1.49	1.38
7	A1	966	2MG	C2-N2	6.47	1.47	1.33
29	W	20	H2U	C2-N3	6.46	1.49	1.38
7	A1	1207	2MG	C2-N2	6.45	1.47	1.33
7	A2	966	2MG	C2-N2	6.45	1.47	1.33
7	A1	1402	4OC	C6-C5	6.43	1.50	1.35
5	72	1835	2MG	C2-N2	6.43	1.47	1.33
29	W	16	H2U	C2-N3	6.42	1.49	1.38
7	A2	1516	2MG	C2-N2	6.41	1.47	1.33
5	72	745	1MG	C2-N2	6.41	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2449	H2U	C2-N3	6.40	1.49	1.38
31	X2	48	3AU	C2-N3	6.38	1.50	1.38
5	72	2445	2MG	C2-N2	6.38	1.47	1.33
7	A2	1402	4OC	C6-C5	6.36	1.49	1.35
7	A2	1402	4OC	C2-N3	6.33	1.49	1.36
7	A1	1402	4OC	C2-N3	6.21	1.48	1.36
7	A1	1498	UR3	C6-C5	6.16	1.49	1.35
7	A2	1498	UR3	C6-C5	6.13	1.49	1.35
5	72	2498	OMC	C6-C5	6.11	1.49	1.35
31	X2	8	4SU	C4-S4	-6.07	1.56	1.68
31	X2	48	3AU	C6-C5	6.04	1.49	1.35
29	W	8	4SU	C4-S4	-5.96	1.57	1.68
30	W1	8	4SU	C4-S4	-5.93	1.57	1.68
32	Y1	46	7MG	C2-N3	5.92	1.47	1.33
31	X2	8	4SU	C2-N1	5.86	1.47	1.38
30	W1	8	4SU	C6-C5	5.84	1.48	1.35
5	72	955	PSU	C6-N1	5.83	1.45	1.36
33	Y2	46	G7M	C2-N3	5.83	1.47	1.33
30	W1	8	4SU	C2-N1	5.83	1.47	1.38
29	W	8	4SU	C6-C5	5.82	1.48	1.35
30	W1	39	PSU	C6-N1	5.82	1.45	1.36
31	X2	8	4SU	C6-C5	5.82	1.48	1.35
30	W1	46	G7M	C2-N3	5.80	1.47	1.33
5	72	2457	PSU	C6-N1	5.80	1.45	1.36
7	A1	527	G7M	C2-N3	5.80	1.47	1.33
5	72	2580	PSU	C6-N1	5.79	1.45	1.36
5	72	2504	PSU	C6-N1	5.79	1.45	1.36
30	W1	32	PSU	C6-N1	5.77	1.45	1.36
5	72	2605	PSU	C6-N1	5.77	1.45	1.36
5	72	2604	PSU	C6-N1	5.76	1.45	1.36
31	X2	47	G7M	C2-N3	5.74	1.47	1.33
7	A2	527	G7M	C2-N3	5.74	1.47	1.33
5	72	2069	G7M	C2-N3	5.74	1.47	1.33
29	W	46	G7M	C2-N3	5.74	1.47	1.33
29	W	32	PSU	C6-N1	5.73	1.45	1.36
29	W	8	4SU	C2-N1	5.72	1.47	1.38
32	Y1	46	7MG	C4-N9	5.67	1.44	1.37
7	A1	967	5MC	C4-N4	5.66	1.48	1.34
7	A1	1407	5MC	C4-N4	5.66	1.48	1.34
7	A2	1407	5MC	C4-N4	5.64	1.48	1.34
7	A2	967	5MC	C4-N4	5.63	1.48	1.34
5	72	1962	5MC	C4-N4	5.62	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A1	1407	5MC	C6-N1	5.61	1.47	1.38
32	Y1	46	7MG	C4-N3	5.59	1.47	1.34
5	72	2445	2MG	C4-N3	5.55	1.50	1.37
7	A1	966	2MG	C4-N3	5.54	1.50	1.37
7	A2	1407	5MC	C6-N1	5.53	1.47	1.38
5	71	1915	3TD	C6-N1	5.53	1.45	1.36
7	A1	1516	2MG	C4-N3	5.52	1.50	1.37
5	72	2498	OMC	C4-N3	5.51	1.45	1.34
7	A2	1207	2MG	C4-N3	5.51	1.50	1.37
7	A1	967	5MC	C6-N1	5.49	1.47	1.38
5	72	1915	3TD	C6-N1	5.49	1.45	1.36
5	72	1962	5MC	C6-N1	5.47	1.47	1.38
7	A2	966	2MG	C4-N3	5.47	1.50	1.37
5	72	2552	OMU	C6-C5	5.47	1.47	1.35
5	72	1835	2MG	C4-N3	5.46	1.50	1.37
7	A2	967	5MC	C6-N1	5.44	1.47	1.38
7	A1	1207	2MG	C4-N3	5.42	1.50	1.37
7	A1	1207	2MG	C2-N1	5.42	1.45	1.36
31	X2	33	RSP	C4-N3	5.41	1.45	1.34
7	A1	966	2MG	C2-N1	5.40	1.45	1.36
7	A2	1207	2MG	C2-N1	5.40	1.45	1.36
7	A2	966	2MG	C2-N1	5.39	1.45	1.36
7	A2	1516	2MG	C4-N3	5.38	1.50	1.37
7	A1	1516	2MG	C2-N1	5.38	1.45	1.36
7	A2	1516	2MG	C2-N1	5.36	1.45	1.36
30	W1	46	G7M	C4-N3	5.34	1.50	1.37
31	X2	47	G7M	C4-N3	5.33	1.50	1.37
31	X2	38	2MA	C4-N3	5.30	1.50	1.37
5	72	2445	2MG	C2-N1	5.29	1.45	1.36
29	W	46	G7M	C4-N3	5.28	1.50	1.37
5	72	1835	2MG	C2-N1	5.24	1.45	1.36
5	72	2498	OMC	C4-N4	5.21	1.46	1.33
33	Y2	46	G7M	C4-N3	5.21	1.50	1.37
5	72	2251	OMG	C2-N3	5.18	1.45	1.33
7	A1	1498	UR3	C2-N3	5.13	1.48	1.39
5	72	2503	2MA	C4-N3	5.12	1.49	1.37
7	A2	1402	4OC	C4-N4	5.12	1.46	1.35
5	72	2069	G7M	C4-N3	5.11	1.49	1.37
7	A2	527	G7M	C4-N3	5.11	1.49	1.37
5	72	745	1MG	C4-N3	5.09	1.49	1.37
7	A1	527	G7M	C4-N3	5.09	1.49	1.37
7	A1	1402	4OC	C4-N4	5.09	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A2	1498	UR3	C2-N3	5.03	1.48	1.39
29	W	20	H2U	C4-N3	4.97	1.46	1.37
29	W	17	H2U	C4-N3	4.97	1.46	1.37
31	X2	21	H2U	C4-N3	4.92	1.46	1.37
31	X2	17	H2U	C4-N3	4.92	1.46	1.37
5	72	2449	H2U	C4-N3	4.90	1.45	1.37
33	Y2	17	H2U	C4-N3	4.90	1.45	1.37
29	W	16	H2U	C4-N3	4.86	1.45	1.37
32	Y1	46	7MG	C2-N2	4.74	1.45	1.34
5	72	2552	OMU	C4-N3	4.64	1.46	1.38
7	A2	967	5MC	C2-N1	4.56	1.49	1.40
7	A1	1407	5MC	C2-N1	4.56	1.49	1.40
5	72	1962	5MC	C2-N1	4.55	1.49	1.40
5	72	2251	OMG	C4-N3	4.53	1.48	1.37
32	Y1	34	CM0	C6-N1	4.53	1.45	1.38
7	A1	967	5MC	C2-N1	4.52	1.49	1.40
5	72	2552	OMU	O4-C4	-4.49	1.15	1.24
7	A2	1407	5MC	C2-N1	4.48	1.49	1.40
33	Y2	46	G7M	C6-N1	4.46	1.44	1.37
5	72	2498	OMC	C2-N1	4.45	1.49	1.40
5	72	2504	PSU	C4-N3	4.40	1.47	1.38
5	72	2580	PSU	C4-N3	4.39	1.47	1.38
30	W1	32	PSU	C4-N3	4.38	1.47	1.38
7	A1	527	G7M	C6-N1	4.37	1.44	1.37
5	72	955	PSU	C4-N3	4.35	1.46	1.38
5	72	2605	PSU	C4-N3	4.34	1.46	1.38
5	72	2457	PSU	C4-N3	4.33	1.46	1.38
30	W1	46	G7M	C6-N1	4.33	1.44	1.37
30	W1	39	PSU	C4-N3	4.32	1.46	1.38
29	W	32	PSU	C4-N3	4.32	1.46	1.38
5	72	2069	G7M	C6-N1	4.31	1.44	1.37
29	W	46	G7M	C6-N1	4.30	1.44	1.37
7	A2	527	G7M	C6-N1	4.29	1.44	1.37
31	X2	47	G7M	C6-N1	4.29	1.44	1.37
5	72	2604	PSU	C4-N3	4.28	1.46	1.38
7	A2	1402	4OC	C2-N1	4.26	1.49	1.40
5	71	1915	3TD	C2-N3	4.21	1.47	1.38
7	A1	1402	4OC	C2-N1	4.20	1.49	1.40
5	72	1915	3TD	C2-N3	4.18	1.47	1.38
7	A1	966	2MG	C6-N1	4.14	1.44	1.37
5	72	2498	OMC	O2-C2	-4.13	1.16	1.23
7	A2	1516	2MG	C6-N1	4.08	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A2	966	2MG	C6-N1	4.07	1.43	1.37
7	A1	1516	2MG	C6-N1	4.03	1.43	1.37
5	72	2445	2MG	C6-N1	4.03	1.43	1.37
7	A2	1207	2MG	C6-N1	4.01	1.43	1.37
5	72	1835	2MG	C6-N1	3.99	1.43	1.37
7	A1	1402	4OC	C5-C4	3.97	1.49	1.40
7	A1	1207	2MG	C6-N1	3.96	1.43	1.37
7	A2	966	2MG	C5-C6	3.87	1.55	1.47
7	A2	1402	4OC	C5-C4	3.86	1.49	1.40
32	Y1	46	7MG	C2-N1	3.84	1.47	1.37
7	A1	966	2MG	C5-C6	3.81	1.55	1.47
5	72	2445	2MG	C5-C6	3.80	1.55	1.47
5	72	2498	OMC	C6-N1	3.79	1.47	1.38
5	72	1835	2MG	C5-C6	3.79	1.55	1.47
7	A2	1207	2MG	C5-C6	3.78	1.55	1.47
7	A1	1207	2MG	C5-C6	3.78	1.55	1.47
7	A1	1516	2MG	C5-C6	3.76	1.55	1.47
7	A2	1516	2MG	C5-C6	3.75	1.55	1.47
32	Y1	34	CM0	C4-N3	3.71	1.45	1.38
5	72	2552	OMU	C6-N1	3.70	1.46	1.38
5	72	2552	OMU	O2-C2	-3.57	1.16	1.23
31	X2	48	3AU	C4-N3	3.57	1.46	1.40
31	X2	33	RSP	C5-C4	3.56	1.51	1.42
