



## Full wwPDB EM Validation Report ⓘ

Feb 4, 2025 – 09:44 AM EST

PDB ID : 8EMM  
EMDB ID : EMD-28254  
Title : Composite 70S ribosome structure for "Atomistic simulations of the E. coli ribosome provide selection criteria for translationally active substrates"  
Authors : Watson, Z.L.; Cate, J.H.D.  
Deposited on : 2022-09-28  
Resolution : 2.10 Å(reported)

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

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

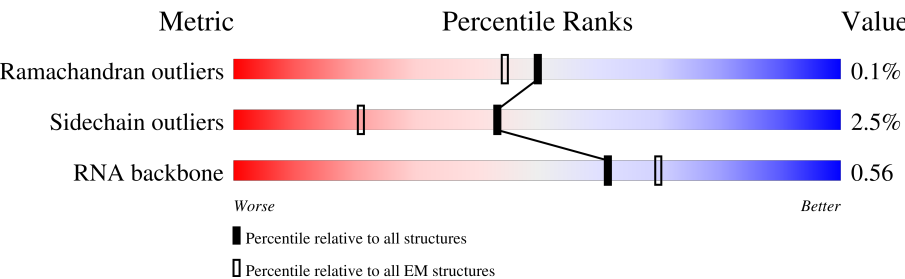
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 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 2.10 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.



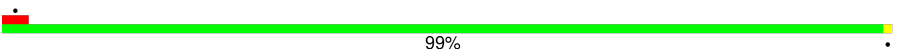

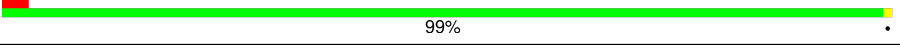
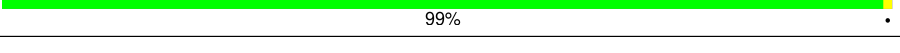
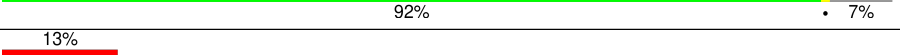
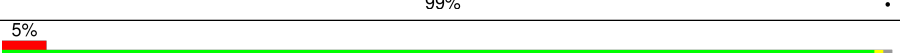
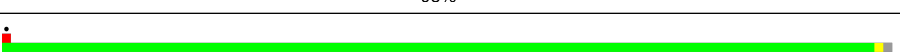
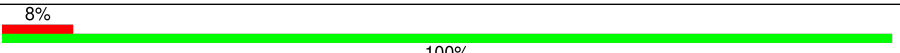

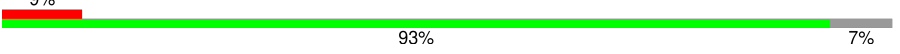
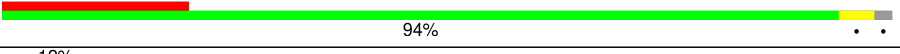
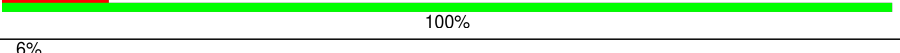
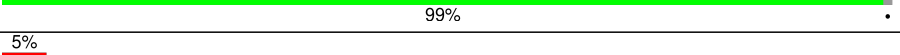
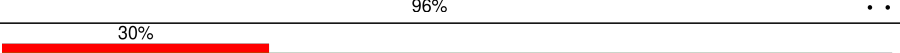
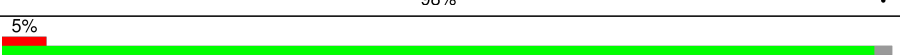
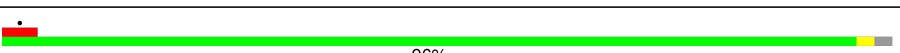
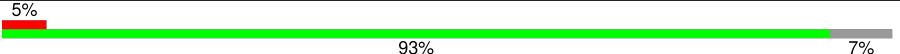
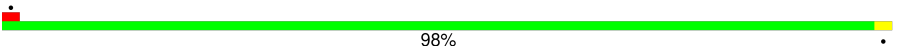
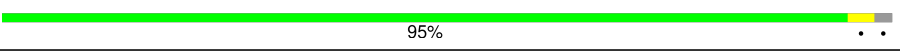
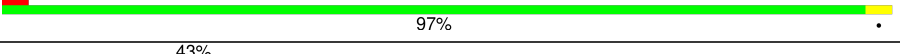

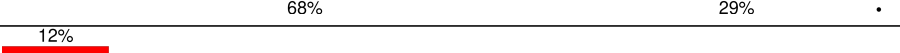



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	a	2904	
2	b	120	
3	c	273	
4	d	209	
5	e	201	
6	f	179	
7	g	177	
8	h	149	

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Mol	Chain	Length	Quality of chain
9	i	142	 99%
10	j	123	 100%
11	k	144	 99%
12	l	136	 99%
13	m	127	 92% 7%
14	n	117	 13% 99%
15	o	115	 5% 98% ..
16	p	118	 98% ..
17	q	103	 8% 100%
18	r	110	 6% 100%
19	s	100	 9% 93% 7%
20	t	104	 21% 94% ..
21	u	94	 12% 100%
22	v	85	 6% 99%
23	w	78	 5% 96% ..
24	x	63	 30% 98%
25	y	59	 5% 98%
26	z	57	 96% ..
27	0	55	 5% 93% 7%
28	1	46	 98%
29	2	65	 95% ..
30	3	38	 97%
31	4	70	 43% 81% 14%
32	Y	76	 43% 68% 29%
32	Z	76	 12% 67% 29%

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Mol	Chain	Length	Quality of chain
33	A	1542	
34	B	241	
35	C	233	
36	D	206	
37	E	167	
38	F	135	
39	G	179	
40	H	130	
41	I	130	
42	J	103	
43	K	129	
44	L	124	
45	M	118	
46	N	101	
47	O	89	
48	P	82	
49	Q	84	
50	R	75	
51	S	92	
52	T	87	
53	U	71	
54	X	28	

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 145735 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP A0A7U9B8R8

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called Ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	t	102	Total	C	N	O		
			779	492	146	141	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	v	84	Total	C	N	O	S	
			628	388	126	113	1	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	x	62	Total	C	N	O	S	
			501	308	98	94	1	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

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

- Molecule 27 is a protein called 50S ribosomal protein L33.



Mol	Chain	Residues	Atoms				AltConf	Trace
27	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 32 is a RNA chain called Met-NH-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	76	Total	C	N	O	P	0	0
			1623	723	295	529	76		
32	Z	76	Total	C	N	O	P	0	0
			1623	723	295	529	76		

- Molecule 33 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

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

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

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

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP A0A0H3PWX2

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

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

- Molecule 47 is a protein called 30S ribosomal protein S15.

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

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

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

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

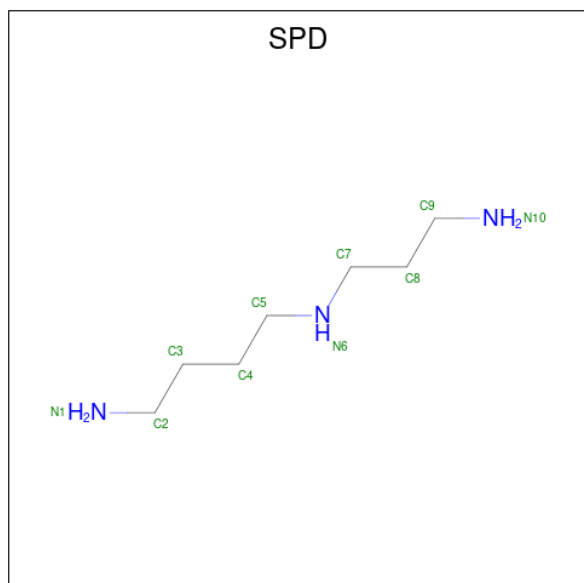
- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	X	15	Total	C	N	O	P	0	0
			322	145	61	101	15		

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

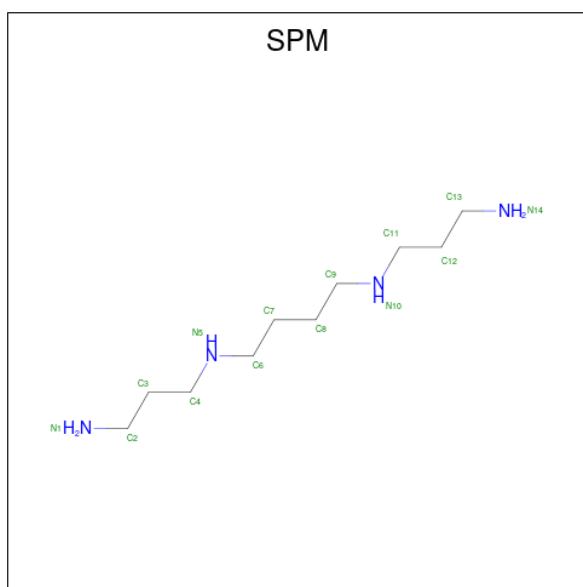
Mol	Chain	Residues	Atoms		AltConf
55	a	217	Total	Mg	0
			217	217	
55	b	5	Total	Mg	0
			5	5	
55	c	1	Total	Mg	0
			1	1	
55	d	1	Total	Mg	0
			1	1	
55	k	1	Total	Mg	0
			1	1	
55	m	1	Total	Mg	0
			1	1	
55	z	1	Total	Mg	0
			1	1	
55	Z	1	Total	Mg	0
			1	1	
55	A	92	Total	Mg	0
			92	92	
55	N	1	Total	Mg	0
			1	1	

- Molecule 56 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
56	a	1	Total	C	N	0
			10	7	3	
56	a	1	Total	C	N	0
			10	7	3	
56	a	1	Total	C	N	0
			10	7	3	
56	a	1	Total	C	N	0
			10	7	3	
56	a	1	Total	C	N	0
			10	7	3	
56	a	1	Total	C	N	0
			10	7	3	
56	a	1	Total	C	N	0
			10	7	3	
56	a	1	Total	C	N	0
			10	7	3	
56	a	1	Total	C	N	0
			10	7	3	
56	a	1	Total	C	N	0
			10	7	3	
56	a	1	Total	C	N	0
			10	7	3	
56	A	1	Total	C	N	0
			10	7	3	

- Molecule 57 is SPERMINE (three-letter code: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			AltConf
57	a	1	Total	C	N	0
			14	10	4	

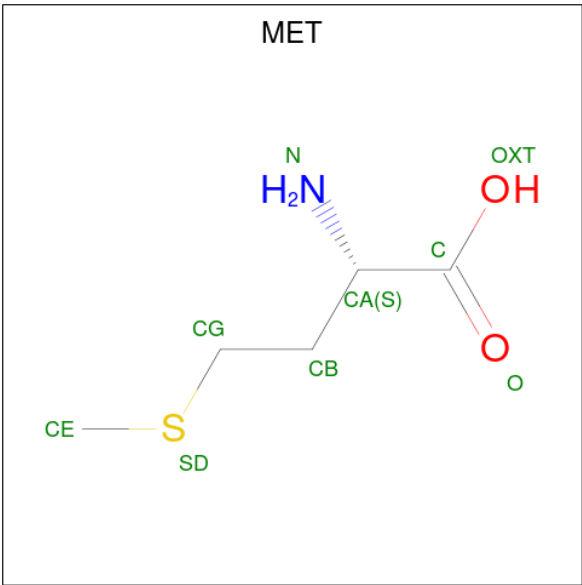
- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	a	9	Total	K	0
			9	9	
58	c	1	Total	K	0
			1	1	

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

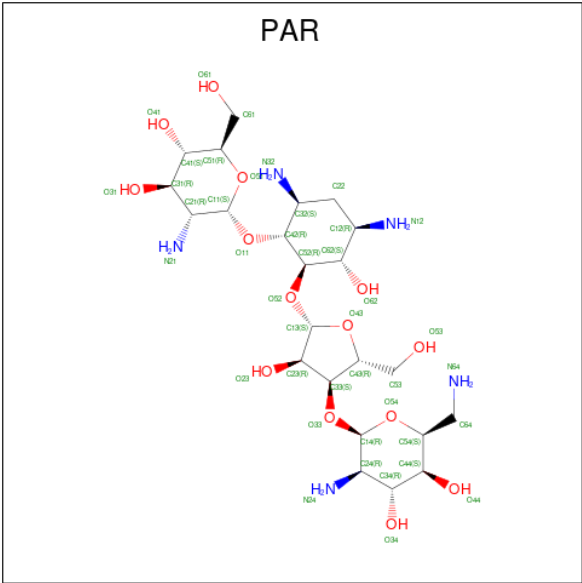
Mol	Chain	Residues	Atoms		AltConf
59	3	1	Total	Zn	0
			1	1	
59	4	1	Total	Zn	0
			1	1	

- Molecule 60 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					AltConf
60	Y	1	Total	C	N	O	S	0
			8	5	1	1	1	
60	Z	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 61 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				AltConf
61	A	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 62 is water.