30	W1	46	G7M	C5-C6	3.53	1.54	1.45
32	Y1	46	7MG	C5-C6	3.52	1.52	1.43
31	X2	47	G7M	C5-C6	3.50	1.54	1.45
29	W	8	4SU	C5-C4	3.49	1.47	1.42
30	W1	8	4SU	C6-N1	3.48	1.46	1.38
30	W1	8	4SU	C5-C4	3.48	1.47	1.42
29	W	46	G7M	C5-C6	3.47	1.54	1.45
31	X2	8	4SU	C5-C4	3.47	1.47	1.42
7	A1	527	G7M	C5-C6	3.47	1.54	1.45
33	Y2	46	G7M	C5-C6	3.45	1.54	1.45
32	Y1	46	7MG	C6-N1	3.44	1.45	1.38
33	Y2	55	PSU	C6-C5	3.43	1.39	1.35
31	X2	8	4SU	C6-N1	3.38	1.46	1.38
5	72	2069	G7M	C5-C6	3.38	1.54	1.45
29	W	8	4SU	C6-N1	3.38	1.46	1.38
7	A2	527	G7M	C5-C6	3.37	1.54	1.45
31	X2	56	PSU	C6-C5	3.34	1.39	1.35
5	72	2251	OMG	C2-N1	3.30	1.45	1.37
7	A1	1402	4OC	C6-N1	3.28	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X2	48	3AU	C6-N1	3.27	1.45	1.38
29	W	55	PSU	C6-C5	3.25	1.39	1.35
5	72	955	PSU	O4-C4	-3.24	1.17	1.23
30	W1	32	PSU	O4-C4	-3.22	1.17	1.23
30	W1	39	PSU	O4-C4	-3.21	1.17	1.23
5	72	2604	PSU	O4-C4	-3.21	1.17	1.23
7	A2	1402	4OC	C6-N1	3.21	1.45	1.38
29	W	32	PSU	O4-C4	-3.18	1.17	1.23
5	72	2605	PSU	O4-C4	-3.18	1.17	1.23
5	72	2457	PSU	O4-C4	-3.17	1.17	1.23
31	X2	33	RSP	C2-S2	-3.17	1.59	1.67
5	72	2580	PSU	O4-C4	-3.15	1.17	1.23
5	72	2504	PSU	O4-C4	-3.13	1.17	1.23
5	72	2503	2MA	C6-N1	3.12	1.44	1.38
31	X2	38	2MA	C6-N1	3.10	1.44	1.38
31	X2	33	RSP	C6-N1	3.10	1.45	1.38
33	Y2	46	G7M	C2-N1	3.09	1.45	1.37
5	72	746	PSU	C6-C5	3.06	1.38	1.35
7	A1	1498	UR3	C6-N1	3.03	1.45	1.38
31	X2	48	3AU	C11-C10	3.03	1.59	1.52
5	72	2069	G7M	C2-N1	3.02	1.45	1.37
5	72	2251	OMG	C6-N1	3.02	1.42	1.37
7	A1	527	G7M	C2-N1	3.00	1.45	1.37
7	A2	527	G7M	C2-N1	3.00	1.45	1.37
7	A2	1498	UR3	C6-N1	2.99	1.45	1.38
30	W1	46	G7M	C2-N1	2.97	1.45	1.37
29	W	46	G7M	C2-N1	2.97	1.45	1.37
31	X2	47	G7M	C2-N1	2.95	1.45	1.37
5	72	2251	OMG	C5-C6	2.85	1.53	1.47
5	72	2498	OMC	C5-C4	2.81	1.49	1.42
7	A1	1402	4OC	O2-C2	-2.81	1.18	1.23
5	72	2580	PSU	C1'-C5	2.79	1.56	1.50
5	72	2604	PSU	C1'-C5	2.78	1.56	1.50
5	72	2605	PSU	C1'-C5	2.76	1.56	1.50
31	X2	38	2MA	C2-N1	2.75	1.45	1.36
30	W1	32	PSU	C1'-C5	2.74	1.56	1.50
5	72	2457	PSU	C1'-C5	2.73	1.56	1.50
5	72	2503	2MA	C2-N1	2.73	1.45	1.36
7	A2	1402	4OC	O2-C2	-2.72	1.18	1.23
31	X2	48	3AU	C5-C4	2.72	1.50	1.43
5	72	955	PSU	C1'-C5	2.72	1.56	1.50
7	A1	1519	MA6	C2-N3	2.71	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2504	PSU	C1'-C5	2.70	1.56	1.50
30	W1	39	PSU	C1'-C5	2.67	1.56	1.50
5	72	2604	PSU	O2-C2	-2.65	1.17	1.23
5	72	955	PSU	O2-C2	-2.65	1.17	1.23
29	W	32	PSU	C1'-C5	2.64	1.56	1.50
7	A1	1518	MA6	C2-N3	2.63	1.36	1.32
7	A2	1519	MA6	C2-N3	2.61	1.36	1.32
30	W1	39	PSU	O2-C2	-2.61	1.17	1.23
29	W	32	PSU	O2-C2	-2.61	1.17	1.23
5	71	1915	3TD	C1'-C5	2.61	1.56	1.50
32	Y1	34	CM0	O5-C7	-2.60	1.38	1.44
5	72	2580	PSU	O2-C2	-2.60	1.17	1.23
5	72	2457	PSU	O2-C2	-2.59	1.18	1.23
5	72	2605	PSU	O2-C2	-2.59	1.18	1.23
5	72	2504	PSU	O2-C2	-2.58	1.18	1.23
7	A2	1518	MA6	C2-N3	2.57	1.36	1.32
30	W1	32	PSU	O2-C2	-2.57	1.18	1.23
7	A2	966	2MG	C5-C4	-2.56	1.36	1.43
7	A2	1516	2MG	C5-C4	-2.55	1.36	1.43
7	A1	966	2MG	C5-C4	-2.53	1.36	1.43
7	A1	1516	2MG	C5-C4	-2.53	1.36	1.43
29	W	37	MIA	C5-C4	-2.53	1.34	1.40
7	A1	1207	2MG	C5-C4	-2.52	1.36	1.43
5	71	1915	3TD	C4-N3	2.52	1.45	1.40
5	72	1915	3TD	C4-N3	2.50	1.45	1.40
7	A2	1207	2MG	C5-C4	-2.49	1.36	1.43
5	72	1835	2MG	C5-C4	-2.46	1.36	1.43
32	Y1	46	7MG	O6-C6	-2.46	1.18	1.23
5	72	746	PSU	C4-C5	-2.43	1.37	1.44
5	72	2445	2MG	C5-C4	-2.43	1.36	1.43
5	72	1915	3TD	C1'-C5	2.43	1.55	1.50
5	72	745	1MG	C5-C4	-2.42	1.36	1.43
5	72	2251	OMG	C5-C4	-2.41	1.36	1.43
30	W1	37	MIA	C5-C4	-2.40	1.34	1.40
7	A2	1519	MA6	C5-C4	-2.39	1.34	1.40
5	72	745	1MG	C6-N1	2.36	1.43	1.39
7	A2	1407	5MC	O2-C2	-2.35	1.19	1.23
7	A1	1518	MA6	C5-C4	-2.34	1.34	1.40
7	A2	1518	MA6	C5-C4	-2.34	1.34	1.40
5	72	2552	OMU	C5-C4	2.33	1.48	1.43
29	W	16	H2U	O2-C2	-2.29	1.18	1.23
5	71	1915	3TD	O4-C4	-2.29	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A1	1519	MA6	C5-C4	-2.29	1.34	1.40
5	72	1915	3TD	O4-C4	-2.28	1.18	1.23
31	X2	17	H2U	O2-C2	-2.27	1.18	1.23
7	A2	967	5MC	O2-C2	-2.26	1.19	1.23
7	A1	967	5MC	O2-C2	-2.25	1.19	1.23
5	72	745	1MG	C5-C6	2.25	1.54	1.47
29	W	17	H2U	O2-C2	-2.25	1.18	1.23
32	Y1	37	6MZ	C5-C4	-2.25	1.35	1.40
5	72	2449	H2U	O2-C2	-2.25	1.18	1.23
5	72	1962	5MC	O2-C2	-2.24	1.19	1.23
33	Y2	17	H2U	O2-C2	-2.24	1.19	1.23
29	W	20	H2U	O2-C2	-2.23	1.19	1.23
5	72	2030	6MZ	C5-C4	-2.22	1.35	1.40
7	A1	1498	UR3	C5-C4	2.22	1.49	1.43
30	W1	46	G7M	O6-C6	-2.22	1.18	1.23
7	A1	1407	5MC	O2-C2	-2.21	1.19	1.23
5	72	1618	6MZ	C5-C4	-2.20	1.35	1.40
31	X2	21	H2U	O2-C2	-2.20	1.19	1.23
7	A2	527	G7M	O6-C6	-2.19	1.18	1.23
5	72	2503	2MA	C5-C4	-2.19	1.37	1.43
31	X2	47	G7M	O6-C6	-2.19	1.18	1.23
7	A2	1498	UR3	O4-C4	-2.19	1.18	1.23
7	A2	1498	UR3	C5-C4	2.18	1.49	1.43
31	X2	21	H2U	O4-C4	-2.17	1.18	1.23
7	A2	1498	UR3	O2-C2	-2.16	1.18	1.22
7	A1	527	G7M	O6-C6	-2.16	1.18	1.23
7	A1	1498	UR3	O4-C4	-2.15	1.18	1.23
5	72	2449	H2U	O4-C4	-2.14	1.18	1.23
29	W	46	G7M	O6-C6	-2.13	1.19	1.23
7	A1	1498	UR3	C4-N3	2.13	1.45	1.40
33	Y2	17	H2U	O4-C4	-2.13	1.18	1.23
7	A1	1498	UR3	O2-C2	-2.12	1.18	1.22
5	72	2069	G7M	O6-C6	-2.12	1.19	1.23
29	W	17	H2U	O4-C4	-2.12	1.19	1.23
29	W	20	H2U	O4-C4	-2.12	1.19	1.23
29	W	16	H2U	O4-C4	-2.12	1.19	1.23
31	X2	17	H2U	O4-C4	-2.11	1.19	1.23
31	X2	38	2MA	C5-C4	-2.10	1.37	1.43
7	A2	1498	UR3	C4-N3	2.09	1.45	1.40
33	Y2	46	G7M	O6-C6	-2.09	1.19	1.23
7	A2	1207	2MG	O6-C6	-2.09	1.19	1.23
7	A1	527	G7M	C8-N7	2.08	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A1	1207	2MG	O6-C6	-2.08	1.19	1.23
32	Y1	37	6MZ	C2-N3	2.07	1.35	1.32
5	72	1835	2MG	O6-C6	-2.07	1.19	1.23
33	Y2	46	G7M	C8-N7	2.06	1.36	1.33
7	A1	1516	2MG	O6-C6	-2.05	1.19	1.23
7	A2	1516	2MG	O6-C6	-2.05	1.19	1.23
5	72	2445	2MG	O6-C6	-2.04	1.19	1.23
7	A2	966	2MG	O6-C6	-2.04	1.19	1.23
7	A1	966	2MG	O6-C6	-2.04	1.19	1.23
5	72	2030	6MZ	C2-N3	2.04	1.35	1.32

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	1519	MA6	N1-C6-N6	-12.56	103.84	117.06
7	A1	1519	MA6	N1-C6-N6	-12.55	103.85	117.06
7	A2	1518	MA6	N1-C6-N6	-12.40	104.00	117.06
7	A1	1518	MA6	N1-C6-N6	-12.15	104.26	117.06
30	W1	37	MIA	C11-S10-C2	10.55	110.15	102.27
29	W	37	MIA	C11-S10-C2	8.92	108.93	102.27
29	W	8	4SU	C4-N3-C2	-7.97	119.60	127.34
31	X2	8	4SU	C4-N3-C2	-7.92	119.65	127.34
30	W1	8	4SU	C4-N3-C2	-7.71	119.85	127.34
31	X2	21	H2U	C4-N3-C2	-7.16	119.85	125.79
5	72	2449	H2U	C4-N3-C2	-7.14	119.87	125.79
29	W	20	H2U	C4-N3-C2	-7.02	119.97	125.79
33	Y2	17	H2U	C4-N3-C2	-7.00	119.98	125.79
29	W	17	H2U	C4-N3-C2	-6.89	120.07	125.79
29	W	16	H2U	C4-N3-C2	-6.81	120.15	125.79
31	X2	17	H2U	C4-N3-C2	-6.76	120.18	125.79
7	A1	1519	MA6	C1'-N9-C4	6.09	137.34	126.64
7	A1	1518	MA6	C1'-N9-C4	5.79	136.82	126.64
31	X2	8	4SU	C5-C4-N3	5.64	119.92	114.69
7	A2	1519	MA6	N3-C2-N1	-5.62	119.89	128.68
32	Y1	37	6MZ	C1'-N9-C4	-5.61	116.79	126.64
7	A2	1518	MA6	C1'-N9-C4	5.60	136.48	126.64
29	W	8	4SU	C5-C4-N3	5.59	119.87	114.69
5	72	1618	6MZ	N3-C2-N1	-5.57	119.98	128.68
7	A2	1518	MA6	N3-C2-N1	-5.52	120.05	128.68
7	A1	1518	MA6	N3-C2-N1	-5.50	120.09	128.68
32	Y1	37	6MZ	N3-C2-N1	-5.49	120.10	128.68
5	72	1915	3TD	N1-C2-N3	5.47	120.45	116.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A1	1519	MA6	N3-C2-N1	-5.46	120.14	128.68
30	W1	8	4SU	C5-C4-N3	5.45	119.74	114.69
5	72	2030	6MZ	N3-C2-N1	-5.44	120.17	128.68
5	72	2030	6MZ	C1'-N9-C4	-5.44	117.09	126.64
32	Y1	34	CM0	C4-N3-C2	-5.41	120.34	127.35
5	71	1915	3TD	N1-C2-N3	5.30	120.32	116.14
7	A2	1519	MA6	C1'-N9-C4	5.19	135.76	126.64
5	72	2552	OMU	C4-N3-C2	-5.06	119.91	126.58
32	Y1	46	7MG	C5-C6-N1	5.01	119.82	110.99
5	72	955	PSU	C4-N3-C2	-4.74	119.51	126.34
5	72	2504	PSU	C4-N3-C2	-4.71	119.55	126.34
29	W	37	MIA	C1'-N9-C4	-4.71	118.37	126.64
7	A2	1498	UR3	C4-N3-C2	-4.67	120.17	124.56
5	72	2604	PSU	C4-N3-C2	-4.67	119.61	126.34
5	72	2580	PSU	C4-N3-C2	-4.64	119.65	126.34
5	72	2605	PSU	C4-N3-C2	-4.63	119.67	126.34
7	A1	1498	UR3	C4-N3-C2	-4.63	120.21	124.56
5	72	2457	PSU	C4-N3-C2	-4.61	119.69	126.34
30	W1	39	PSU	C4-N3-C2	-4.54	119.80	126.34
29	W	32	PSU	C4-N3-C2	-4.53	119.81	126.34
30	W1	32	PSU	C4-N3-C2	-4.51	119.83	126.34
32	Y1	46	7MG	C2-N3-C4	4.50	120.31	112.30
5	72	2504	PSU	N1-C2-N3	4.34	120.05	115.13
5	72	2030	6MZ	C2-N1-C6	4.27	120.25	116.59
5	72	2457	PSU	N1-C2-N3	4.20	119.89	115.13
5	72	955	PSU	N1-C2-N3	4.19	119.88	115.13
5	72	2605	PSU	N1-C2-N3	4.19	119.88	115.13
32	Y1	46	7MG	C5-C4-N3	-4.17	120.18	128.13
5	72	1915	3TD	C4-N3-C2	-4.16	120.10	124.61
30	W1	39	PSU	N1-C2-N3	4.15	119.83	115.13
29	W	32	PSU	N1-C2-N3	4.14	119.82	115.13
32	Y1	37	6MZ	C2-N1-C6	4.14	120.14	116.59
5	72	2604	PSU	N1-C2-N3	4.11	119.79	115.13
5	72	2580	PSU	N1-C2-N3	4.11	119.78	115.13
30	W1	32	PSU	N1-C2-N3	4.09	119.76	115.13
5	72	745	1MG	C5-C6-N1	4.08	120.03	113.90
5	71	1915	3TD	C4-N3-C2	-4.04	120.22	124.61
29	W	8	4SU	N3-C2-N1	3.85	120.00	114.89
5	72	1618	6MZ	C1'-N9-C4	-3.82	119.93	126.64
31	X2	8	4SU	N3-C2-N1	3.82	119.96	114.89
30	W1	8	4SU	N3-C2-N1	3.78	119.90	114.89
5	72	1618	6MZ	C9-N6-C6	-3.77	119.62	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2552	OMU	N3-C2-N1	3.76	119.89	114.89
31	X2	48	3AU	C4-N3-C2	-3.74	119.94	124.63
29	W	37	MIA	N3-C2-N1	-3.70	120.17	126.98
30	W1	37	MIA	C12-C13-C14	-3.69	119.96	127.14
5	72	1618	6MZ	C2-N1-C6	3.68	119.74	116.59
5	72	2445	2MG	C5-C6-N1	3.61	120.33	113.95
5	72	1835	2MG	C5-C6-N1	3.60	120.31	113.95
32	Y1	34	CM0	N3-C2-N1	3.59	119.65	114.89
30	W1	37	MIA	N3-C2-N1	-3.59	120.38	126.98
7	A1	966	2MG	C5-C6-N1	3.55	120.21	113.95
7	A1	1516	2MG	C5-C6-N1	3.52	120.17	113.95
5	72	2251	OMG	C5-C6-N1	3.50	120.14	113.95
30	W1	8	4SU	C5-C4-S4	-3.50	119.96	124.47
29	W	37	MIA	C12-C13-C14	-3.49	120.34	127.14
7	A2	966	2MG	C5-C6-N1	3.48	120.10	113.95
7	A2	1207	2MG	C5-C6-N1	3.48	120.10	113.95
29	W	8	4SU	C5-C4-S4	-3.47	120.00	124.47
5	72	1962	5MC	C5-C6-N1	-3.47	119.77	123.34
31	X2	8	4SU	C5-C4-S4	-3.45	120.02	124.47
30	W1	37	MIA	C2-N3-C4	3.44	120.07	115.32
7	A1	967	5MC	C5-C6-N1	-3.43	119.81	123.34
5	72	2503	2MA	C5-C6-N1	3.40	119.89	114.02
7	A2	1516	2MG	C5-C6-N1	3.40	119.95	113.95
5	72	2504	PSU	C6-C5-C4	3.38	120.56	118.20
7	A1	1207	2MG	C5-C6-N1	3.38	119.92	113.95
29	W	32	PSU	C6-C5-C4	3.37	120.55	118.20
31	X2	38	2MA	C5-C6-N1	3.35	119.80	114.02
5	72	1939	5MU	O3'-C3'-C2'	-3.34	101.02	111.82
31	X2	48	3AU	C5-C4-N3	3.33	119.89	115.50
29	W	37	MIA	C2-N3-C4	3.33	119.91	115.32
5	72	2457	PSU	C6-C5-C4	3.28	120.49	118.20
5	72	2552	OMU	C5-C4-N3	3.27	119.74	114.84
30	W1	39	PSU	C6-C5-C4	3.25	120.47	118.20
32	Y1	46	7MG	C4-C5-N7	3.21	109.99	105.53
5	72	2449	H2U	N3-C2-N1	3.21	120.05	116.65
31	X2	21	H2U	N3-C2-N1	3.19	120.02	116.65
29	W	17	H2U	N3-C2-N1	3.17	120.01	116.65
29	W	20	H2U	N3-C2-N1	3.16	120.00	116.65
7	A2	967	5MC	C5-C6-N1	-3.15	120.09	123.34
31	X2	17	H2U	N3-C2-N1	3.14	119.97	116.65
33	Y2	17	H2U	N3-C2-N1	3.14	119.97	116.65
30	W1	46	G7M	C2-N1-C6	-3.12	119.35	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2580	PSU	C6-C5-C4	3.12	120.38	118.20
29	W	46	G7M	C2-N1-C6	-3.11	119.37	125.10
5	72	955	PSU	C6-C5-C4	3.07	120.34	118.20
30	W1	37	MIA	C1'-N9-C4	-3.03	121.31	126.64
31	X2	47	G7M	C2-N1-C6	-3.01	119.56	125.10
5	72	2251	OMG	C2-N1-C6	-3.00	119.56	125.10
30	W1	32	PSU	C6-C5-C4	3.00	120.30	118.20
7	A2	527	G7M	C2-N1-C6	-2.99	119.60	125.10
7	A1	527	G7M	C2-N1-C6	-2.99	119.60	125.10
29	W	16	H2U	C5-C4-N3	2.98	119.99	116.65
29	W	16	H2U	N3-C2-N1	2.98	119.80	116.65
5	72	2504	PSU	C6-N1-C2	-2.97	119.65	122.68
5	72	2604	PSU	C6-C5-C4	2.97	120.27	118.20
32	Y1	46	7MG	C5-C4-N9	2.96	110.19	106.35
5	72	2605	PSU	C6-N1-C2	-2.96	119.66	122.68
5	72	2069	G7M	C2-N1-C6	-2.92	119.72	125.10
33	Y2	46	G7M	C2-N1-C6	-2.91	119.73	125.10
30	W1	32	PSU	C6-N1-C2	-2.91	119.71	122.68
5	72	1939	5MU	O2'-C2'-C1'	-2.90	100.34	110.02
5	72	2552	OMU	O4-C4-C5	-2.89	120.08	125.16
7	A1	1407	5MC	C5-C6-N1	-2.89	120.37	123.34
29	W	32	PSU	C6-N1-C2	-2.89	119.73	122.68
5	72	2449	H2U	C5-C4-N3	2.88	119.89	116.65
32	Y1	46	7MG	C2-N1-C6	-2.88	119.86	125.10
30	W1	39	PSU	C6-N1-C2	-2.87	119.74	122.68
5	72	2251	OMG	C8-N7-C5	2.87	108.46	102.99
29	W	37	MIA	S10-C2-N3	2.86	126.03	116.10
31	X2	21	H2U	C5-C4-N3	2.85	119.85	116.65
5	72	2457	PSU	C6-N1-C2	-2.85	119.77	122.68
32	Y1	46	7MG	O6-C6-C5	-2.85	120.55	127.54
5	72	2605	PSU	C6-C5-C4	2.84	120.18	118.20
29	W	17	H2U	C5-C4-N3	2.82	119.82	116.65
33	Y2	17	H2U	C5-C4-N3	2.80	119.79	116.65
5	72	955	PSU	C6-N1-C2	-2.79	119.83	122.68
29	W	20	H2U	C5-C4-N3	2.79	119.78	116.65
32	Y1	46	7MG	N9-C4-N3	2.78	129.62	125.47
29	W	16	H2U	C5-C6-N1	2.77	120.73	111.61
29	W	17	H2U	C5-C6-N1	2.75	120.69	111.61
31	X2	17	H2U	C5-C4-N3	2.73	119.71	116.65
30	W1	37	MIA	S10-C2-N3	2.72	125.54	116.10
31	X2	17	H2U	C5-C6-N1	2.72	120.58	111.61
7	A2	1407	5MC	C5-C6-N1	-2.71	120.55	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2580	PSU	C6-N1-C2	-2.70	119.92	122.68
5	72	745	1MG	C8-N7-C5	2.70	108.14	102.99
7	A2	966	2MG	C8-N7-C5	2.68	108.10	102.99
5	72	2604	PSU	C6-N1-C2	-2.67	119.96	122.68
5	72	2503	2MA	C8-N7-C5	2.66	108.06	102.99
7	A1	966	2MG	C8-N7-C5	2.66	108.05	102.99
7	A1	1516	2MG	C8-N7-C5	2.63	108.00	102.99
29	W	20	H2U	C5-C6-N1	2.62	120.26	111.61
33	Y2	17	H2U	C5-C6-N1	2.62	120.24	111.61
7	A1	1207	2MG	C8-N7-C5	2.61	107.97	102.99
7	A2	1516	2MG	C8-N7-C5	2.61	107.97	102.99
31	X2	38	2MA	C8-N7-C5	2.61	107.95	102.99
5	72	2449	H2U	C5-C6-N1	2.61	120.20	111.61
31	X2	21	H2U	C5-C6-N1	2.58	120.11	111.61
5	72	2445	2MG	C8-N7-C5	2.57	107.89	102.99
7	A2	1207	2MG	C8-N7-C5	2.57	107.89	102.99
5	72	2605	PSU	O2-C2-N1	-2.55	119.98	122.79
7	A1	1402	4OC	C6-C5-C4	2.55	120.08	116.96
5	72	1835	2MG	C8-N7-C5	2.54	107.83	102.99
29	W	32	PSU	O2-C2-N1	-2.54	119.99	122.79
5	72	955	PSU	O2-C2-N1	-2.51	120.03	122.79
5	72	2457	PSU	O2-C2-N1	-2.51	120.03	122.79
5	72	2504	PSU	O2-C2-N1	-2.50	120.03	122.79
29	W	17	H2U	O2-C2-N1	-2.48	120.00	123.11
5	72	745	1MG	O6-C6-C5	-2.45	119.85	124.19
29	W	20	H2U	O2-C2-N1	-2.45	120.03	123.11
32	Y1	46	7MG	N9-C8-N7	2.41	106.83	103.38
5	72	2580	PSU	O2-C2-N1	-2.41	120.14	122.79
33	Y2	17	H2U	O2-C2-N1	-2.41	120.09	123.11
30	W1	39	PSU	O2-C2-N1	-2.40	120.14	122.79
30	W1	32	PSU	O2-C2-N1	-2.39	120.16	122.79
5	72	2604	PSU	O2-C2-N1	-2.39	120.16	122.79
29	W	16	H2U	O2-C2-N1	-2.39	120.11	123.11
29	W	37	MIA	C16-C14-C15	2.37	119.83	114.60
30	W1	37	MIA	C16-C14-C15	2.36	119.83	114.60
29	W	55	PSU	C2'-C3'-C4'	-2.36	98.05	102.64
5	72	1835	2MG	O6-C6-C5	-2.36	119.76	124.37
7	A2	1402	4OC	C6-C5-C4	2.35	119.83	116.96
7	A1	1516	2MG	O6-C6-C5	-2.34	119.80	124.37
5	72	2445	2MG	O6-C6-C5	-2.33	119.81	124.37
5	72	1915	3TD	C6-C5-C4	2.32	119.82	118.22
32	Y1	37	6MZ	C9-N6-C6	-2.32	120.88	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	1516	2MG	O6-C6-C5	-2.31	119.87	124.37
7	A1	966	2MG	O6-C6-C5	-2.30	119.89	124.37
31	X2	21	H2U	O2-C2-N1	-2.29	120.23	123.11
5	72	2449	H2U	O2-C2-N1	-2.28	120.25	123.11
7	A2	966	2MG	O6-C6-C5	-2.26	119.95	124.37
7	A2	1207	2MG	O6-C6-C5	-2.25	119.98	124.37
7	A1	1207	2MG	O6-C6-C5	-2.23	120.01	124.37
5	72	2251	OMG	O6-C6-C5	-2.23	120.02	124.37
5	72	746	PSU	C5-C6-N1	-2.17	118.85	122.11
7	A1	1407	5MC	CM5-C5-C6	-2.15	119.97	122.85
7	A2	1407	5MC	CM5-C5-C6	-2.13	120.00	122.85
5	72	2580	PSU	O4'-C1'-C2'	2.12	108.14	105.14
5	72	2552	OMU	O2-C2-N1	-2.12	119.97	122.79
7	A1	1498	UR3	C6-N1-C2	-2.12	119.89	121.79
7	A1	967	5MC	CM5-C5-C6	-2.11	120.03	122.85
29	W	8	4SU	O2-C2-N1	-2.09	120.01	122.79
5	72	2445	2MG	CM2-N2-C2	-2.08	119.26	123.86
7	A1	1498	UR3	C1'-N1-C2	2.08	120.50	116.99
5	72	1962	5MC	CM5-C5-C6	-2.08	120.07	122.85
7	A2	1498	UR3	C6-N1-C2	-2.07	119.93	121.79
5	72	1835	2MG	CM2-N2-C2	-2.06	119.31	123.86
31	X2	48	3AU	C6-N1-C2	-2.04	119.96	121.79
7	A2	967	5MC	CM5-C5-C6	-2.02	120.15	122.85
31	X2	17	H2U	O2-C2-N1	-2.01	120.59	123.11