Mol	Chain	Residues	Atoms		AltConf
62	a	3031	Total 3031	O 3031	0
62	b	39	Total 39	O 39	0
62	c	86	Total 86	O 86	0
62	d	33	Total 33	O 33	0
62	e	28	Total 28	O 28	0
62	h	1	Total 1	O 1	0
62	i	10	Total 10	O 10	0
62	j	15	Total 15	O 15	0
62	k	30	Total 30	O 30	0
62	l	19	Total 19	O 19	0
62	m	21	Total 21	O 21	0
62	o	15	Total 15	O 15	0
62	p	24	Total 24	O 24	0
62	q	15	Total 15	O 15	0
62	r	23	Total 23	O 23	0
62	s	5	Total 5	O 5	0
62	t	1	Total 1	O 1	0
62	u	4	Total 4	O 4	0
62	v	12	Total 12	O 12	0
62	w	9	Total 9	O 9	0
62	x	1	Total 1	O 1	0
62	y	1	Total 1	O 1	0

*Continued on next page...*

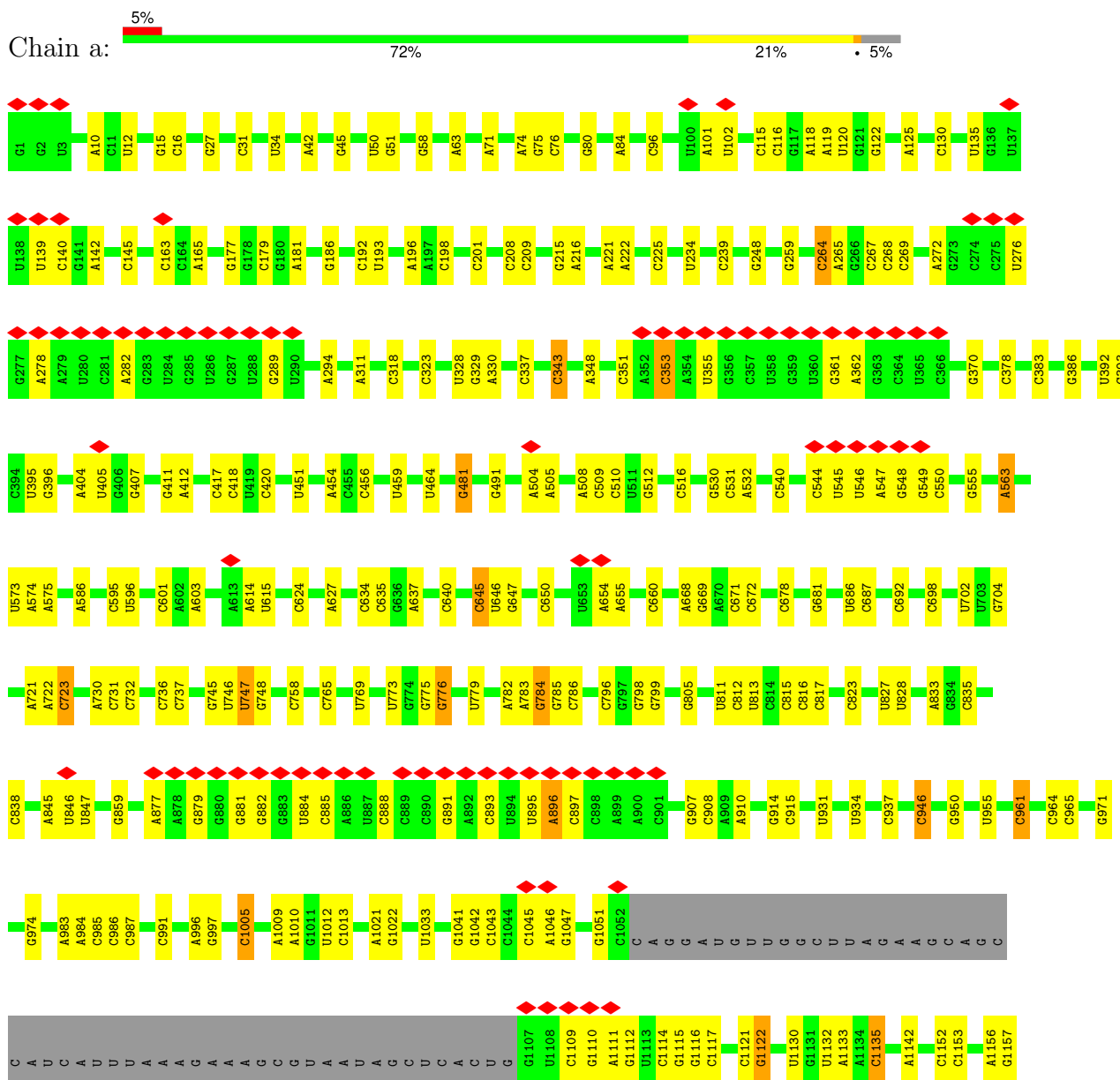
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
62	z	24	Total 24	O 24	0
62	0	1	Total 1	O 1	0
62	1	16	Total 16	O 16	0
62	2	20	Total 20	O 20	0
62	3	4	Total 4	O 4	0
62	Z	2	Total 2	O 2	0
62	A	1	Total 1	O 1	0

### 3 Residue-property plots


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: 23S rRNA





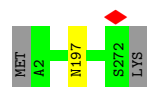
- Molecule 2: 5S rRNA

Chain b: 



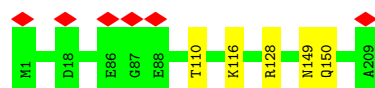
- Molecule 3: 50S ribosomal protein L2

Chain c: 



- Molecule 4: 50S ribosomal protein L3

Chain d: 

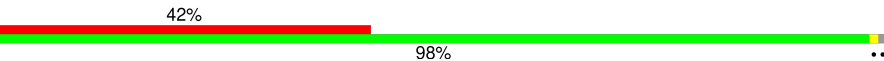


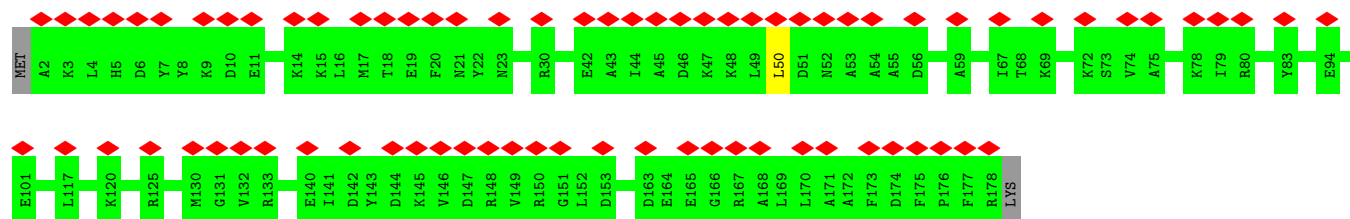
- Molecule 5: 50S ribosomal protein L4

Chain e: 



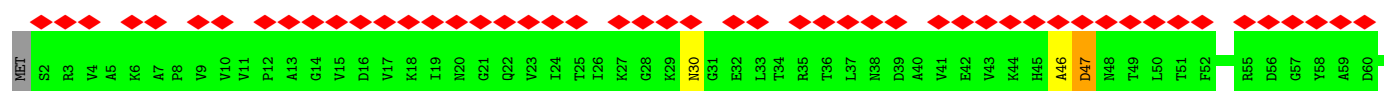
- Molecule 6: 50S ribosomal protein L5

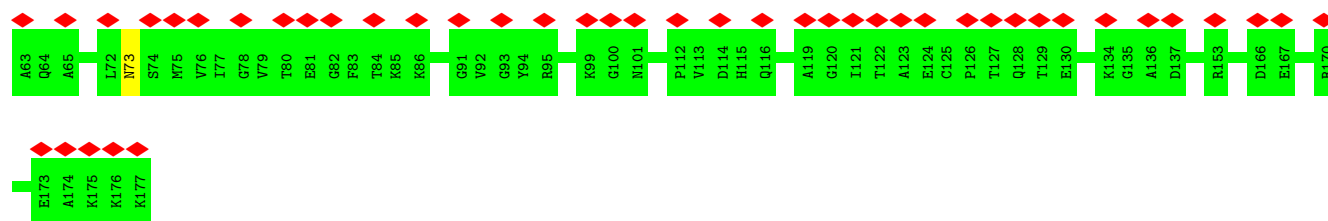
Chain f: 



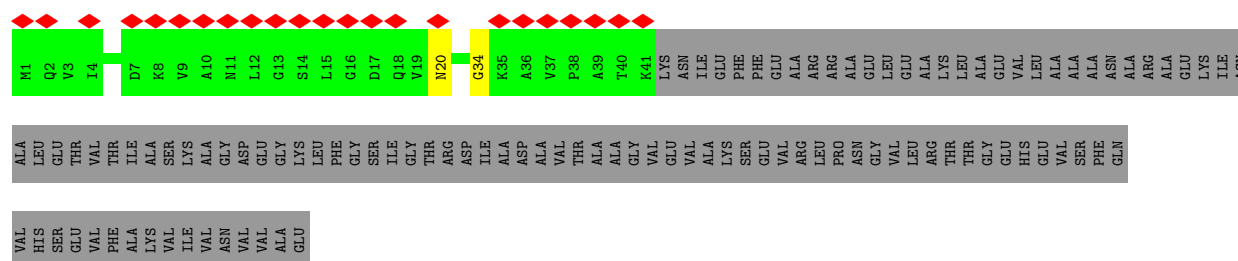
- Molecule 7: 50S ribosomal protein L6

Chain g: 

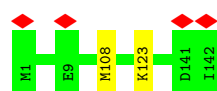




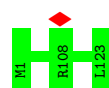
• Molecule 8: 50S ribosomal protein L9



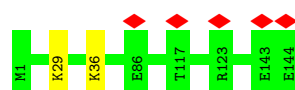
• Molecule 9: 50S ribosomal protein L13



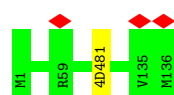
• Molecule 10: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal protein L15

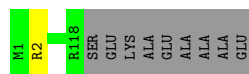


• Molecule 12: 50S ribosomal protein L16



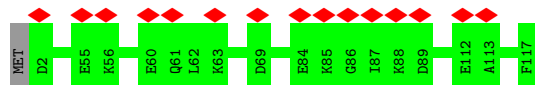
- Molecule 13: 50S ribosomal protein L17

Chain m:  92% 7%



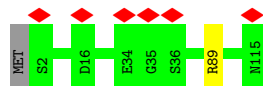
- Molecule 14: 50S ribosomal protein L18

Chain n:  13% 99%



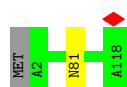
- Molecule 15: 50S ribosomal protein L19

Chain o:  5% 98%



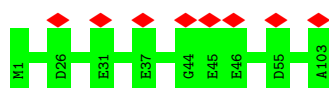
- Molecule 16: 50S ribosomal protein L20

Chain p:  98%



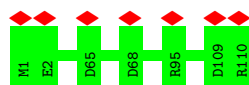
- Molecule 17: Ribosomal protein L21

Chain q:  8% 100%




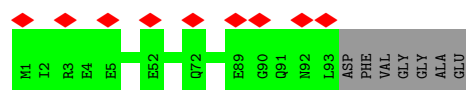
- Molecule 18: 50S ribosomal protein L22

Chain r:  6% 100%

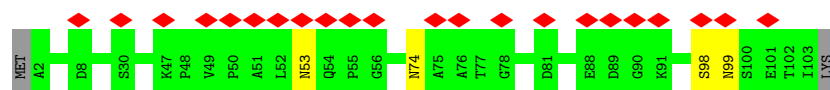


- Molecule 19: 50S ribosomal protein L23

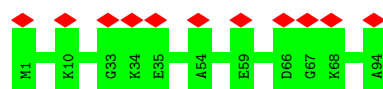
Chain s:  9% 93% 7%



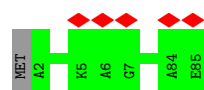
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



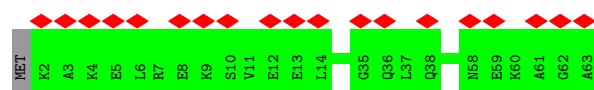
- Molecule 22: 50S ribosomal protein L27



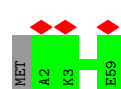
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

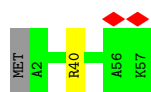


- Molecule 25: 50S ribosomal protein L30

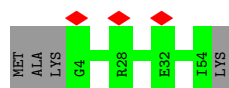
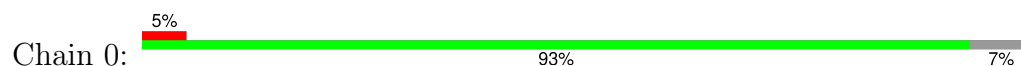


- Molecule 26: 50S ribosomal protein L32

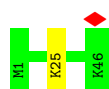




- Molecule 27: 50S ribosomal protein L33



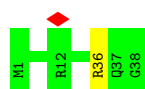
- Molecule 28: 50S ribosomal protein L34



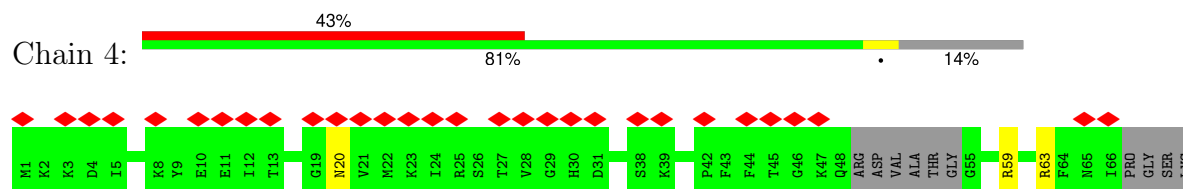
- Molecule 29: 50S ribosomal protein L35



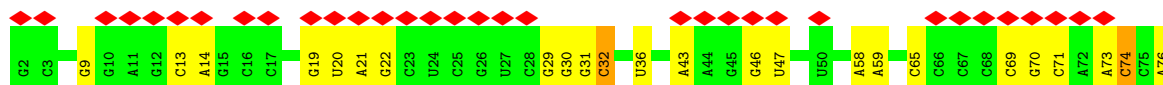
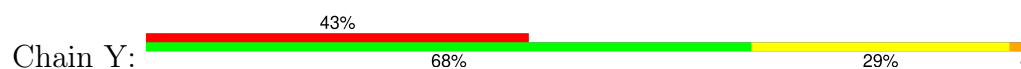
- Molecule 30: 50S ribosomal protein L36



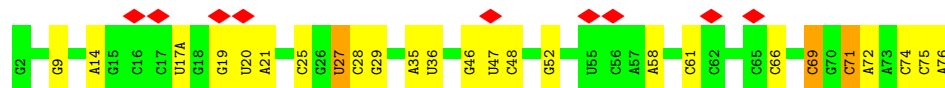
- Molecule 31: 50S ribosomal protein L31