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A1	1402	4OC	C1'-C2'-O2'-CM2
7	A1	1518	MA6	C5-C6-N6-C9
7	A1	1518	MA6	C5-C6-N6-C10
7	A1	1519	MA6	C3'-C4'-C5'-O5'
7	A1	1519	MA6	C5-C6-N6-C10
7	A2	1402	4OC	C1'-C2'-O2'-CM2
5	72	1618	6MZ	N1-C6-N6-C9
5	72	1618	6MZ	O4'-C4'-C5'-O5'
5	72	1618	6MZ	C3'-C4'-C5'-O5'
5	72	1939	5MU	C3'-C4'-C5'-O5'
5	72	1939	5MU	O4'-C4'-C5'-O5'
5	72	2030	6MZ	C5-C6-N6-C9
5	72	2030	6MZ	N1-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
5	72	2251	OMG	O4'-C4'-C5'-O5'
5	72	2251	OMG	C1'-C2'-O2'-CM2
30	W1	37	MIA	O4'-C4'-C5'-O5'
30	W1	37	MIA	C3'-C4'-C5'-O5'
30	W1	37	MIA	N1-C2-S10-C11
30	W1	37	MIA	N3-C2-S10-C11
31	X2	8	4SU	C3'-C4'-C5'-O5'
31	X2	8	4SU	O4'-C4'-C5'-O5'
31	X2	17	H2U	O4'-C1'-N1-C6
31	X2	33	RSP	C4'-C5'-O5'-P
31	X2	47	G7M	O4'-C4'-C5'-O5'
31	X2	47	G7M	C3'-C4'-C5'-O5'
31	X2	48	3AU	C10-C11-C12-N40
31	X2	55	5MU	C3'-C4'-C5'-O5'
32	Y1	34	CM0	O5-C7-C8-O8
32	Y1	37	6MZ	N1-C6-N6-C9
33	Y2	17	H2U	O4'-C4'-C5'-O5'
33	Y2	17	H2U	C3'-C4'-C5'-O5'
33	Y2	17	H2U	O4'-C1'-N1-C6
33	Y2	17	H2U	C2'-C1'-N1-C2
33	Y2	17	H2U	C2'-C1'-N1-C6
32	Y1	34	CM0	O5-C7-C8-O9
31	X2	47	G7M	C4'-C5'-O5'-P
7	A1	1498	UR3	O4'-C4'-C5'-O5'
7	A1	1498	UR3	C3'-C4'-C5'-O5'
7	A1	1519	MA6	O4'-C4'-C5'-O5'
7	A2	1498	UR3	O4'-C4'-C5'-O5'
7	A2	1498	UR3	C3'-C4'-C5'-O5'
7	A2	1519	MA6	O4'-C4'-C5'-O5'
5	72	2251	OMG	C3'-C4'-C5'-O5'
5	72	2498	OMC	C3'-C4'-C5'-O5'
5	72	2498	OMC	O4'-C4'-C5'-O5'
29	W	8	4SU	C3'-C4'-C5'-O5'
29	W	8	4SU	O4'-C4'-C5'-O5'
30	W1	8	4SU	O4'-C4'-C5'-O5'
33	Y2	46	G7M	C3'-C4'-C5'-O5'
30	W1	8	4SU	C3'-C4'-C5'-O5'
31	X2	48	3AU	O4'-C4'-C5'-O5'
31	X2	55	5MU	O4'-C4'-C5'-O5'
7	A1	1518	MA6	N1-C6-N6-C10
7	A2	1519	MA6	C3'-C4'-C5'-O5'
5	72	1915	3TD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
29	W	54	5MU	C3'-C4'-C5'-O5'
33	Y2	54	5MU	C3'-C4'-C5'-O5'
7	A1	1519	MA6	C4'-C5'-O5'-P
29	W	55	PSU	O4'-C4'-C5'-O5'
31	X2	17	H2U	C3'-C4'-C5'-O5'
31	X2	48	3AU	C3'-C4'-C5'-O5'
7	A1	1519	MA6	C5-C6-N6-C9
31	X2	38	2MA	C4'-C5'-O5'-P
31	X2	17	H2U	C4'-C5'-O5'-P
31	X2	21	H2U	C4'-C5'-O5'-P
29	W	55	PSU	C3'-C4'-C5'-O5'
31	X2	17	H2U	O4'-C4'-C5'-O5'
33	Y2	46	G7M	O4'-C4'-C5'-O5'
33	Y2	54	5MU	O4'-C4'-C5'-O5'
5	72	1618	6MZ	C5-C6-N6-C9
32	Y1	37	6MZ	C5-C6-N6-C9
30	W1	46	G7M	O4'-C4'-C5'-O5'
7	A1	527	G7M	C4'-C5'-O5'-P
29	W	46	G7M	C4'-C5'-O5'-P
30	W1	46	G7M	C4'-C5'-O5'-P
31	X2	48	3AU	C4'-C5'-O5'-P
32	Y1	46	7MG	C4'-C5'-O5'-P
29	W	54	5MU	O4'-C4'-C5'-O5'
7	A2	527	G7M	C3'-C4'-C5'-O5'
30	W1	37	MIA	C5-C6-N6-C12
7	A2	527	G7M	C4'-C5'-O5'-P
33	Y2	17	H2U	C4'-C5'-O5'-P
5	72	2069	G7M	C4'-C5'-O5'-P
29	W	16	H2U	C4'-C5'-O5'-P
29	W	55	PSU	C4'-C5'-O5'-P
29	W	46	G7M	O4'-C4'-C5'-O5'
31	X2	38	2MA	C3'-C4'-C5'-O5'
30	W1	37	MIA	N1-C6-N6-C12
5	72	1915	3TD	C3'-C4'-C5'-O5'
33	Y2	17	H2U	O4'-C1'-N1-C2
29	W	37	MIA	N6-C12-C13-C14
5	72	2069	G7M	O4'-C4'-C5'-O5'
5	72	746	PSU	O4'-C1'-C5-C4
5	72	2457	PSU	O4'-C1'-C5-C4
5	72	2504	PSU	O4'-C1'-C5-C4
31	X2	56	PSU	O4'-C1'-C5-C4
7	A1	1519	MA6	N1-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
31	X2	48	3AU	C11-C12-C13-O31
7	A2	527	G7M	O4'-C4'-C5'-O5'
7	A2	967	5MC	O4'-C4'-C5'-O5'
29	W	17	H2U	O4'-C4'-C5'-O5'
30	W1	46	G7M	C3'-C4'-C5'-O5'
31	X2	38	2MA	O4'-C4'-C5'-O5'
31	X2	48	3AU	C11-C12-C13-O30
5	72	2449	H2U	O4'-C1'-N1-C6
5	72	2457	PSU	O4'-C1'-C5-C6
31	X2	21	H2U	O4'-C1'-N1-C6
31	X2	56	PSU	O4'-C1'-C5-C6
29	W	54	5MU	C2'-C1'-N1-C2
31	X2	17	H2U	O4'-C1'-N1-C2
29	W	20	H2U	C4'-C5'-O5'-P
31	X2	17	H2U	C2'-C1'-N1-C2
7	A1	1402	4OC	O4'-C4'-C5'-O5'
5	71	1915	3TD	C3'-C4'-C5'-O5'
5	72	2030	6MZ	O4'-C4'-C5'-O5'
29	W	46	G7M	C3'-C4'-C5'-O5'
31	X2	21	H2U	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 302 ligands modelled in this entry, 298 are monoatomic - leaving 4 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
47	PUT	72	3002	-	5,5,5	0.24	0	4,4,4	0.56	0
50	ALA	Y2	102	33	3,4,5	0.48	0	2,4,6	2.56	2 (100%)
48	SPD	72	3003	-	9,9,9	0.32	0	8,8,8	0.87	0
47	PUT	72	3001	-	5,5,5	0.26	0	4,4,4	0.52	0

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
47	PUT	72	3002	-	-	0/3/3/3	-
50	ALA	Y2	102	33	-	0/0/2/4	-
48	SPD	72	3003	-	-	0/7/7/7	-
47	PUT	72	3001	-	-	1/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	Y2	102	ALA	CB-CA-N	-3.01	100.32	109.85
50	Y2	102	ALA	O-C-CA	-2.02	117.88	124.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	72	3001	PUT	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

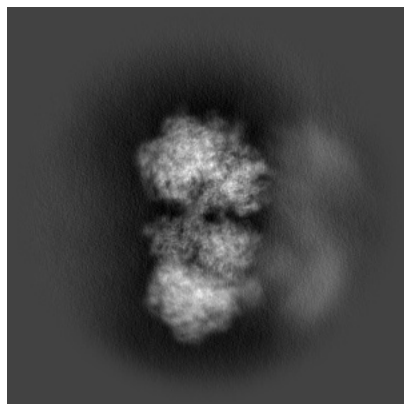
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19054. These allow visual inspection of the internal detail of the map and identification of artifacts.

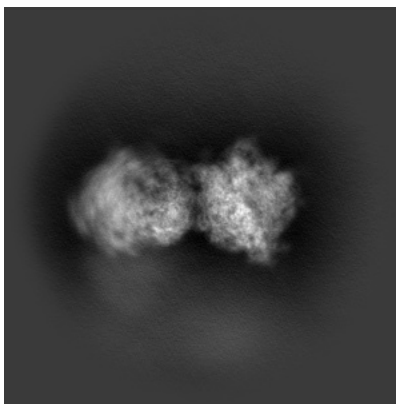
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

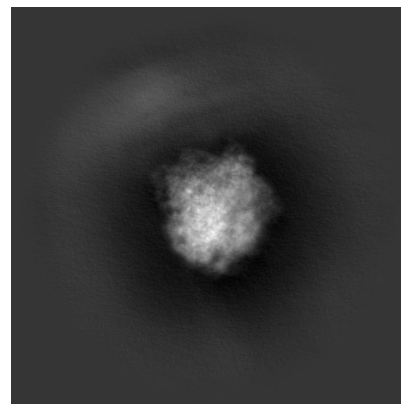
#### 6.1.1 Primary map



X

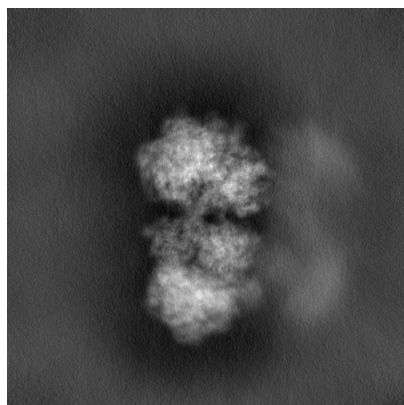


Y

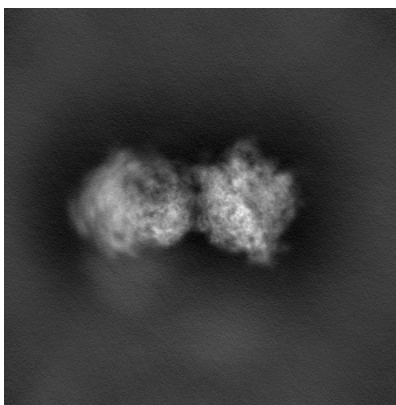


Z

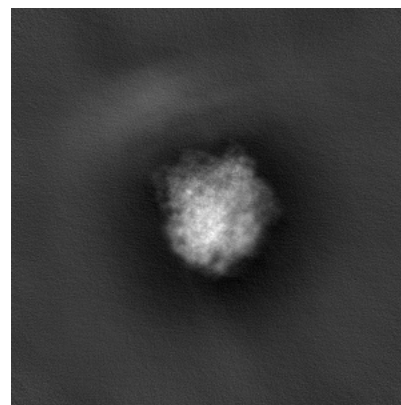
#### 6.1.2 Raw map



X



Y

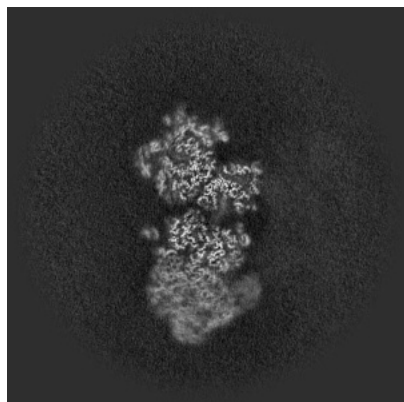


Z

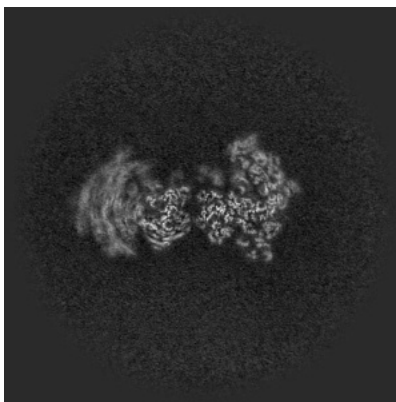
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

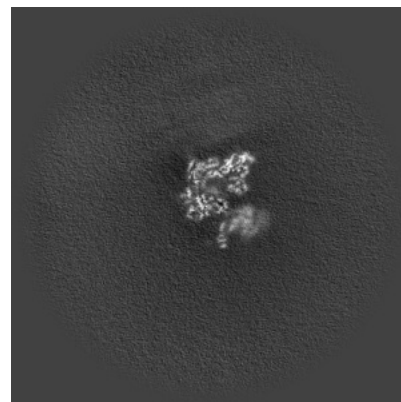
### 6.2.1 Primary map



X Index: 234

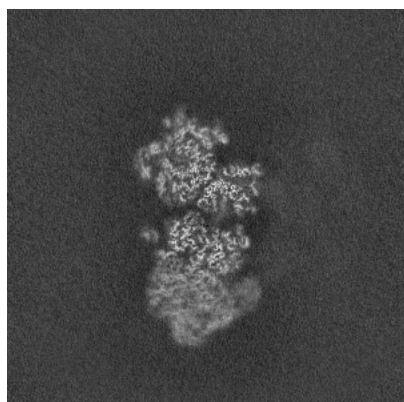


Y Index: 234

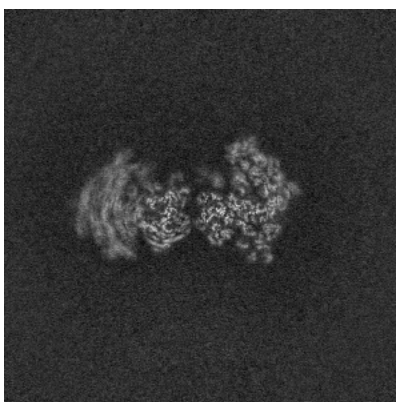


Z Index: 234

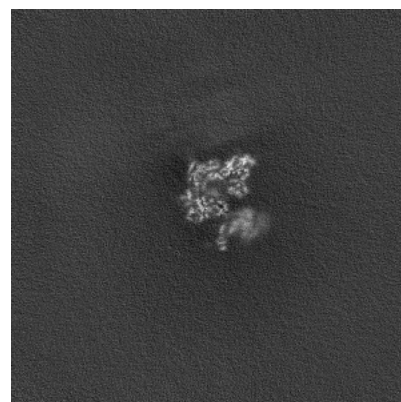
### 6.2.2 Raw map



X Index: 234



Y Index: 234

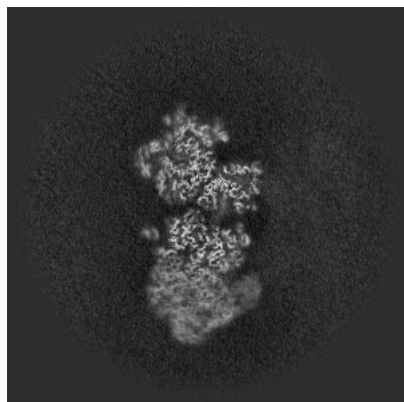


Z Index: 234

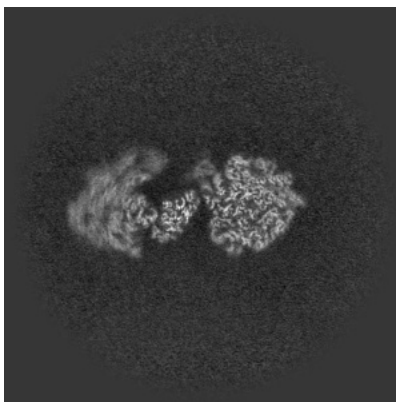
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

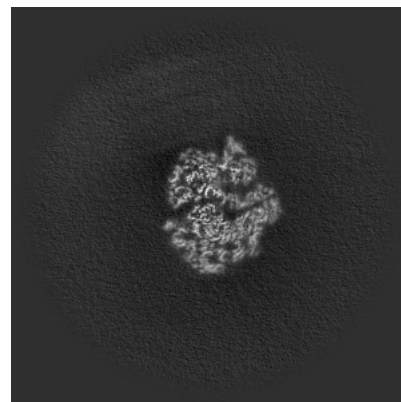
### 6.3.1 Primary map



X Index: 234

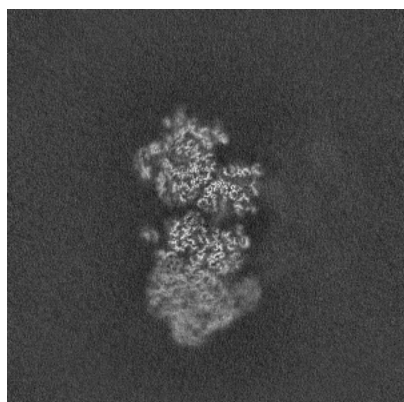


Y Index: 208

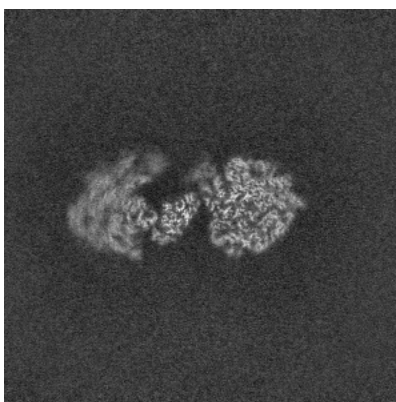


Z Index: 274

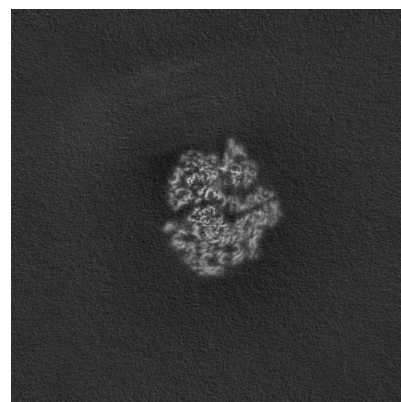
### 6.3.2 Raw map



X Index: 234



Y Index: 208

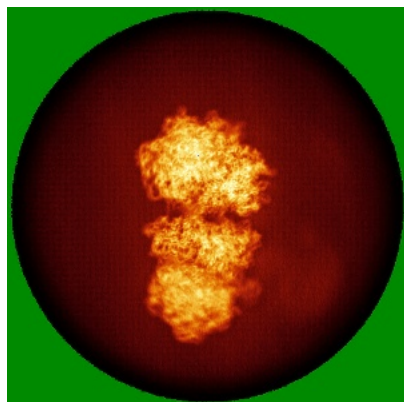


Z Index: 274

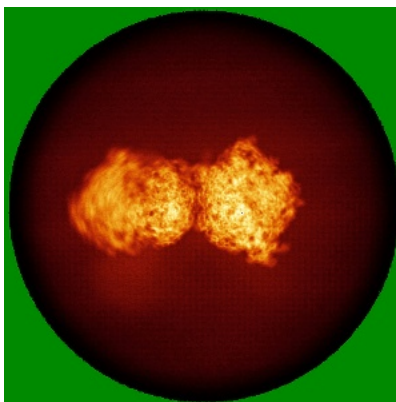
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