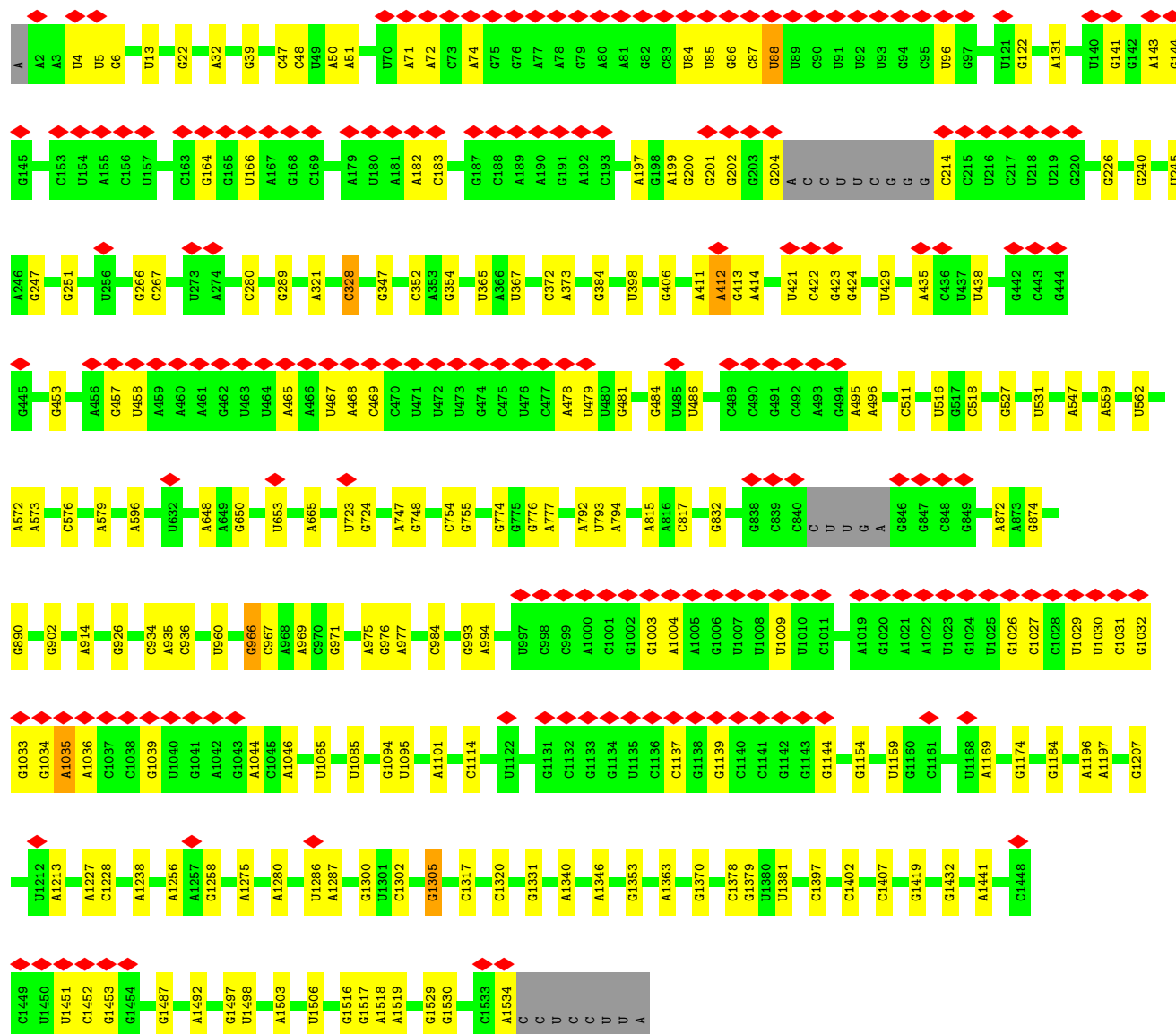
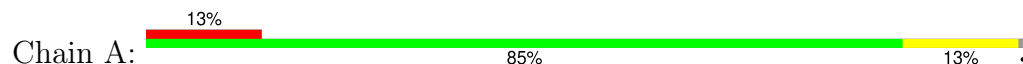
- Molecule 32: Met-NH-tRNA



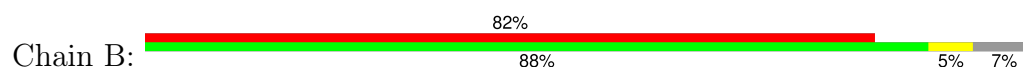
- Molecule 32: Met-NH-tRNA

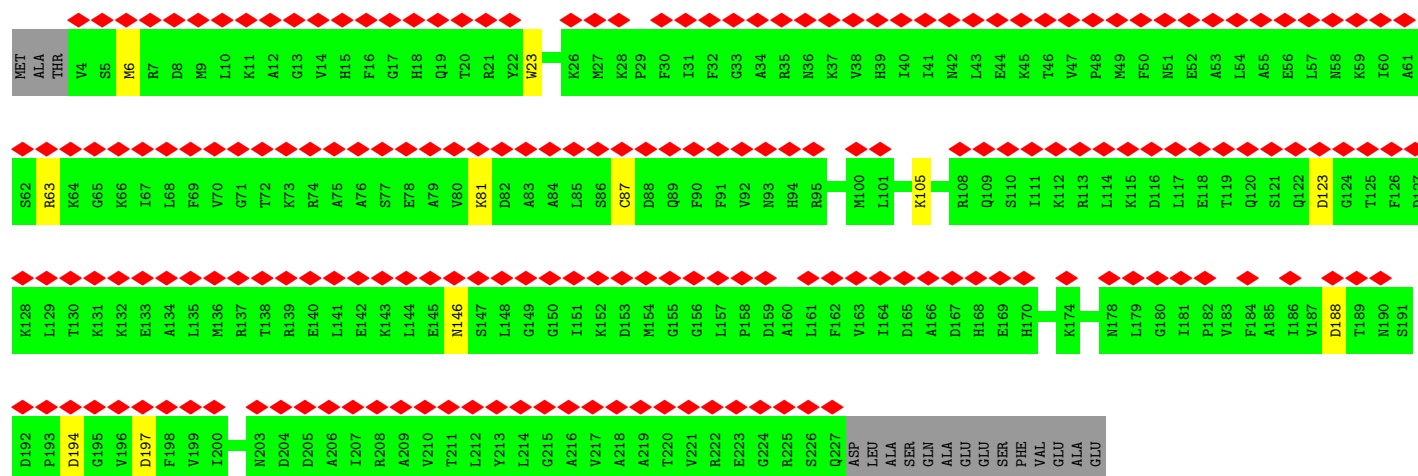


- Molecule 33: 16S rRNA

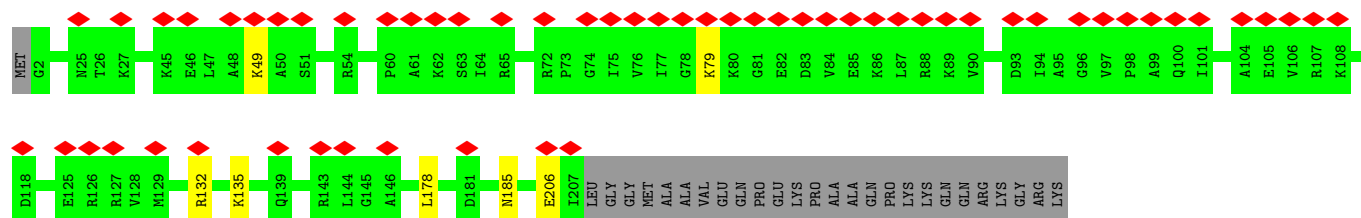
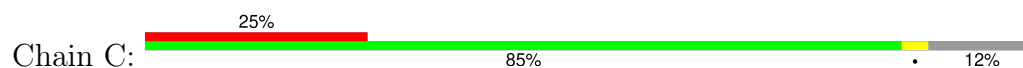


- Molecule 34: 30S ribosomal protein S2

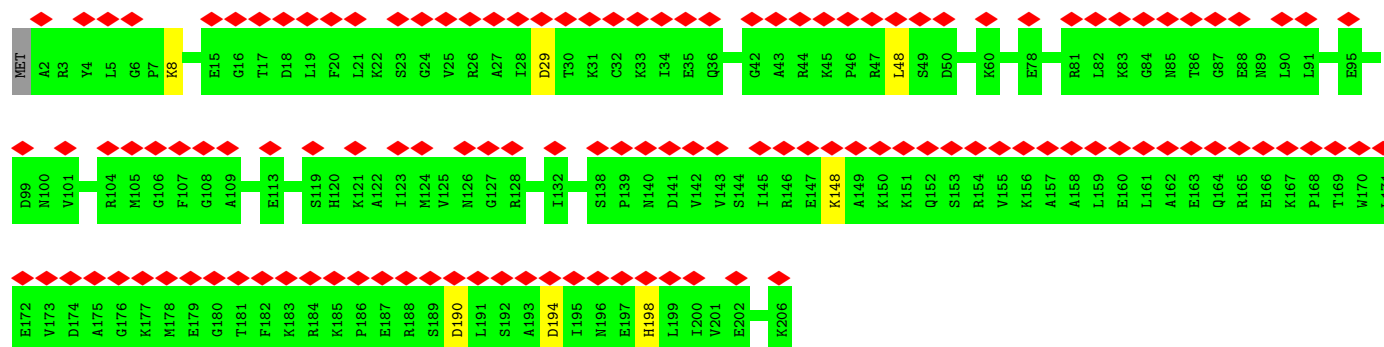




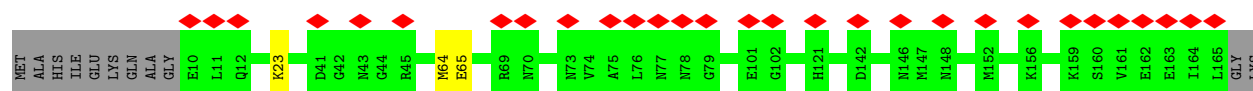
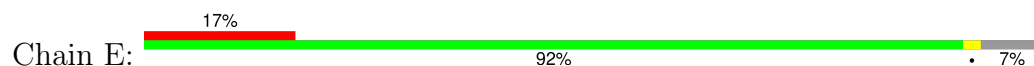
• Molecule 35: 30S ribosomal protein S3