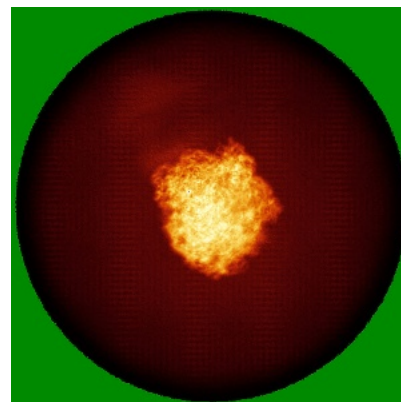
### 6.4.1 Primary map



X

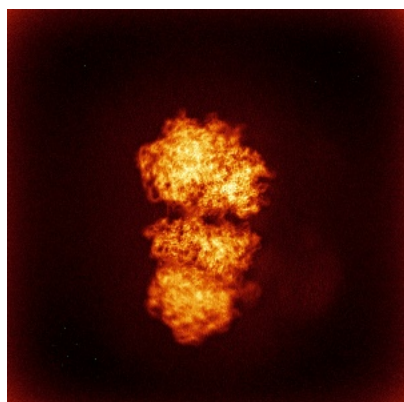


Y

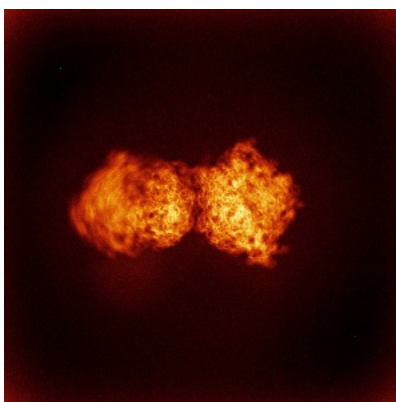


Z

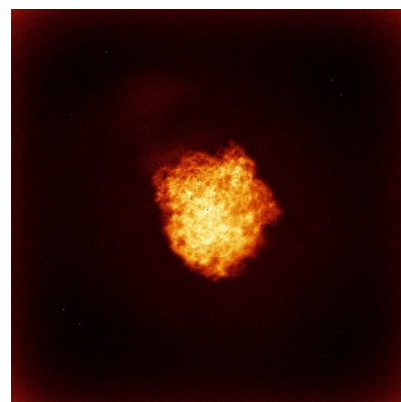
### 6.4.2 Raw map



X



Y

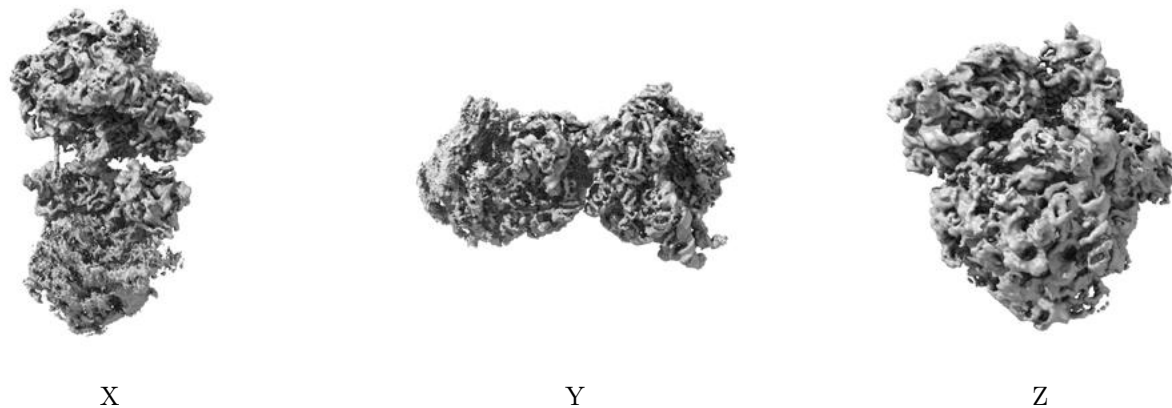


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

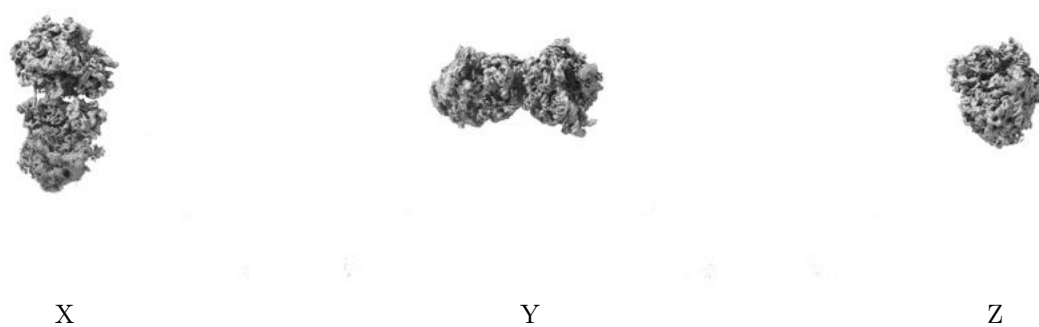
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 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.

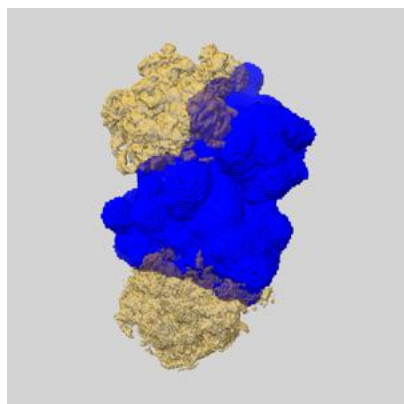
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

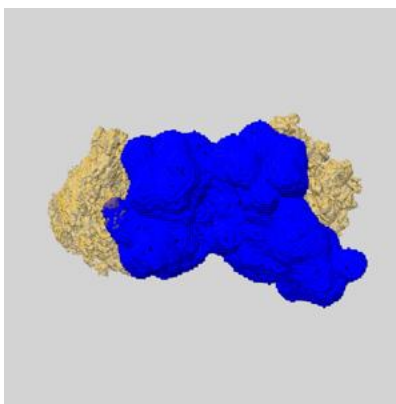
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

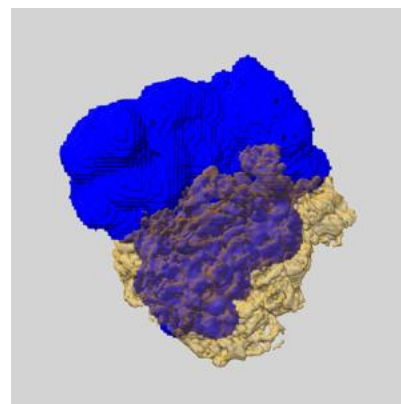
### 6.6.1 emd\_19054\_msk\_1.map [i](#)