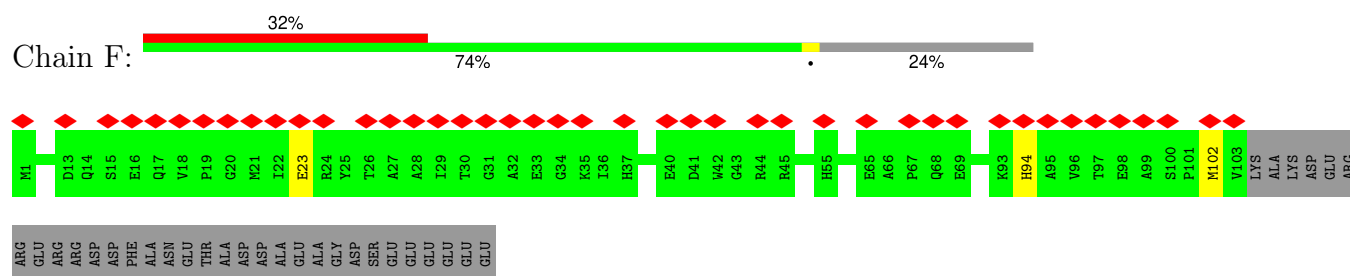
• Molecule 36: 30S ribosomal protein S4



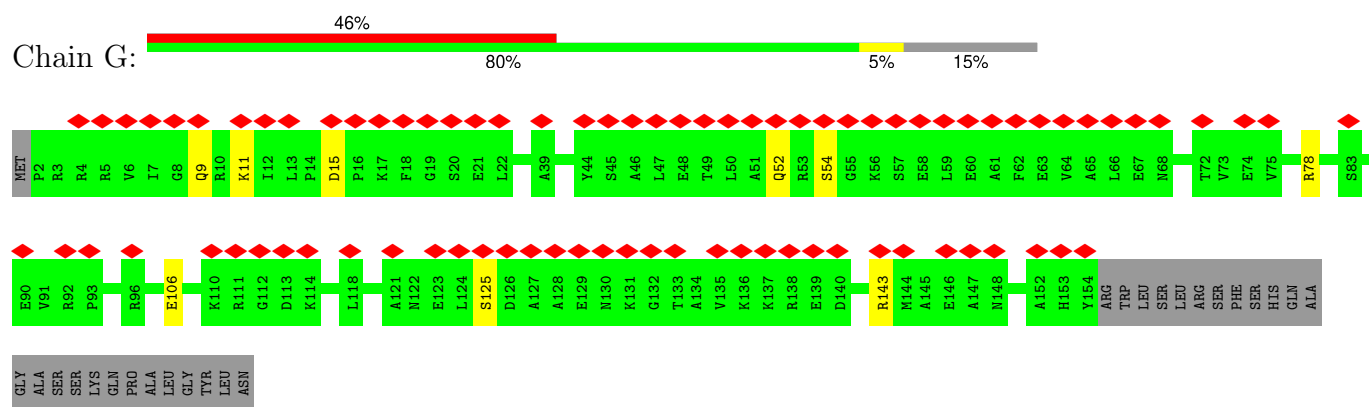
• Molecule 37: 30S ribosomal protein S5



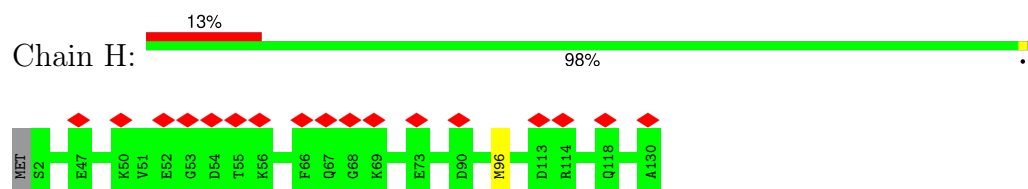
• Molecule 38: 30S ribosomal protein S6



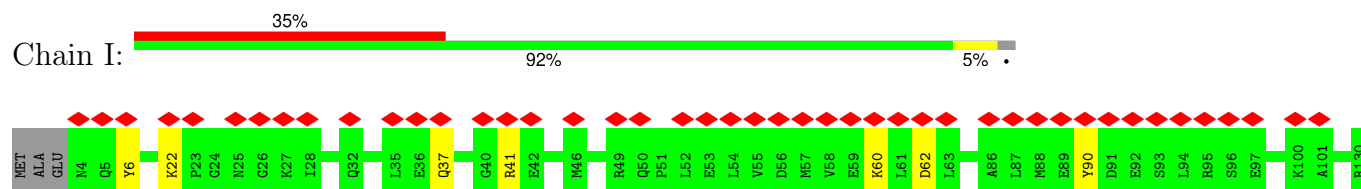
- Molecule 39: 30S ribosomal protein S7



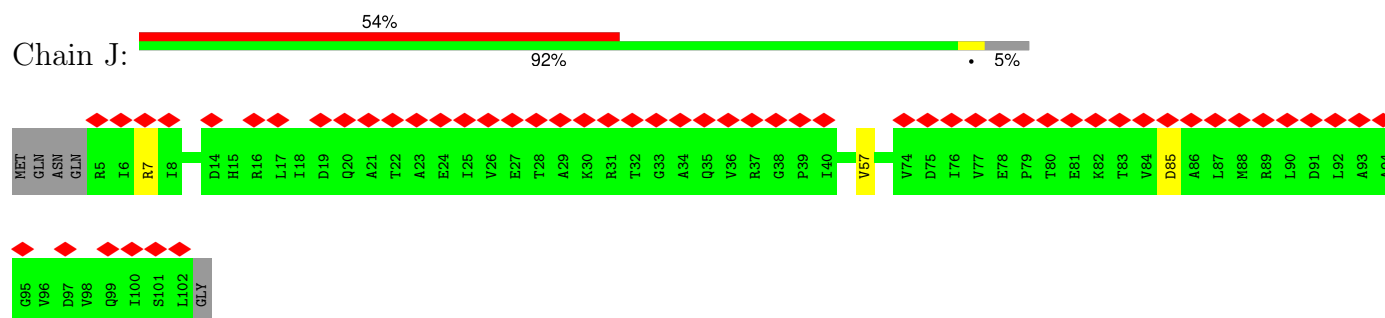
- Molecule 40: 30S ribosomal protein S8



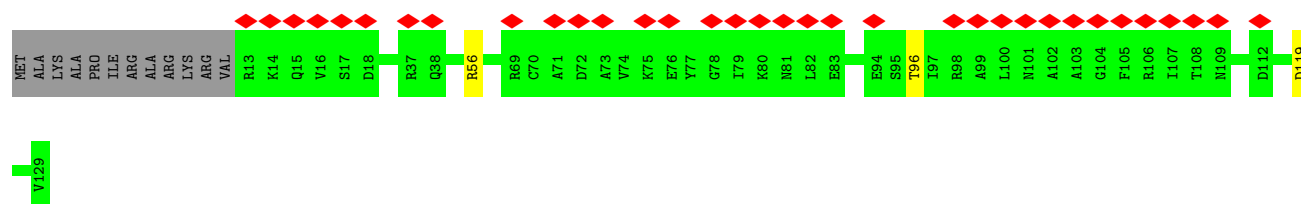
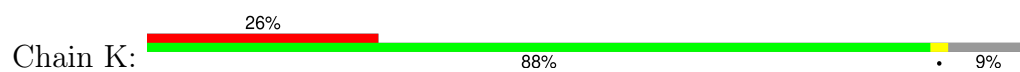
- Molecule 41: 30S ribosomal protein S9



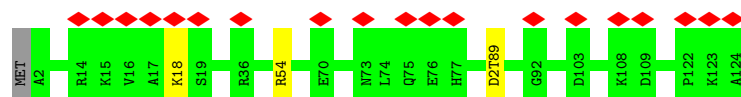
- Molecule 42: 30S ribosomal protein S10



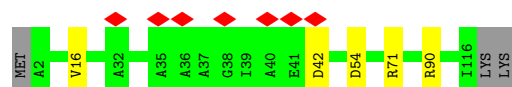
- Molecule 43: 30S ribosomal protein S11



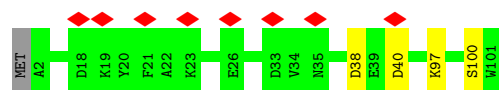
- Molecule 44: 30S ribosomal protein S12



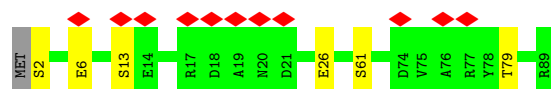
- Molecule 45: 30S ribosomal protein S13



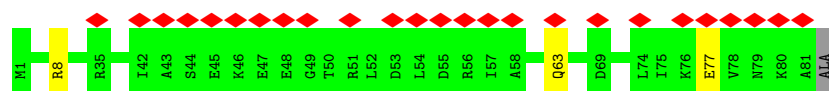
- Molecule 46: 30S ribosomal protein S14



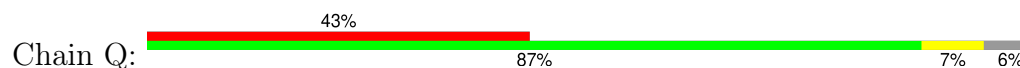
- Molecule 47: 30S ribosomal protein S15

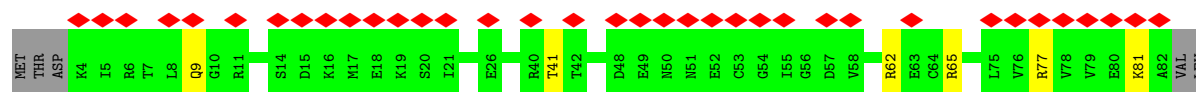


- Molecule 48: 30S ribosomal protein S16

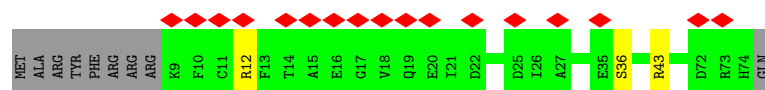
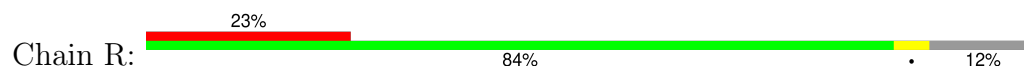


- Molecule 49: 30S ribosomal protein S17

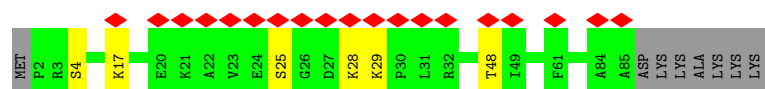
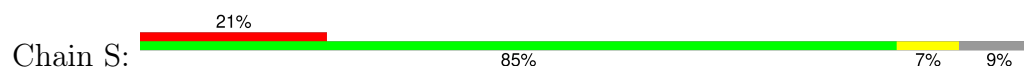




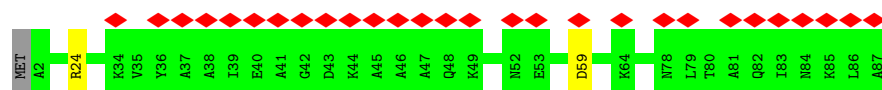
- Molecule 50: 30S ribosomal protein S18



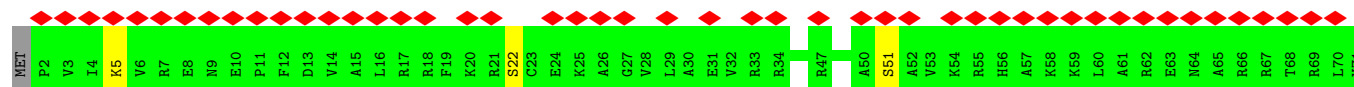
- Molecule 51: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S21



- Molecule 54: mRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129455	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0151	Depositor
Map size (Å)	378.29758, 378.29758, 378.29758	wwPDB
Map dimensions	456, 456, 456	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8296, 0.8296, 0.8296	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8AN, 3TD, 2MA, ZN, SPM, K, OMU, G7M, 5MU, 4OC, PSU, OMC, 6MZ, SPD, D2T, MA6, H2U, 2MG, 5MC, OMG, PAR, MS6, 1MG, 4D4, UR3, IAS, MEQ, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	a	1.19	2/65651 (0.0%)	1.25	456/102413 (0.4%)
2	b	0.89	0/2850	1.09	12/4444 (0.3%)
3	c	0.54	0/2121	0.67	0/2852
4	d	0.56	0/1576	0.63	0/2119
5	e	0.47	0/1571	0.63	0/2113
6	f	0.38	0/1434	0.61	1/1926 (0.1%)
7	g	0.40	0/1343	0.65	0/1816
8	h	0.38	0/306	0.69	0/413
9	i	0.53	1/1152 (0.1%)	0.58	0/1551
10	j	0.54	0/955	0.71	0/1279
11	k	0.49	0/1062	0.66	0/1413
12	l	0.53	0/1073	0.68	0/1433
13	m	0.53	0/958	0.69	0/1281
14	n	0.48	0/902	0.62	0/1209
15	o	0.51	0/929	0.60	0/1242
16	p	0.55	0/960	0.66	0/1278
17	q	0.50	0/829	0.64	0/1107
18	r	0.47	0/864	0.58	0/1156
19	s	0.44	0/744	0.61	0/994
20	t	0.45	0/787	0.66	1/1051 (0.1%)
21	u	0.49	0/766	0.59	0/1025
22	v	0.51	0/636	0.64	0/841
23	w	0.47	0/635	0.63	0/848
24	x	0.37	0/502	0.53	0/667
25	y	0.42	0/453	0.62	0/605
26	z	0.52	0/450	0.82	2/599 (0.3%)
27	0	0.52	0/424	0.65	0/565
28	1	0.49	0/380	0.65	0/498
29	2	0.52	0/513	0.63	0/676
30	3	0.53	0/303	0.59	0/397
31	4	0.41	0/488	0.59	0/649



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Y	0.51	0/1788	0.98	8/2786 (0.3%)
32	Z	0.61	0/1788	1.06	10/2786 (0.4%)
33	A	0.61	0/36236	0.87	16/56520 (0.0%)
34	B	0.32	0/1784	0.58	1/2403 (0.0%)
35	C	0.33	0/1651	0.57	0/2225
36	D	0.32	0/1665	0.58	0/2227
37	E	0.35	0/1165	0.58	0/1568
38	F	0.36	0/858	0.58	0/1160
39	G	0.32	0/1219	0.58	0/1635
40	H	0.36	0/989	0.59	0/1326
41	I	0.35	0/1034	0.61	0/1375
42	J	0.37	0/796	0.64	0/1077
43	K	0.33	0/884	0.58	0/1191
44	L	0.36	0/960	0.64	0/1286
45	M	0.34	0/900	0.62	0/1204
46	N	0.34	0/817	0.59	0/1088
47	O	0.32	0/722	0.58	0/964
48	P	0.33	0/653	0.61	0/877
49	Q	0.36	0/650	0.61	0/871
50	R	0.39	0/553	0.60	0/742
51	S	0.34	0/685	0.57	0/922
52	T	0.32	0/676	0.52	0/895
53	U	0.31	0/597	0.62	0/792
54	X	0.46	0/361	0.75	0/560
All	All	0.88	3/153048 (0.0%)	1.02	507/228940 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	g	0	2
8	h	0	1
23	w	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	2576	G	C6-O6	-5.63	1.19	1.24
9	i	108	MET	C-N	-5.38	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1269	A	N7-C5	-5.00	1.36	1.39

All (507) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1313	U	N1-C2-O2	13.27	132.09	122.80
1	a	1313	U	N3-C2-O2	-13.25	112.93	122.20
1	a	12	U	N3-C2-O2	-11.88	113.88	122.20
1	a	12	U	C2-N1-C1'	11.74	131.79	117.70
1	a	12	U	N1-C2-O2	11.40	130.78	122.80
1	a	2646	C	C6-N1-C2	-11.05	115.88	120.30
1	a	512	G	O4'-C1'-N9	11.05	117.04	108.20
1	a	672	C	C6-N1-C2	-9.11	116.66	120.30
1	a	1804	C	C6-N1-C2	-8.95	116.72	120.30
1	a	624	C	C6-N1-C2	-8.61	116.86	120.30
1	a	198	C	C6-N1-C2	-8.41	116.94	120.30
1	a	2723	C	C6-N1-C2	-8.39	116.94	120.30
1	a	1121	C	C6-N1-C2	-8.37	116.95	120.30
1	a	2443	C	N1-C2-O2	8.30	123.88	118.90
1	a	1782	U	O5'-P-OP1	-8.28	98.25	105.70
1	a	2023	C	C6-N1-C2	-8.23	117.01	120.30
1	a	698	C	C6-N1-C2	-8.21	117.02	120.30
1	a	783	A	C2-N3-C4	8.12	114.66	110.60
1	a	1997	C	N1-C2-O2	8.09	123.75	118.90
1	a	2870	C	C6-N1-C2	-7.90	117.14	120.30
1	a	672	C	C5-C6-N1	7.84	124.92	121.00
1	a	650	C	C6-N1-C2	-7.83	117.17	120.30
1	a	1967	C	N1-C2-O2	7.82	123.59	118.90
1	a	2765	A	C2-N3-C4	7.82	114.51	110.60
1	a	1774	C	C6-N1-C2	-7.81	117.18	120.30
1	a	2646	C	C5-C6-N1	7.79	124.90	121.00
1	a	264	C	N3-C2-O2	-7.72	116.50	121.90
1	a	2615	U	N3-C2-O2	-7.70	116.81	122.20
1	a	601	C	C6-N1-C2	-7.61	117.25	120.30
1	a	1314	C	C2-N1-C1'	7.61	127.17	118.80
1	a	1816	C	N1-C2-O2	7.60	123.46	118.90
2	b	97	C	C6-N1-C2	-7.56	117.28	120.30
1	a	1879	C	C6-N1-C2	-7.54	117.28	120.30
1	a	984	A	O4'-C1'-N9	7.54	114.23	108.20
1	a	351	C	C6-N1-C2	-7.53	117.29	120.30
1	a	2562	U	N3-C2-O2	-7.50	116.95	122.20
1	a	965	C	C6-N1-C2	-7.49	117.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	816	C	C6-N1-C2	-7.47	117.31	120.30
1	a	2626	C	N1-C2-O2	7.43	123.36	118.90
1	a	635	C	C6-N1-C2	-7.43	117.33	120.30
1	a	2025	C	C6-N1-C2	-7.31	117.38	120.30
1	a	12	U	C6-N1-C2	-7.30	116.62	121.00
32	Z	27	U	C2-N1-C1'	7.27	126.42	117.70
1	a	786	C	N1-C2-O2	7.25	123.25	118.90
1	a	16	C	N1-C2-O2	7.25	123.25	118.90
1	a	1764	C	C6-N1-C2	-7.24	117.41	120.30
1	a	12	U	C5-C6-N1	7.24	126.32	122.70
1	a	417	C	C6-N1-C2	-7.22	117.41	120.30
1	a	799	G	C2-N3-C4	7.22	115.51	111.90
1	a	1662	U	N3-C2-O2	-7.19	117.17	122.20
1	a	634	C	C6-N1-C2	-7.17	117.43	120.30
1	a	1330	C	N1-C2-O2	7.12	123.17	118.90
1	a	2450	A	C6-N1-C2	7.09	122.86	118.60
1	a	378	C	C6-N1-C2	-7.07	117.47	120.30
32	Y	71	C	N1-C2-O2	7.05	123.13	118.90
1	a	1984	G	C5-C6-O6	7.04	132.83	128.60
1	a	1997	C	N3-C2-O2	-6.99	117.01	121.90
1	a	2006	C	C6-N1-C2	-6.93	117.53	120.30
1	a	12	U	C6-N1-C1'	-6.92	111.51	121.20
1	a	1822	C	C6-N1-C2	-6.92	117.53	120.30
34	B	123	ASP	CB-CG-OD1	6.92	124.52	118.30
1	a	737	C	C6-N1-C2	-6.88	117.55	120.30
1	a	264	C	N1-C2-O2	6.87	123.02	118.90
1	a	1984	G	N1-C6-O6	-6.87	115.78	119.90
1	a	838	C	C6-N1-C2	-6.87	117.55	120.30
26	z	40	ARG	CG-CD-NE	6.86	126.21	111.80
1	a	946	C	C6-N1-C2	-6.86	117.56	120.30
1	a	1289	C	C6-N1-C2	-6.84	117.56	120.30
33	A	412	A	O4'-C1'-N9	6.84	113.67	108.20
1	a	1005	C	C6-N1-C2	-6.84	117.57	120.30
1	a	2403	C	N1-C2-O2	6.84	123.00	118.90
1	a	1952	A	N1-C2-N3	-6.79	125.90	129.30
1	a	370	G	O4'-C1'-N9	-6.79	102.77	108.20
1	a	2403	C	C6-N1-C2	-6.79	117.58	120.30
1	a	2880	C	N1-C2-O2	6.77	122.96	118.90
1	a	198	C	C5-C6-N1	6.76	124.38	121.00
1	a	393	C	C6-N1-C2	-6.76	117.59	120.30
1	a	1314	C	C6-N1-C2	-6.75	117.60	120.30
1	a	2043	C	N1-C2-O2	6.74	122.95	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1313	U	C2-N1-C1'	6.74	125.78	117.70
1	a	1351	C	N3-C2-O2	-6.73	117.19	121.90
1	a	1547	C	C6-N1-C2	-6.72	117.61	120.30
1	a	116	C	N1-C2-O2	6.69	122.92	118.90
1	a	16	C	N3-C2-O2	-6.66	117.24	121.90
1	a	1965	C	C6-N1-C2	-6.64	117.64	120.30
1	a	122	G	O5'-P-OP2	-6.62	99.74	105.70
1	a	1338	G	N1-C6-O6	-6.62	115.93	119.90
1	a	2562	U	N1-C2-O2	6.62	127.43	122.80
1	a	1813	G	N1-C6-O6	-6.61	115.94	119.90
1	a	1348	C	C6-N1-C2	-6.61	117.66	120.30
1	a	1357	C	C6-N1-C2	-6.59	117.66	120.30
1	a	1533	C	N1-C2-O2	6.57	122.84	118.90
32	Z	69	C	C6-N1-C2	-6.57	117.67	120.30
1	a	908	C	C6-N1-C2	-6.55	117.68	120.30
1	a	896	A	P-O3'-C3'	-6.55	111.84	119.70
1	a	2473	U	N1-C2-O2	6.55	127.39	122.80
1	a	1774	C	N3-C2-O2	-6.54	117.32	121.90
26	z	40	ARG	CA-CB-CG	6.54	127.79	113.40
1	a	2579	C	O5'-P-OP1	-6.54	99.81	105.70
1	a	1936	A	O4'-C1'-N9	6.54	113.43	108.20
1	a	2646	C	N3-C2-O2	-6.54	117.33	121.90
1	a	2576	G	C2-N3-C4	6.53	115.17	111.90
1	a	1774	C	N1-C2-O2	6.53	122.82	118.90
1	a	1437	C	C6-N1-C2	-6.50	117.70	120.30
1	a	225	C	N1-C2-O2	6.50	122.80	118.90
1	a	796	C	C6-N1-C2	-6.48	117.71	120.30
1	a	2452	C	C6-N1-C2	-6.47	117.71	120.30
1	a	1315	C	C6-N1-C2	-6.45	117.72	120.30
1	a	2043	C	C5-C6-N1	6.45	124.22	121.00
1	a	783	A	N3-C4-N9	6.43	132.54	127.40
1	a	1967	C	N3-C2-O2	-6.42	117.41	121.90
1	a	2795	C	C6-N1-C2	-6.42	117.73	120.30
1	a	815	C	N3-C2-O2	-6.41	117.41	121.90
1	a	2615	U	N1-C2-O2	6.41	127.29	122.80
2	b	37	C	N1-C2-O2	6.40	122.74	118.90
1	a	1816	C	N3-C2-O2	-6.40	117.42	121.90
1	a	1670	C	N3-C2-O2	-6.40	117.42	121.90
20	t	98	SER	C-N-CA	6.38	137.66	121.70
32	Y	74	C	N1-C2-O2	6.38	122.73	118.90
1	a	2473	U	N3-C2-O2	-6.38	117.74	122.20
1	a	1330	C	N3-C2-O2	-6.37	117.44	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	234	U	N3-C2-O2	-6.36	117.75	122.20
1	a	823	C	C6-N1-C2	-6.34	117.76	120.30
1	a	1956	U	N3-C2-O2	-6.34	117.76	122.20
1	a	2072	C	C6-N1-C2	-6.34	117.77	120.30
6	f	50	LEU	CA-CB-CG	6.33	129.87	115.30
1	a	1324	G	O4'-C1'-N9	6.33	113.26	108.20
1	a	784	G	P-O3'-C3'	6.32	127.29	119.70
1	a	395	U	O4'-C1'-N1	6.32	113.25	108.20
1	a	971	G	N1-C6-O6	-6.30	116.12	119.90
1	a	1686	C	N1-C2-O2	6.30	122.68	118.90
33	A	214	C	C2-N1-C1'	6.30	125.73	118.80
1	a	510	C	N1-C2-O2	6.28	122.67	118.90
1	a	2055	C	C6-N1-C2	-6.27	117.79	120.30
1	a	239	C	N1-C2-O2	6.24	122.64	118.90
1	a	783	A	N3-C4-C5	-6.24	122.43	126.80
1	a	1670	C	C6-N1-C2	-6.24	117.81	120.30
1	a	835	C	C6-N1-C2	-6.23	117.81	120.30
1	a	343	C	C6-N1-C2	-6.21	117.82	120.30
2	b	37	C	C6-N1-C2	-6.20	117.82	120.30
1	a	2617	U	N3-C2-O2	-6.20	117.86	122.20
1	a	2232	C	C6-N1-C2	-6.20	117.82	120.30
1	a	815	C	N1-C2-O2	6.19	122.61	118.90
1	a	2283	C	C6-N1-C2	-6.17	117.83	120.30
1	a	2771	C	N1-C2-O2	6.17	122.60	118.90
1	a	318	C	N1-C2-O2	6.16	122.60	118.90
1	a	2043	C	C6-N1-C2	-6.16	117.84	120.30
1	a	2450	A	C5-C6-N6	6.15	128.62	123.70
1	a	2576	G	C5-C6-N1	6.14	114.57	111.50
1	a	2676	C	C6-N1-C2	-6.14	117.84	120.30
1	a	208	C	C6-N1-C2	-6.12	117.85	120.30
1	a	1843	C	C6-N1-C2	-6.12	117.85	120.30
1	a	2044	C	C5-C6-N1	6.12	124.06	121.00
1	a	2044	C	C6-N1-C2	-6.12	117.85	120.30
1	a	2403	C	N3-C2-O2	-6.11	117.62	121.90
1	a	555	G	N3-C4-N9	6.11	129.67	126.00
32	Z	71	C	C6-N1-C2	-6.11	117.86	120.30
1	a	209	C	C6-N1-C2	-6.10	117.86	120.30
1	a	1306	C	N1-C2-O2	6.09	122.56	118.90
1	a	1893	C	C6-N1-C2	-6.09	117.86	120.30
1	a	2456	C	C6-N1-C2	-6.09	117.86	120.30
1	a	383	C	N1-C2-O2	6.09	122.55	118.90
1	a	2880	C	N3-C2-O2	-6.09	117.64	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	2591	C	C6-N1-C2	-6.09	117.87	120.30
1	a	2720	U	N3-C2-O2	-6.08	117.94	122.20
1	a	669	G	C2-N3-C4	6.08	114.94	111.90
1	a	2556	C	N1-C2-O2	6.07	122.54	118.90
32	Z	75	C	C6-N1-C2	-6.07	117.87	120.30
1	a	1157	G	N3-C4-N9	6.06	129.63	126.00
1	a	799	G	N1-C6-O6	-6.05	116.27	119.90
1	a	946	C	N1-C2-O2	6.03	122.52	118.90
1	a	646	U	N3-C2-O2	-6.02	117.99	122.20
1	a	404	A	P-O3'-C3'	6.01	126.91	119.70
1	a	2626	C	N3-C2-O2	-6.01	117.69	121.90
32	Z	69	C	C5-C6-N1	6.01	124.00	121.00
1	a	2238	G	N3-C4-C5	-6.00	125.60	128.60
1	a	2848	G	O4'-C1'-N9	6.00	113.00	108.20
1	a	192	C	C6-N1-C2	-5.99	117.90	120.30
2	b	71	C	C6-N1-C2	-5.99	117.90	120.30
2	b	37	C	N3-C2-O2	-5.99	117.71	121.90
1	a	1985	C	N3-C2-O2	-5.98	117.71	121.90
1	a	516	C	C6-N1-C2	-5.98	117.91	120.30
1	a	2491	U	O5'-P-OP1	5.95	117.84	110.70
1	a	1993	U	N3-C2-O2	-5.95	118.03	122.20
1	a	225	C	N3-C2-O2	-5.95	117.74	121.90
1	a	779	U	N3-C2-O2	-5.94	118.04	122.20
1	a	2815	C	C6-N1-C2	-5.94	117.92	120.30
1	a	985	C	N1-C2-O2	5.93	122.46	118.90
1	a	2517	C	O4'-C1'-N1	5.93	112.94	108.20
1	a	1257	C	C6-N1-C2	-5.92	117.93	120.30
1	a	645	C	N1-C2-O2	5.92	122.45	118.90
1	a	574	A	O5'-P-OP1	-5.92	100.37	105.70
1	a	1643	G	N1-C6-O6	-5.91	116.35	119.90
1	a	1899	A	C8-N9-C4	-5.91	103.44	105.80
1	a	595	C	C6-N1-C2	-5.90	117.94	120.30
1	a	1352	U	N3-C2-O2	-5.90	118.07	122.20
1	a	1820	U	O5'-P-OP1	-5.90	100.39	105.70
1	a	459	U	C5-C6-N1	5.90	125.65	122.70
1	a	813	U	N1-C2-O2	5.89	126.93	122.80
1	a	698	C	N3-C4-C5	-5.89	119.54	121.90
1	a	2023	C	C5-C6-N1	5.88	123.94	121.00
1	a	813	U	N3-C2-O2	-5.88	118.08	122.20
1	a	1158	C	C6-N1-C2	-5.87	117.95	120.30
1	a	31	C	C6-N1-C2	-5.87	117.95	120.30
1	a	660	C	C6-N1-C2	-5.87	117.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	269	C	N3-C2-O2	-5.87	117.79	121.90
1	a	634	C	N1-C2-O2	5.87	122.42	118.90
1	a	748	G	O4'-C1'-N9	5.86	112.89	108.20
1	a	2619	C	C6-N1-C2	-5.86	117.96	120.30
1	a	2616	C	N1-C2-O2	5.86	122.41	118.90
1	a	2646	C	N1-C2-O2	5.85	122.41	118.90
1	a	1908	C	C6-N1-C2	-5.84	117.96	120.30
1	a	1314	C	N1-C2-O2	5.84	122.40	118.90
1	a	2238	G	C2-N3-C4	5.83	114.82	111.90
2	b	31	C	N1-C2-O2	5.83	122.40	118.90
1	a	193	U	N3-C2-O2	-5.83	118.12	122.20
1	a	1826	G	N1-C6-O6	-5.82	116.41	119.90
1	a	1547	C	N1-C2-O2	5.81	122.39	118.90
1	a	634	C	N3-C2-O2	-5.81	117.83	121.90
1	a	681	G	N9-C4-C5	-5.81	103.08	105.40
1	a	816	C	N3-C2-O2	-5.81	117.83	121.90
1	a	838	C	N3-C2-O2	-5.81	117.83	121.90
1	a	1021	A	C2-N3-C4	5.81	113.50	110.60
1	a	1627	G	C2-N3-C4	5.81	114.80	111.90
1	a	702	U	N3-C2-O2	-5.80	118.14	122.20
1	a	2243	U	C6-N1-C2	-5.80	117.52	121.00
1	a	563	A	C2-N3-C4	5.79	113.50	110.60
1	a	784	G	OP1-P-O3'	5.79	117.94	105.20
1	a	2430	A	O4'-C1'-N9	5.79	112.83	108.20
1	a	1741	C	C6-N1-C2	-5.78	117.99	120.30
1	a	811	U	N3-C2-O2	-5.78	118.16	122.20
1	a	16	C	C6-N1-C2	-5.78	117.99	120.30
33	A	1035	A	P-O3'-C3'	5.77	126.62	119.70
32	Z	74	C	N3-C2-O2	-5.76	117.86	121.90
1	a	1200	C	C6-N1-C2	-5.76	118.00	120.30
1	a	1833	C	C6-N1-C2	-5.75	118.00	120.30
1	a	937	C	C6-N1-C2	-5.75	118.00	120.30
1	a	758	C	C6-N1-C2	-5.75	118.00	120.30
1	a	1518	C	C6-N1-C2	-5.75	118.00	120.30
1	a	2027	G	N1-C6-O6	-5.74	116.45	119.90
32	Z	27	U	C6-N1-C1'	-5.74	113.17	121.20
33	A	438	U	O4'-C1'-N1	5.73	112.78	108.20
1	a	769	U	N3-C2-O2	-5.72	118.19	122.20
1	a	1153	C	N3-C2-O2	-5.72	117.90	121.90
1	a	2196	C	N3-C2-O2	-5.71	117.90	121.90
1	a	2282	G	O4'-C1'-N9	5.71	112.77	108.20
1	a	2466	C	N1-C2-O2	5.71	122.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1311	G	O4'-C1'-N9	5.71	112.77	108.20
1	a	2689	U	N3-C2-O2	-5.71	118.20	122.20
1	a	351	C	C5-C6-N1	5.70	123.85	121.00
1	a	991	C	C6-N1-C2	-5.70	118.02	120.30
33	A	872	A	O4'-C1'-N9	5.70	112.76	108.20
1	a	2394	C	C6-N1-C2	-5.69	118.02	120.30
1	a	786	C	N3-C2-O2	-5.69	117.92	121.90
1	a	946	C	N3-C2-O2	-5.69	117.92	121.90
1	a	1297	C	C6-N1-C2	-5.69	118.02	120.30
1	a	2395	C	C6-N1-C2	-5.69	118.02	120.30
1	a	2805	C	N1-C2-O2	5.68	122.31	118.90
33	A	1035	A	O4'-C1'-N9	5.67	112.74	108.20
1	a	2501	C	C6-N1-C1'	5.66	127.60	120.80
1	a	2516	A	N1-C2-N3	-5.66	126.47	129.30
1	a	2047	C	N3-C2-O2	-5.66	117.94	121.90
1	a	2870	C	C5-C6-N1	5.66	123.83	121.00
1	a	2616	C	N3-C2-O2	-5.64	117.95	121.90
1	a	1931	U	N3-C2-O2	-5.63	118.26	122.20
1	a	817	C	C6-N1-C2	-5.62	118.05	120.30
1	a	668	A	N9-C4-C5	-5.62	103.55	105.80
1	a	915	C	C6-N1-C2	-5.61	118.05	120.30
1	a	234	U	N1-C2-O2	5.61	126.73	122.80
1	a	2767	C	C6-N1-C2	-5.61	118.06	120.30
1	a	2447	G	C8-N9-C4	5.60	108.64	106.40
1	a	2703	C	C6-N1-C2	-5.60	118.06	120.30
1	a	1233	C	N1-C2-O2	5.60	122.26	118.90
1	a	1005	C	N3-C2-O2	-5.59	117.99	121.90
1	a	1135	C	N1-C2-O2	5.58	122.25	118.90
1	a	1836	C	C6-N1-C2	-5.58	118.07	120.30
1	a	1743	G	C5-C6-O6	-5.58	125.25	128.60
1	a	1670	C	N1-C2-O2	5.58	122.25	118.90
1	a	393	C	N3-C2-O2	-5.58	118.00	121.90
1	a	451	U	C5-C6-N1	-5.57	119.92	122.70
1	a	2200	C	N1-C2-O2	5.57	122.24	118.90
1	a	731	C	C6-N1-C2	-5.57	118.07	120.30
1	a	259	G	N1-C6-O6	-5.56	116.56	119.90
1	a	2043	C	N3-C2-O2	-5.56	118.01	121.90
33	A	792	A	O4'-C1'-N9	5.56	112.65	108.20
33	A	993	G	N3-C4-N9	5.55	129.33	126.00
1	a	692	C	C6-N1-C2	-5.55	118.08	120.30
1	a	2236	U	N1-C2-O2	5.55	126.69	122.80
1	a	1338	G	C5-C6-O6	5.55	131.93	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	687	C	N1-C2-O2	5.53	122.22	118.90
1	a	2689	U	N1-C2-O2	5.53	126.67	122.80
1	a	1378	A	N1-C2-N3	-5.53	126.53	129.30
1	a	640	C	C5-C6-N1	5.53	123.76	121.00
1	a	2023	C	N3-C2-O2	-5.52	118.03	121.90
1	a	2023	C	N1-C2-O2	5.51	122.21	118.90
1	a	2214	C	C6-N1-C2	-5.51	118.09	120.30
1	a	1836	C	N1-C2-O2	5.51	122.20	118.90
1	a	2055	C	C5-C6-N1	5.51	123.75	121.00
1	a	2016	U	C6-N1-C2	-5.50	117.70	121.00
1	a	2036	C	N1-C2-O2	5.50	122.20	118.90
1	a	2064	C	C6-N1-C2	-5.49	118.10	120.30
1	a	991	C	N3-C2-O2	-5.49	118.06	121.90
1	a	732	C	C6-N1-C2	-5.49	118.11	120.30
1	a	668	A	N1-C6-N6	5.49	121.89	118.60
2	b	28	C	C6-N1-C2	-5.48	118.11	120.30
1	a	2678	C	C6-N1-C2	-5.48	118.11	120.30
32	Y	65	C	C6-N1-C2	-5.48	118.11	120.30
1	a	2501	C	C2-N1-C1'	-5.48	112.77	118.80
1	a	2649	C	C5-C6-N1	5.48	123.74	121.00
1	a	2510	C	N1-C2-O2	5.47	122.18	118.90
1	a	407	G	C5-C6-O6	5.47	131.88	128.60
1	a	1314	C	N3-C2-O2	-5.46	118.08	121.90
1	a	723	C	N1-C2-O2	5.46	122.18	118.90
1	a	2806	C	C6-N1-C2	-5.46	118.11	120.30
1	a	1805	A	C2-N3-C4	5.46	113.33	110.60
2	b	17	C	N1-C2-O2	5.45	122.17	118.90