X



Y



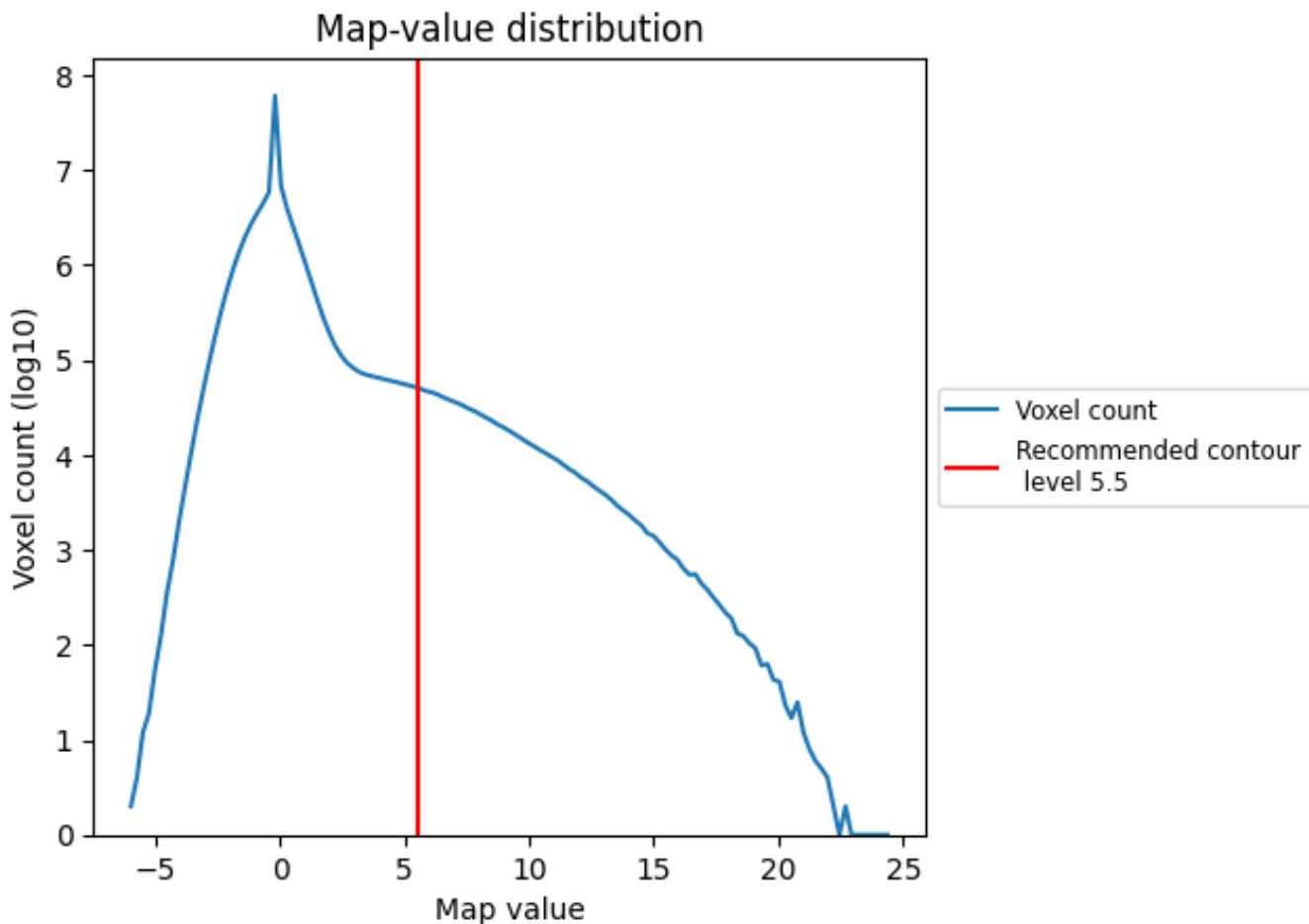
Z



## 7 Map analysis [i](#)

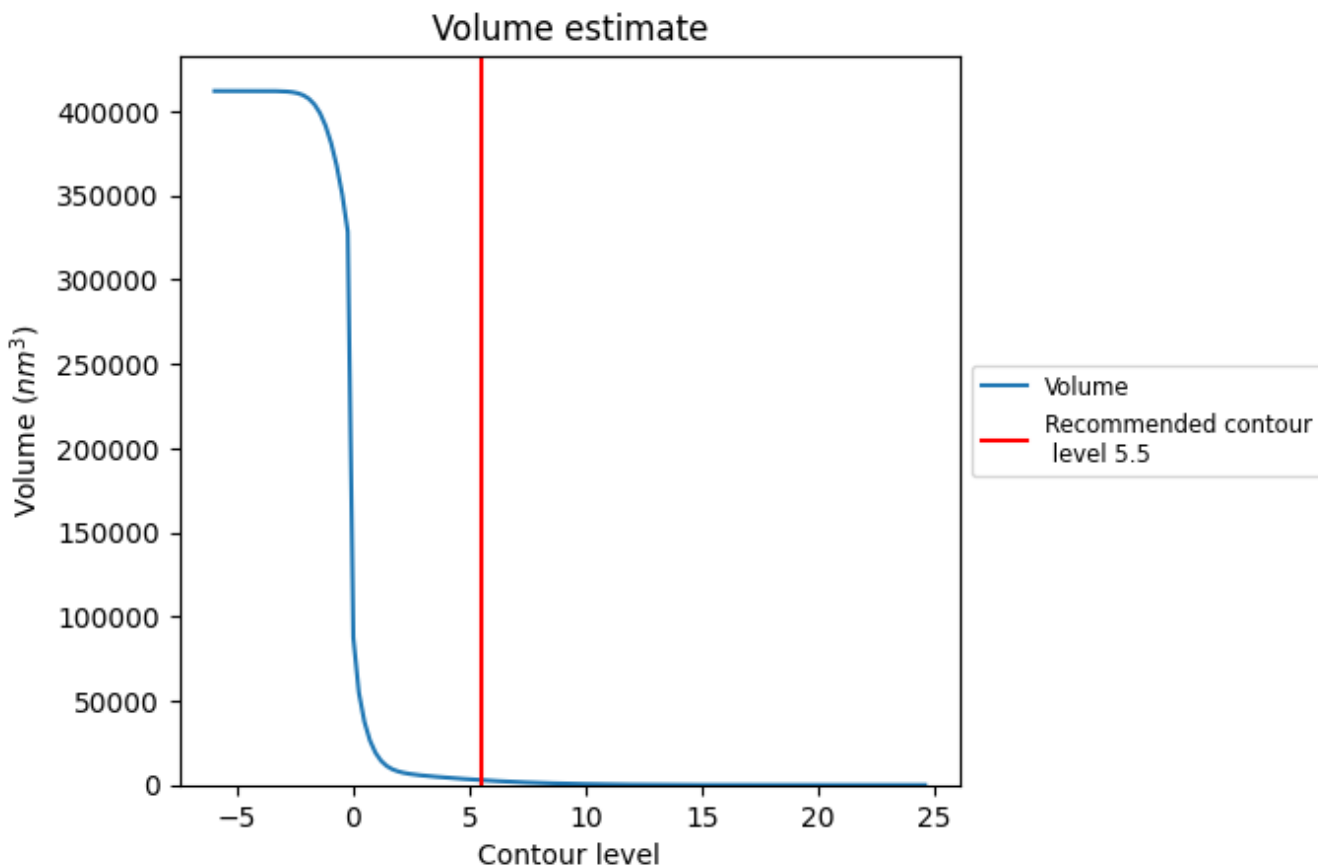
This section contains the results of statistical analysis of the map.

### 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.

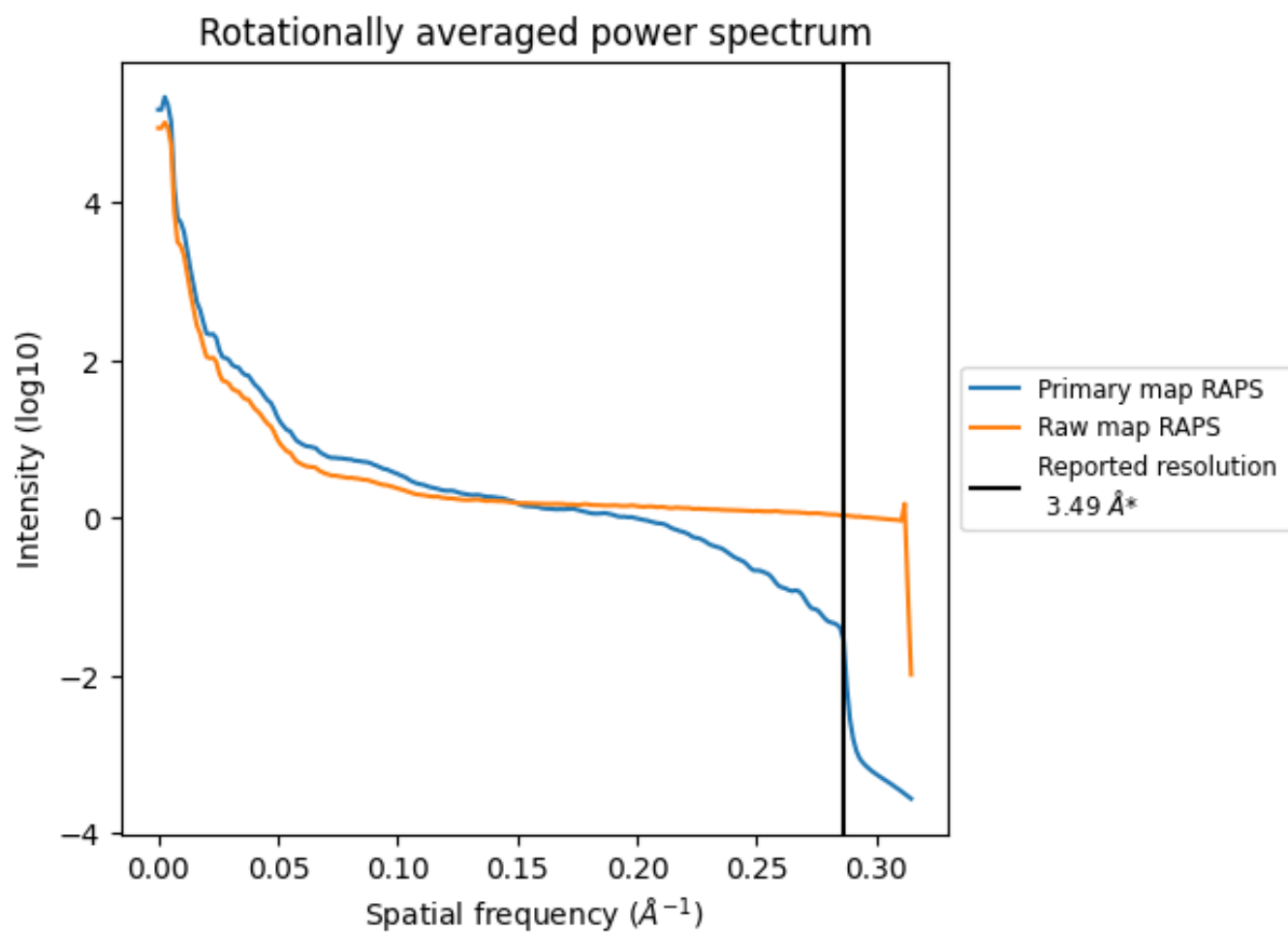
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2896  $\text{nm}^3$ ; this corresponds to an approximate mass of 2616 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