1	a	225	C	C6-N1-C2	-5.45	118.12	120.30
1	a	987	C	N1-C2-O2	5.45	122.17	118.90
1	a	392	U	N3-C2-O2	-5.44	118.39	122.20
1	a	984	A	N1-C6-N6	-5.44	115.34	118.60
32	Y	32	C	N3-C2-O2	-5.44	118.09	121.90
1	a	1611	C	C6-N1-C2	-5.44	118.12	120.30
2	b	91	C	N1-C2-O2	5.43	122.16	118.90
33	A	88	U	N1-C2-O2	5.43	126.61	122.80
1	a	451	U	C2-N1-C1'	-5.43	111.18	117.70
1	a	2450	A	N1-C2-N3	-5.43	126.59	129.30
1	a	1278	C	C6-N1-C2	-5.42	118.13	120.30
1	a	1533	C	N3-C2-O2	-5.41	118.11	121.90
1	a	1547	C	N3-C2-O2	-5.40	118.12	121.90
1	a	1975	G	C5-C6-N1	5.40	114.20	111.50
33	A	1305	G	O4'-C1'-N9	5.40	112.52	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1288	G	O4'-C1'-N9	5.40	112.52	108.20
1	a	1315	C	N3-C2-O2	-5.40	118.12	121.90
1	a	1229	C	C6-N1-C2	-5.40	118.14	120.30
1	a	1437	C	N3-C2-O2	-5.39	118.12	121.90
1	a	1956	U	N1-C2-O2	5.39	126.57	122.80
1	a	2575	C	C5-C6-N1	5.39	123.69	121.00
1	a	328	U	OP1-P-O3'	5.38	117.05	105.20
1	a	239	C	N3-C2-O2	-5.38	118.13	121.90
1	a	96	C	N1-C2-O2	5.38	122.13	118.90
1	a	417	C	N3-C2-O2	-5.37	118.14	121.90
1	a	671	C	N1-C2-O2	5.37	122.12	118.90
1	a	201	C	N1-C2-O2	5.37	122.12	118.90
1	a	2089	C	C6-N1-C2	-5.37	118.15	120.30
1	a	343	C	C5-C6-N1	5.37	123.68	121.00
1	a	404	A	OP2-P-O3'	5.36	117.00	105.20
1	a	1394	U	C5-C6-N1	5.36	125.38	122.70
1	a	2266	A	C2-N3-C4	5.36	113.28	110.60
1	a	417	C	N1-C2-O2	5.36	122.11	118.90
1	a	179	C	N1-C2-O2	5.36	122.11	118.90
1	a	2896	C	C6-N1-C2	-5.36	118.16	120.30
1	a	1771	C	C6-N1-C2	-5.35	118.16	120.30
1	a	1941	C	C6-N1-C2	-5.35	118.16	120.30
1	a	2001	C	C6-N1-C2	-5.35	118.16	120.30
1	a	417	C	C5-C6-N1	5.35	123.67	121.00
1	a	2591	C	N3-C2-O2	-5.34	118.16	121.90
1	a	481	G	O4'-C1'-N9	5.34	112.47	108.20
1	a	596	U	N1-C2-O2	5.34	126.53	122.80
1	a	671	C	N3-C2-O2	-5.33	118.17	121.90
1	a	353	C	N1-C2-O2	5.33	122.10	118.90
1	a	984	A	C2-N3-C4	5.33	113.26	110.60
1	a	2527	C	N1-C2-O2	5.33	122.09	118.90
1	a	1768	C	C6-N1-C2	-5.32	118.17	120.30
1	a	671	C	C6-N1-C2	-5.32	118.17	120.30
1	a	1994	C	C6-N1-C2	-5.32	118.17	120.30
1	a	634	C	C5-C6-N1	5.32	123.66	121.00
1	a	986	C	N1-C2-O2	5.32	122.09	118.90
1	a	2678	C	C2-N3-C4	5.32	122.56	119.90
1	a	758	C	C5-C6-N1	5.31	123.66	121.00
1	a	2765	A	N1-C6-N6	-5.31	115.42	118.60
1	a	964	C	C6-N1-C2	-5.30	118.18	120.30
1	a	1881	C	C6-N1-C2	-5.30	118.18	120.30
1	a	269	C	N1-C2-O2	5.30	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1558	C	C6-N1-C2	-5.30	118.18	120.30
1	a	318	C	N3-C2-O2	-5.30	118.19	121.90
1	a	2385	C	C6-N1-C2	-5.30	118.18	120.30
1	a	1837	C	C6-N1-C2	-5.29	118.18	120.30
32	Y	69	C	C6-N1-C2	-5.29	118.18	120.30
1	a	811	U	N3-C4-O4	-5.29	115.70	119.40
1	a	1394	U	C6-N1-C1'	5.29	128.60	121.20
1	a	961	C	C6-N1-C2	-5.29	118.19	120.30
1	a	2880	C	C6-N1-C2	-5.28	118.19	120.30
1	a	1575	C	C6-N1-C2	-5.28	118.19	120.30
1	a	2611	C	N3-C2-O2	-5.28	118.21	121.90
1	a	1779	U	N1-C2-O2	5.27	126.49	122.80
1	a	268	C	C6-N1-C2	-5.27	118.19	120.30
1	a	1612	C	C6-N1-C2	-5.27	118.19	120.30
1	a	2556	C	N3-C2-O2	-5.27	118.21	121.90
1	a	177	G	C8-N9-C4	-5.26	104.30	106.40
1	a	2064	C	N3-C4-C5	-5.26	119.80	121.90
1	a	1152	C	N1-C2-O2	5.25	122.05	118.90
1	a	418	C	N1-C2-O2	5.25	122.05	118.90
1	a	1476	U	N3-C2-O2	-5.25	118.52	122.20
1	a	1639	C	C6-N1-C2	-5.25	118.20	120.30
1	a	2027	G	C2-N3-C4	5.25	114.52	111.90
1	a	2206	C	C6-N1-C2	-5.25	118.20	120.30
1	a	2047	C	C6-N1-C2	-5.24	118.20	120.30
1	a	731	C	C5-C6-N1	5.24	123.62	121.00
1	a	1376	C	C6-N1-C2	-5.24	118.21	120.30
1	a	2558	C	C6-N1-C2	-5.24	118.21	120.30
1	a	635	C	N3-C2-O2	-5.23	118.24	121.90
32	Z	66	C	C6-N1-C2	-5.23	118.21	120.30
32	Y	69	C	N3-C2-O2	-5.23	118.24	121.90
1	a	2859	G	N3-C4-N9	5.22	129.13	126.00
32	Z	74	C	N1-C2-O2	5.22	122.03	118.90
1	a	1409	U	C5-C6-N1	5.22	125.31	122.70
1	a	2467	C	C6-N1-C2	-5.21	118.21	120.30
1	a	2391	G	C5-C6-N1	5.21	114.11	111.50
1	a	1351	C	N1-C2-O2	5.20	122.02	118.90
1	a	418	C	N3-C2-O2	-5.20	118.26	121.90
1	a	1836	C	N3-C2-O2	-5.20	118.26	121.90
1	a	2515	C	C6-N1-C2	-5.20	118.22	120.30
1	a	915	C	N3-C2-O2	-5.20	118.26	121.90
1	a	1774	C	C5-C6-N1	5.20	123.60	121.00
1	a	2026	U	C5-C6-N1	5.20	125.30	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	116	C	N3-C2-O2	-5.19	118.27	121.90
1	a	186	G	N1-C6-O6	-5.19	116.79	119.90
1	a	1005	C	N1-C2-O2	5.18	122.01	118.90
1	a	1153	C	N1-C2-O2	5.18	122.01	118.90
33	A	214	C	C5-C6-N1	5.18	123.59	121.00
1	a	76	C	N1-C2-O2	5.17	122.00	118.90
1	a	323	C	N1-C2-O2	5.17	122.00	118.90
1	a	1569	A	N1-C6-N6	-5.17	115.50	118.60
1	a	2443	C	N3-C2-O2	-5.17	118.28	121.90
1	a	1362	C	C6-N1-C2	-5.17	118.23	120.30
1	a	2446	G	N1-C6-O6	-5.17	116.80	119.90
1	a	748	G	C4-N9-C1'	-5.16	119.79	126.50
1	a	1122	G	C2-N3-C4	5.16	114.48	111.90
1	a	704	G	O4'-C1'-N9	5.15	112.32	108.20
1	a	692	C	C5-C6-N1	5.15	123.58	121.00
1	a	2795	C	C5-C6-N1	5.15	123.58	121.00
32	Y	71	C	C2-N1-C1'	5.15	124.47	118.80
1	a	2044	C	N1-C2-O2	5.15	121.99	118.90
1	a	2061	G	C8-N9-C4	5.15	108.46	106.40
1	a	540	C	N3-C2-O2	-5.14	118.30	121.90
1	a	1741	C	N3-C2-O2	-5.14	118.30	121.90
1	a	2594	C	C6-N1-C2	-5.14	118.24	120.30
1	a	635	C	C5-C6-N1	5.14	123.57	121.00
1	a	997	G	O5'-P-OP1	-5.14	101.07	105.70
33	A	88	U	N3-C2-O2	-5.14	118.60	122.20
1	a	115	C	N1-C2-O2	5.13	121.98	118.90
1	a	736	C	C6-N1-C2	-5.13	118.25	120.30
33	A	365	U	C2-N1-C1'	5.13	123.86	117.70
1	a	1352	U	C6-N1-C2	-5.13	117.92	121.00
1	a	1463	C	C6-N1-C2	-5.13	118.25	120.30
1	a	946	C	N3-C4-C5	-5.12	119.85	121.90
1	a	1159	U	N3-C2-O2	-5.12	118.61	122.20
32	Y	71	C	N3-C2-O2	-5.12	118.31	121.90
1	a	1786	A	O4'-C1'-N9	5.12	112.30	108.20
1	a	27	G	O4'-C1'-N9	5.12	112.30	108.20
1	a	2861	U	N3-C2-O2	-5.12	118.61	122.20
33	A	328	C	O4'-C1'-N1	5.12	112.30	108.20
1	a	1533	C	C6-N1-C2	-5.11	118.25	120.30
1	a	179	C	N3-C2-O2	-5.11	118.32	121.90
1	a	1547	C	C5-C6-N1	5.11	123.56	121.00
1	a	2235	G	C2-N3-C4	5.11	114.45	111.90
1	a	76	C	C6-N1-C2	-5.11	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	748	G	C8-N9-C1'	5.11	133.64	127.00
1	a	798	G	C2-N3-C4	5.10	114.45	111.90
1	a	681	G	C5-C6-O6	-5.10	125.54	128.60
1	a	1158	C	C5-C4-N4	5.10	123.77	120.20
1	a	2196	C	N1-C2-O2	5.09	121.96	118.90
1	a	833	A	C2-N3-C4	5.09	113.15	110.60
1	a	2645	G	O4'-C1'-N9	5.09	112.27	108.20
33	A	754	C	C2-N1-C1'	5.09	124.40	118.80
1	a	950	G	C5-C6-N1	5.08	114.04	111.50
1	a	2450	A	N1-C6-N6	-5.08	115.55	118.60
1	a	464	U	N3-C2-O2	-5.08	118.64	122.20
1	a	1547	C	C2-N1-C1'	5.08	124.39	118.80
1	a	2527	C	C6-N1-C2	-5.08	118.27	120.30
1	a	811	U	C5-C4-O4	5.08	128.94	125.90
1	a	1788	C	C5-C6-N1	5.08	123.54	121.00
1	a	1947	C	C6-N1-C2	-5.07	118.27	120.30
1	a	2875	C	C6-N1-C2	-5.07	118.27	120.30
1	a	1758	U	N3-C2-O2	-5.07	118.65	122.20
1	a	2403	C	C5-C6-N1	5.07	123.53	121.00
1	a	1434	A	O4'-C1'-N9	5.05	112.24	108.20
1	a	2822	G	C5-C6-O6	-5.05	125.57	128.60
33	A	1331	G	O4'-C1'-N9	5.05	112.24	108.20
1	a	946	C	C2-N3-C4	5.05	122.43	119.90
1	a	1986	C	C6-N1-C2	-5.05	118.28	120.30
1	a	2385	C	C5-C6-N1	5.05	123.53	121.00
1	a	337	C	C6-N1-C2	-5.04	118.28	120.30
1	a	1644	C	N1-C2-O2	5.04	121.93	118.90
1	a	2822	G	C5-C6-N1	5.04	114.02	111.50
1	a	130	C	N1-C2-O2	5.04	121.92	118.90
1	a	1289	C	N3-C2-O2	-5.04	118.37	121.90
1	a	1301	A	N1-C6-N6	-5.04	115.58	118.60
1	a	420	C	N1-C2-O2	5.04	121.92	118.90
1	a	2442	C	C6-N1-C2	-5.04	118.28	120.30
1	a	776	G	O4'-C1'-N9	-5.04	104.17	108.20
1	a	2463	C	N1-C2-O2	5.04	121.92	118.90
1	a	145	C	C6-N1-C2	-5.03	118.29	120.30
1	a	668	A	C5-C6-N6	-5.03	119.68	123.70
1	a	2050	C	N3-C4-N4	-5.03	114.48	118.00
2	b	91	C	C6-N1-C2	-5.03	118.29	120.30
1	a	678	C	N3-C4-C5	5.02	123.91	121.90
32	Z	69	C	C2-N1-C1'	5.02	124.32	118.80
1	a	986	C	C6-N1-C2	-5.02	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1768	C	C5-C6-N1	5.01	123.51	121.00
2	b	30	C	C6-N1-C2	-5.01	118.29	120.30
1	a	2747	G	C5-C6-O6	-5.01	125.59	128.60
2	b	38	C	N1-C2-O2	5.01	121.91	118.90
1	a	512	G	N1-C6-O6	-5.01	116.90	119.90
1	a	773	U	C5-C4-O4	-5.01	122.90	125.90
1	a	2617	U	N1-C2-O2	5.01	126.30	122.80
1	a	2806	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	g	46	ALA	Peptide
7	g	47	ASP	Peptide
8	h	34	GLY	Peptide
23	w	16	ASN	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
3	c	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
4	d	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	25	23
5	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
6	f	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
7	g	174/177 (98%)	158 (91%)	15 (9%)	1 (1%)	22	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
9	i	140/142 (99%)	140 (100%)	0	0	100	100
10	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
11	k	142/144 (99%)	137 (96%)	4 (3%)	1 (1%)	19	16
12	l	132/136 (97%)	129 (98%)	3 (2%)	0	100	100
13	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
14	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
15	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
16	p	115/118 (98%)	115 (100%)	0	0	100	100
17	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
18	r	108/110 (98%)	108 (100%)	0	0	100	100
19	s	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
20	t	100/104 (96%)	93 (93%)	6 (6%)	1 (1%)	13	9
21	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
22	v	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
23	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
24	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
25	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
26	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
27	0	49/55 (89%)	49 (100%)	0	0	100	100
28	1	44/46 (96%)	44 (100%)	0	0	100	100
29	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	3	36/38 (95%)	36 (100%)	0	0	100	100
31	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
34	B	222/241 (92%)	209 (94%)	13 (6%)	0	100	100
35	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
36	D	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
37	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
38	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
39	G	151/179 (84%)	138 (91%)	13 (9%)	0	100	100
40	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	I	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
42	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	13	9
43	K	113/129 (88%)	105 (93%)	8 (7%)	0	100	100
44	L	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
45	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
46	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
47	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
48	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
49	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
50	R	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
51	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
52	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
53	U	68/71 (96%)	68 (100%)	0	0	100	100
All	All	5487/5913 (93%)	5291 (96%)	191 (4%)	5 (0%)	50	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	k	36	LYS
7	g	47	ASP
42	J	57	VAL
20	t	99	ASN
4	d	149	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	216/218 (99%)	215 (100%)	1 (0%)	86	91
4	d	163/163 (100%)	160 (98%)	3 (2%)	54	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	165/165 (100%)	163 (99%)	2 (1%)	67	74
6	f	148/150 (99%)	148 (100%)	0	100	100
7	g	137/138 (99%)	135 (98%)	2 (2%)	60	67
8	h	32/114 (28%)	31 (97%)	1 (3%)	35	39
9	i	116/116 (100%)	115 (99%)	1 (1%)	75	82
10	j	104/104 (100%)	104 (100%)	0	100	100
11	k	103/103 (100%)	102 (99%)	1 (1%)	73	79
12	l	107/107 (100%)	107 (100%)	0	100	100
13	m	98/103 (95%)	97 (99%)	1 (1%)	73	79
14	n	86/87 (99%)	86 (100%)	0	100	100
15	o	99/100 (99%)	98 (99%)	1 (1%)	73	79
16	p	89/90 (99%)	88 (99%)	1 (1%)	70	77
17	q	84/84 (100%)	84 (100%)	0	100	100
18	r	93/93 (100%)	93 (100%)	0	100	100
19	s	80/84 (95%)	80 (100%)	0	100	100
20	t	83/85 (98%)	81 (98%)	2 (2%)	44	49
21	u	78/78 (100%)	78 (100%)	0	100	100
22	v	61/63 (97%)	61 (100%)	0	100	100
23	w	67/68 (98%)	66 (98%)	1 (2%)	60	67
24	x	54/55 (98%)	54 (100%)	0	100	100
25	y	48/49 (98%)	48 (100%)	0	100	100
26	z	47/48 (98%)	47 (100%)	0	100	100
27	0	46/49 (94%)	46 (100%)	0	100	100
28	1	38/38 (100%)	37 (97%)	1 (3%)	41	46
29	2	51/52 (98%)	49 (96%)	2 (4%)	27	29
30	3	34/34 (100%)	33 (97%)	1 (3%)	37	41
31	4	55/62 (89%)	52 (94%)	3 (6%)	18	16
34	B	186/199 (94%)	176 (95%)	10 (5%)	18	17
35	C	170/190 (90%)	163 (96%)	7 (4%)	26	27
36	D	172/173 (99%)	165 (96%)	7 (4%)	26	27
37	E	119/126 (94%)	116 (98%)	3 (2%)	42	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	F	90/116 (78%)	87 (97%)	3 (3%)	33	36
39	G	126/147 (86%)	117 (93%)	9 (7%)	12	10
40	H	104/105 (99%)	103 (99%)	1 (1%)	73	79
41	I	105/107 (98%)	98 (93%)	7 (7%)	13	11
42	J	86/90 (96%)	84 (98%)	2 (2%)	45	51
43	K	89/98 (91%)	87 (98%)	2 (2%)	47	53
44	L	102/103 (99%)	100 (98%)	2 (2%)	50	57
45	M	93/96 (97%)	88 (95%)	5 (5%)	18	17
46	N	83/84 (99%)	79 (95%)	4 (5%)	21	21
47	O	76/77 (99%)	70 (92%)	6 (8%)	10	7
48	P	65/65 (100%)	62 (95%)	3 (5%)	23	23
49	Q	73/78 (94%)	67 (92%)	6 (8%)	9	7
50	R	57/65 (88%)	54 (95%)	3 (5%)	19	18
51	S	72/79 (91%)	66 (92%)	6 (8%)	9	6
52	T	65/66 (98%)	63 (97%)	2 (3%)	35	39
53	U	60/61 (98%)	57 (95%)	3 (5%)	20	20
All	All	4575/4825 (95%)	4460 (98%)	115 (2%)	43	47

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	197	ASN
4	d	110	THR
4	d	116	LYS
4	d	128	ARG
5	e	69	ARG
5	e	163	ASN
7	g	30	ASN
7	g	73	ASN
8	h	20	ASN
9	i	123	LYS
11	k	29	LYS
13	m	2	ARG
15	o	89	ARG
16	p	81	ASN
20	t	53	ASN

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Mol	Chain	Res	Type
20	t	74	ASN
23	w	27	ARG
28	1	25	LYS
29	2	31	HIS
29	2	47	LYS
30	3	36	ARG
31	4	20	ASN
31	4	59	ARG
31	4	63	ARG
34	B	6	MET
34	B	23	TRP
34	B	63	ARG
34	B	81	LYS
34	B	87	CYS
34	B	105	LYS
34	B	146	ASN
34	B	188	ASP
34	B	194	ASP
34	B	197	ASP
35	C	49	LYS
35	C	79	LYS
35	C	132	ARG
35	C	135	LYS
35	C	178	LEU
35	C	185	ASN
35	C	206	GLU
36	D	8	LYS
36	D	29	ASP
36	D	48	LEU
36	D	148	LYS
36	D	190	ASP
36	D	194	ASP
36	D	198	HIS
37	E	23	LYS
37	E	64	MET
37	E	65	GLU
38	F	23	GLU
38	F	94	HIS
38	F	102	MET
39	G	9	GLN
39	G	11	LYS
39	G	15	ASP

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Mol	Chain	Res	Type
39	G	52	GLN
39	G	54	SER
39	G	78	ARG
39	G	106	GLU
39	G	125	SER
39	G	143	ARG
40	H	96	MET
41	I	6	TYR
41	I	22	LYS
41	I	37	GLN
41	I	41	ARG
41	I	60	LYS
41	I	62	ASP
41	I	90	TYR
42	J	7	ARG
42	J	85	ASP
43	K	56	ARG
43	K	96	THR
44	L	18	LYS
44	L	54	ARG
45	M	16	VAL
45	M	42	ASP
45	M	54	ASP
45	M	71	ARG
45	M	90	ARG
46	N	38	ASP
46	N	40	ASP
46	N	97	LYS
46	N	100	SER
47	O	2	SER
47	O	6	GLU
47	O	13	SER
47	O	26	GLU
47	O	61	SER
47	O	79	THR
48	P	8	ARG
48	P	63	GLN
48	P	77	GLU
49	Q	9	GLN
49	Q	41	THR
49	Q	62	ARG
49	Q	65	ARG

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Mol	Chain	Res	Type
49	Q	77	ARG
49	Q	81	LYS
50	R	12	ARG
50	R	36	SER
50	R	43	ARG
51	S	4	SER
51	S	17	LYS
51	S	25	SER
51	S	28	LYS
51	S	29	LYS
51	S	48	THR
52	T	24	ARG
52	T	59	ASP
53	U	5	LYS
53	U	22	SER
53	U	51	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	86	ASN
3	c	197	ASN
3	c	243	HIS
4	d	32	ASN
5	e	163	ASN
6	f	37	ASN
7	g	22	GLN
7	g	30	ASN
7	g	115	HIS
8	h	20	ASN
10	j	93	GLN
12	l	13	HIS
13	m	31	HIS
14	n	98	GLN
14	n	100	HIS
15	o	12	GLN
16	p	37	GLN
16	p	81	ASN
17	q	43	ASN
18	r	7	HIS
19	s	48	GLN
20	t	53	ASN

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Mol	Chain	Res	Type
20	t	74	ASN
21	u	49	ASN
21	u	87	GLN
22	v	57	HIS
23	w	20	HIS
26	z	6	ASN
29	2	31	HIS
31	4	20	ASN
34	B	93	ASN
34	B	120	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	2745/2904 (94%)	362 (13%)	0
2	b	118/120 (98%)	19 (16%)	0
32	Y	74/76 (97%)	20 (27%)	0
32	Z	74/76 (97%)	21 (28%)	1 (1%)
33	A	1513/1542 (98%)	190 (12%)	7 (0%)
54	X	14/28 (50%)	3 (21%)	1 (7%)
All	All	4538/4746 (95%)	615 (13%)	9 (0%)

All (615) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	A
1	a	15	G
1	a	34	U
1	a	42	A
1	a	45	G
1	a	50	U
1	a	51	G
1	a	58	G
1	a	63	A
1	a	71	A
1	a	74	A
1	a	75	G
1	a	80	G
1	a	84	A
1	a	101	A
1	a	102	U