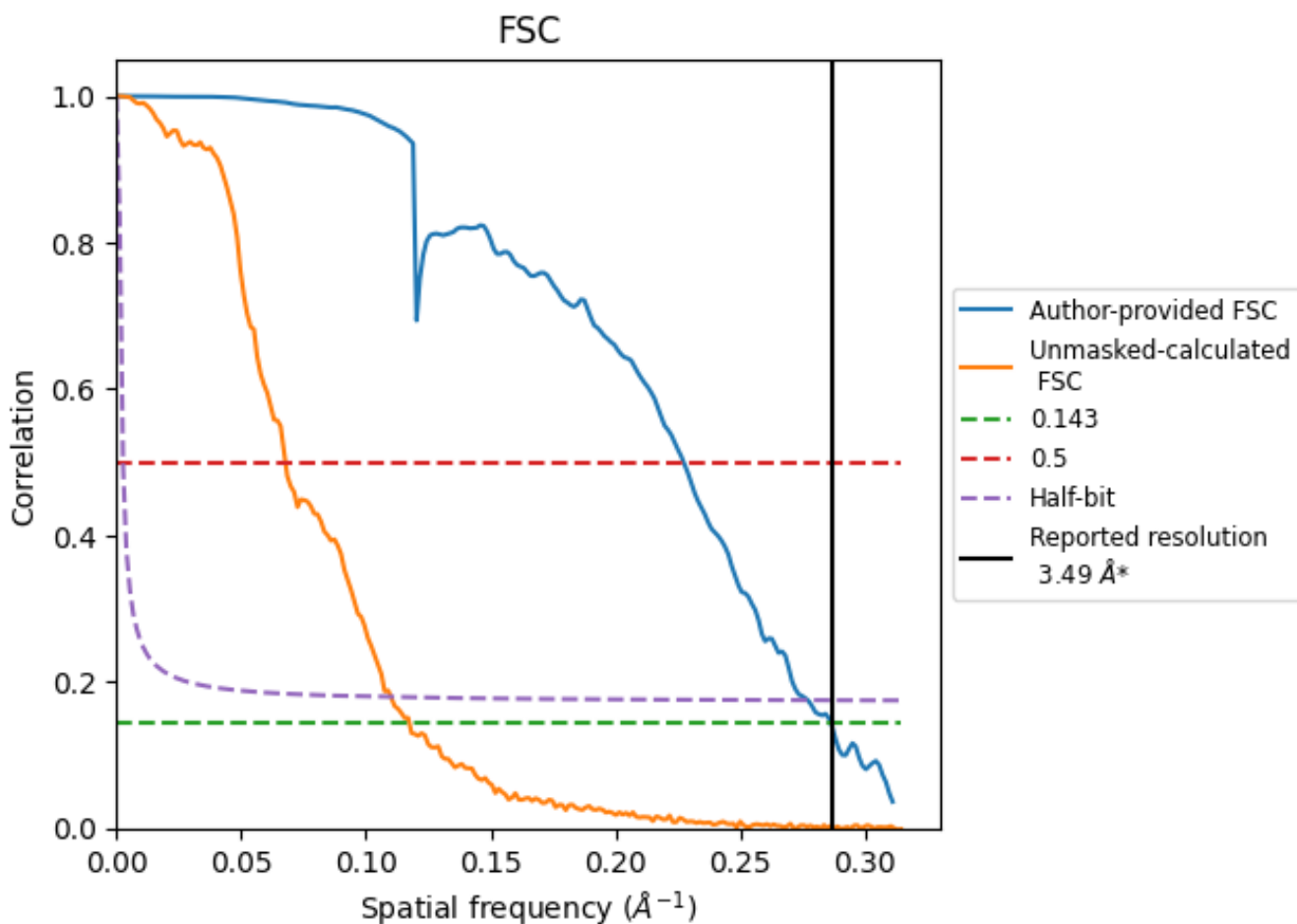


\*Reported resolution corresponds to spatial frequency of 0.287 Å<sup>-1</sup>

## 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 0.287 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

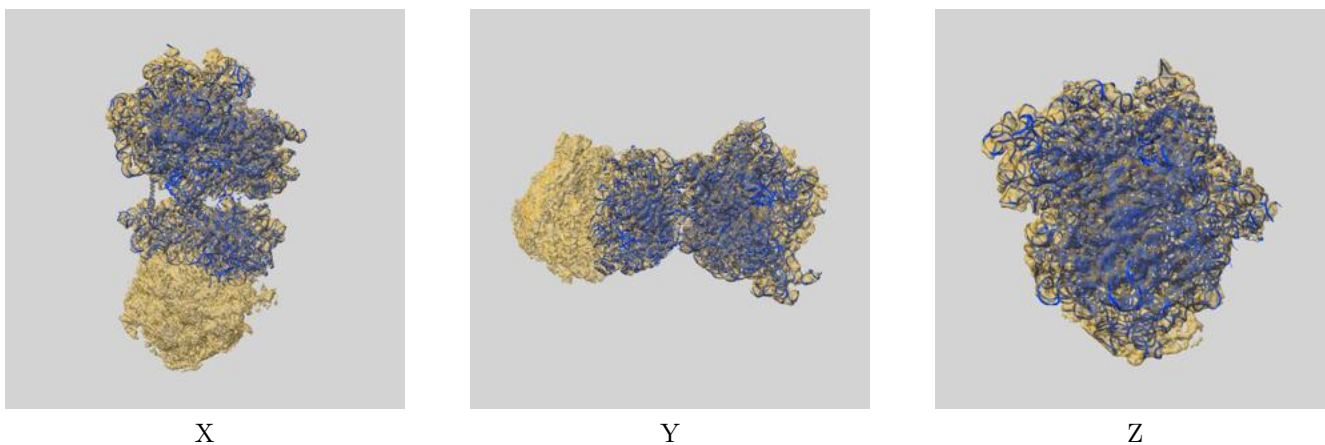
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.49	4.40	3.61
Unmasked-calculated*	8.52	14.75	9.09

\*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 8.52 differs from the reported value 3.49 by more than 10 %

## 9 Map-model fit [i](#)

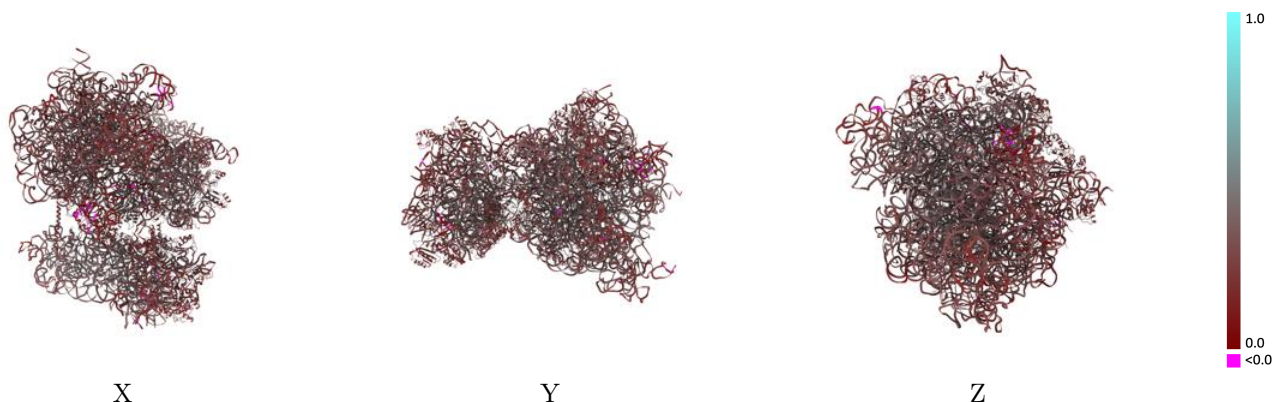
This section contains information regarding the fit between EMDB map EMD-19054 and PDB model 8RCL. Per-residue inclusion information can be found in section 3 on page 16.

### 9.1 Map-model overlay [i](#)



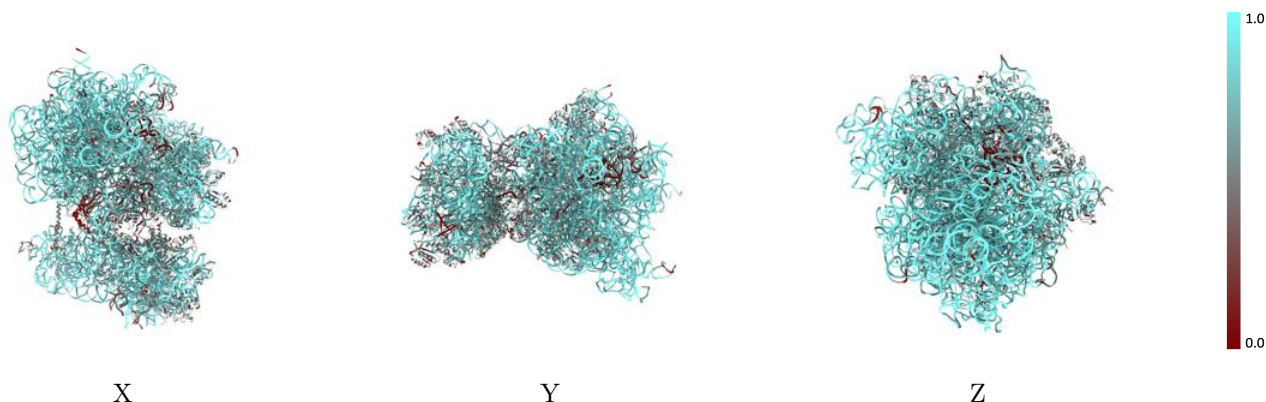
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



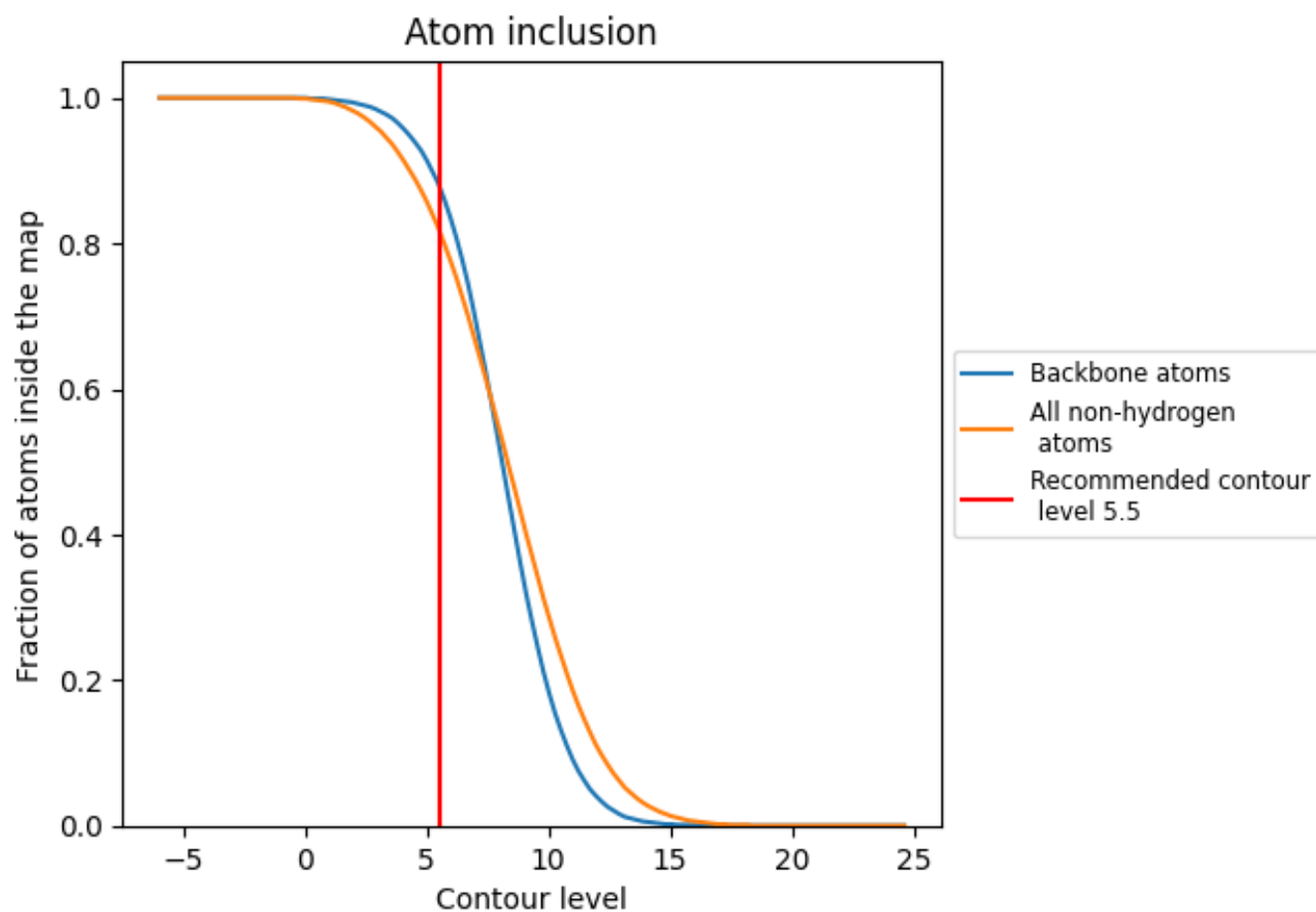
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 88% of all backbone atoms, 82% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.3070
12	 0.5990	 0.2990
32	 0.5950	 0.2170
4	 0.5390	 0.2790
62	 0.6500	 0.2570
71	 0.9210	 0.2890
72	 0.9200	 0.3050
82	 0.8790	 0.2460
A1	 0.9330	 0.3300
A2	 0.9360	 0.3480
B	 0.4920	 0.2480
B2	 0.5520	 0.3030
C1	 0.5530	 0.3100
C2	 0.6350	 0.3220
D1	 0.5610	 0.3160
D2	 0.5160	 0.2670
E1	 0.6000	 0.3100
E2	 0.6380	 0.3470
F1	 0.4210	 0.2320
F2	 0.5910	 0.3360
G1	 0.5310	 0.2340
G2	 0.6120	 0.2960
H1	 0.6220	 0.2890
H2	 0.6310	 0.3190
I1	 0.6230	 0.2570
I2	 0.7020	 0.3240
J1	 0.5780	 0.2960
J2	 0.6170	 0.3170
K1	 0.5380	 0.2640
K2	 0.6220	 0.3420
L1	 0.6840	 0.3460
L2	 0.6830	 0.3310
M1	 0.5310	 0.2140
M2	 0.6480	 0.2890
N1	 0.6330	 0.2480



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
N2	 0.6960	 0.2940
O1	 0.5910	 0.2410
O2	 0.6390	 0.3030
P1	 0.6860	 0.3380
Q1	 0.6010	 0.3070
Q2	 0.5970	 0.3220
R1	 0.4610	 0.2520
R2	 0.5350	 0.3230
S1	 0.5360	 0.2060
S2	 0.6890	 0.2980
T1	 0.6490	 0.2480
U1	 0.4180	 0.2290
U2	 0.5140	 0.3100
V2	 0.3440	 0.2080
W	 0.8200	 0.2970
W1	 0.7250	 0.2590
X2	 0.4320	 0.1680
Y1	 0.5030	 0.2290
Y2	 0.0520	 0.1910
Z1	 0.0000	 0.1390
a2	 0.1140	 0.1090
b2	 0.6830	 0.3540
e2	 0.5920	 0.2350
g2	 0.5750	 0.2450
h2	 0.5720	 0.2770
i2	 0.5200	 0.2870
l2	 0.7070	 0.2840
o2	 0.7590	 0.2820
p	 0.1130	 0.1230
r2	 0.5890	 0.2110
z2	 0.6470	 0.2260