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Mol	Chain	Res	Type
1	a	118	A
1	a	119	A
1	a	120	U
1	a	125	A
1	a	135	U
1	a	139	U
1	a	140	C
1	a	142	A
1	a	163	C
1	a	165	A
1	a	181	A
1	a	196	A
1	a	215	G
1	a	216	A
1	a	221	A
1	a	222	A
1	a	248	G
1	a	264	C
1	a	265	A
1	a	267	C
1	a	272	A
1	a	276	U
1	a	278	A
1	a	282	A
1	a	289	G
1	a	294	A
1	a	311	A
1	a	329	G
1	a	330	A
1	a	343	C
1	a	348	A
1	a	353	C
1	a	355	U
1	a	361	G
1	a	362	A
1	a	386	G
1	a	396	G
1	a	405	U
1	a	411	G
1	a	412	A
1	a	454	A
1	a	456	C

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Mol	Chain	Res	Type
1	a	481	G
1	a	491	G
1	a	504	A
1	a	505	A
1	a	508	A
1	a	509	C
1	a	530	G
1	a	531	C
1	a	532	A
1	a	544	C
1	a	545	U
1	a	546	U
1	a	547	A
1	a	548	G
1	a	549	G
1	a	550	C
1	a	563	A
1	a	573	U
1	a	575	A
1	a	586	A
1	a	603	A
1	a	614	A
1	a	615	U
1	a	627	A
1	a	637	A
1	a	645	C
1	a	647	G
1	a	654	A
1	a	655	A
1	a	686	U
1	a	721	A
1	a	722	A
1	a	723	C
1	a	730	A
1	a	747	5MU
1	a	765	C
1	a	775	G
1	a	776	G
1	a	782	A
1	a	784	G
1	a	785	G
1	a	805	G

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Mol	Chain	Res	Type
1	a	812	C
1	a	827	U
1	a	828	U
1	a	845	A
1	a	846	U
1	a	847	U
1	a	859	G
1	a	877	A
1	a	879	G
1	a	881	G
1	a	882	G
1	a	884	U
1	a	885	C
1	a	888	C
1	a	891	G
1	a	893	C
1	a	895	U
1	a	896	A
1	a	897	C
1	a	907	G
1	a	910	A
1	a	914	G
1	a	931	U
1	a	934	U
1	a	946	C
1	a	961	C
1	a	974	G
1	a	983	A
1	a	996	A
1	a	1005	C
1	a	1009	A
1	a	1010	A
1	a	1012	U
1	a	1013	C
1	a	1022	G
1	a	1033	U
1	a	1041	G
1	a	1042	G
1	a	1043	C
1	a	1045	C
1	a	1046	A
1	a	1047	G

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Mol	Chain	Res	Type
1	a	1051	G
1	a	1109	C
1	a	1110	G
1	a	1111	A
1	a	1112	G
1	a	1114	C
1	a	1115	G
1	a	1116	G
1	a	1117	C
1	a	1122	G
1	a	1130	U
1	a	1132	U
1	a	1133	A
1	a	1135	C
1	a	1142	A
1	a	1156	A
1	a	1169	A
1	a	1171	G
1	a	1178	C
1	a	1218	G
1	a	1247	A
1	a	1248	G
1	a	1250	G
1	a	1253	A
1	a	1256	G
1	a	1271	G
1	a	1272	A
1	a	1273	U
1	a	1300	G
1	a	1301	A
1	a	1329	U
1	a	1352	U
1	a	1365	A
1	a	1379	U
1	a	1383	A
1	a	1403	A
1	a	1409	U
1	a	1414	C
1	a	1415	U
1	a	1416	G
1	a	1419	A
1	a	1420	A

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Mol	Chain	Res	Type
1	a	1427	A
1	a	1428	C
1	a	1437	C
1	a	1451	C
1	a	1452	G
1	a	1453	A
1	a	1460	U
1	a	1482	G
1	a	1483	G
1	a	1485	U
1	a	1490	A
1	a	1493	C
1	a	1497	U
1	a	1504	A
1	a	1509	A
1	a	1515	A
1	a	1524	G
1	a	1529	G
1	a	1533	C
1	a	1535	A
1	a	1536	C
1	a	1559	U
1	a	1560	G
1	a	1566	A
1	a	1569	A
1	a	1578	U
1	a	1581	G
1	a	1584	U
1	a	1585	C
1	a	1586	A
1	a	1607	C
1	a	1608	A
1	a	1609	A
1	a	1647	U
1	a	1648	U
1	a	1674	G
1	a	1715	G
1	a	1728	C
1	a	1729	U
1	a	1730	C
1	a	1738	G
1	a	1744	A

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Mol	Chain	Res	Type
1	a	1764	C
1	a	1773	A
1	a	1782	U
1	a	1791	A
1	a	1800	C
1	a	1801	A
1	a	1808	A
1	a	1816	C
1	a	1829	A
1	a	1847	A
1	a	1858	A
1	a	1869	G
1	a	1870	C
1	a	1871	A
1	a	1872	A
1	a	1873	G
1	a	1876	A
1	a	1906	G
1	a	1907	G
1	a	1929	G
1	a	1930	G
1	a	1937	A
1	a	1938	A
1	a	1955	U
1	a	1967	C
1	a	1970	A
1	a	1971	U
1	a	1972	G
1	a	1991	U
1	a	1993	U
1	a	2020	A
1	a	2023	C
1	a	2031	A
1	a	2033	A
1	a	2043	C
1	a	2049	G
1	a	2055	C
1	a	2056	G
1	a	2060	A
1	a	2061	G
1	a	2062	A
1	a	2069	G7M

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Mol	Chain	Res	Type
1	a	2095	A
1	a	2096	C
1	a	2198	A
1	a	2204	G
1	a	2211	A
1	a	2223	G
1	a	2225	A
1	a	2238	G
1	a	2239	G
1	a	2268	A
1	a	2279	G
1	a	2283	C
1	a	2287	A
1	a	2294	G
1	a	2300	C
1	a	2304	G
1	a	2305	U
1	a	2308	G
1	a	2309	A
1	a	2321	U
1	a	2322	A
1	a	2325	G
1	a	2326	C
1	a	2328	A
1	a	2331	G
1	a	2333	A
1	a	2335	A
1	a	2336	A
1	a	2337	G
1	a	2345	G
1	a	2347	C
1	a	2350	C
1	a	2361	G
1	a	2367	G
1	a	2371	G
1	a	2379	G
1	a	2383	G
1	a	2385	C
1	a	2402	U
1	a	2406	A
1	a	2425	A
1	a	2429	G

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Mol	Chain	Res	Type
1	a	2435	A
1	a	2441	U
1	a	2448	A
1	a	2476	A
1	a	2478	A
1	a	2484	G
1	a	2491	U
1	a	2494	G
1	a	2502	G
1	a	2505	G
1	a	2518	A
1	a	2529	G
1	a	2535	G
1	a	2547	A
1	a	2554	U
1	a	2566	A
1	a	2567	G
1	a	2573	C
1	a	2602	A
1	a	2609	U
1	a	2610	C
1	a	2613	U
1	a	2629	U
1	a	2630	G
1	a	2639	A
1	a	2663	G
1	a	2682	A
1	a	2689	U
1	a	2690	U
1	a	2714	G
1	a	2726	A
1	a	2733	A
1	a	2744	G
1	a	2748	A
1	a	2765	A
1	a	2778	A
1	a	2792	A
1	a	2795	C
1	a	2797	U
1	a	2798	U
1	a	2799	A
1	a	2818	U

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Mol	Chain	Res	Type
1	a	2820	A
1	a	2821	A
1	a	2835	A
1	a	2873	A
1	a	2879	A
1	a	2883	A
1	a	2884	U
1	a	2891	U
1	a	2899	A
1	a	2902	C
2	b	21	G
2	b	24	G
2	b	31	C
2	b	35	C
2	b	36	C
2	b	56	G
2	b	62	C
2	b	64	G
2	b	65	U
2	b	66	A
2	b	67	G
2	b	68	C
2	b	88	C
2	b	89	U
2	b	90	C
2	b	99	A
2	b	105	G
2	b	108	A
2	b	109	A
32	Y	9	G
32	Y	13	C
32	Y	14	A
32	Y	19	G
32	Y	20	U
32	Y	21	A
32	Y	22	G
32	Y	29	G
32	Y	30	G
32	Y	31	G
32	Y	32	C
32	Y	36	U
32	Y	43	A

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Mol	Chain	Res	Type
32	Y	46	G
32	Y	47	U
32	Y	58	A
32	Y	59	A
32	Y	70	G
32	Y	73	A
32	Y	74	C
32	Z	9	G
32	Z	14	A
32	Z	17(A)	U
32	Z	19	G
32	Z	20	U
32	Z	21	A
32	Z	25	C
32	Z	27	U
32	Z	28	C
32	Z	29	G
32	Z	35	A
32	Z	36	U
32	Z	46	G
32	Z	47	U
32	Z	48	C
32	Z	52	G
32	Z	58	A
32	Z	61	C
32	Z	69	C
32	Z	71	C
32	Z	72	A
33	A	4	U
33	A	5	U
33	A	6	G
33	A	13	U
33	A	22	G
33	A	32	A
33	A	39	G
33	A	47	C
33	A	48	C
33	A	50	A
33	A	51	A
33	A	71	A
33	A	72	A
33	A	74	A

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Mol	Chain	Res	Type
33	A	84	U
33	A	85	U
33	A	86	G
33	A	87	C
33	A	88	U
33	A	96	U
33	A	122	G
33	A	131	A
33	A	141	G
33	A	143	A
33	A	144	G
33	A	164	G
33	A	166	U
33	A	182	A
33	A	183	C
33	A	197	A
33	A	200	G
33	A	201	G
33	A	202	G
33	A	204	G
33	A	226	G
33	A	240	G
33	A	245	U
33	A	247	G
33	A	251	G
33	A	266	G
33	A	267	C
33	A	280	C
33	A	289	G
33	A	321	A
33	A	328	C
33	A	347	G
33	A	352	C
33	A	354	G
33	A	367	U
33	A	372	C
33	A	373	A
33	A	384	G
33	A	398	U
33	A	406	G
33	A	411	A
33	A	412	A

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Mol	Chain	Res	Type
33	A	413	G
33	A	414	A
33	A	421	U
33	A	422	C
33	A	423	G
33	A	424	G
33	A	429	U
33	A	435	A
33	A	453	G
33	A	457	G
33	A	458	U
33	A	465	A
33	A	467	U
33	A	468	A
33	A	469	C
33	A	478	A
33	A	479	U
33	A	481	G
33	A	484	G
33	A	486	U
33	A	495	A
33	A	496	A
33	A	511	C
33	A	518	C
33	A	531	U
33	A	547	A
33	A	559	A
33	A	562	U
33	A	572	A
33	A	573	A
33	A	576	C
33	A	579	A
33	A	596	A
33	A	648	A
33	A	650	G
33	A	653	U
33	A	665	A
33	A	723	U
33	A	724	G
33	A	747	A
33	A	748	G
33	A	755	G

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Mol	Chain	Res	Type
33	A	774	G
33	A	777	A
33	A	793	U
33	A	794	A
33	A	815	A
33	A	817	C
33	A	832	G
33	A	874	G
33	A	890	G
33	A	902	G
33	A	914	A
33	A	926	G
33	A	934	C
33	A	935	A
33	A	936	C
33	A	960	U
33	A	966	2MG
33	A	969	A
33	A	971	G
33	A	975	A
33	A	976	G
33	A	977	A
33	A	984	C
33	A	994	A
33	A	1003	G
33	A	1004	A
33	A	1009	U
33	A	1027	C
33	A	1029	U
33	A	1030	U
33	A	1031	C
33	A	1032	G
33	A	1033	G
33	A	1034	G
33	A	1036	A
33	A	1039	G
33	A	1044	A
33	A	1046	A
33	A	1065	U
33	A	1085	U
33	A	1094	G
33	A	1095	U

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Mol	Chain	Res	Type
33	A	1101	A
33	A	1137	C
33	A	1139	G
33	A	1144	G
33	A	1154	G
33	A	1159	U
33	A	1169	A
33	A	1174	G
33	A	1184	G
33	A	1196	A
33	A	1197	A
33	A	1213	A
33	A	1227	A
33	A	1228	C
33	A	1238	A
33	A	1256	A
33	A	1258	G
33	A	1275	A
33	A	1280	A
33	A	1286	U
33	A	1287	A
33	A	1300	G
33	A	1302	C
33	A	1305	G
33	A	1317	C
33	A	1320	C
33	A	1340	A
33	A	1346	A
33	A	1353	G
33	A	1363	A
33	A	1370	G
33	A	1378	C
33	A	1379	G
33	A	1381	U
33	A	1397	C
33	A	1419	G
33	A	1432	G
33	A	1441	A
33	A	1451	U
33	A	1452	C
33	A	1453	G
33	A	1487	G

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Mol	Chain	Res	Type
33	A	1492	A
33	A	1497	G
33	A	1503	A
33	A	1506	U
33	A	1517	G
33	A	1529	G
33	A	1530	G
33	A	1534	A
54	X	24	A
54	X	25	C
54	X	27	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	Z	35	A
33	A	5	U
33	A	199	A
33	A	467	U
33	A	776	G
33	A	1026	G
33	A	1035	A
33	A	1114	C
54	X	24	A

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

41 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
33	2MG	A	966	33	18,26,27	0.92	1 (5%)	16,38,41	1.42	5 (31%)
1	5MU	a	1939	1	19,22,23	1.46	4 (21%)	27,32,35	2.35	8 (29%)
1	5MU	a	747	1	19,22,23	1.50	5 (26%)	27,32,35	2.15	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	4OC	A	1402	33	20,23,24	0.75	0	25,32,35	0.97	1 (4%)
1	3TD	a	1915	1	19,22,23	1.61	5 (26%)	23,32,35	2.20	4 (17%)
1	6MZ	a	2030	1	17,25,26	1.00	1 (5%)	15,36,39	2.56	4 (26%)
1	PSU	a	2504	58,1	18,21,22	1.73	5 (27%)	21,30,33	2.26	6 (28%)
1	H2U	a	2449	1	18,21,22	1.18	3 (16%)	19,30,33	1.04	2 (10%)
1	2MG	a	2445	1	18,26,27	1.24	2 (11%)	16,38,41	0.96	2 (12%)
1	OMC	a	2498	55,1	19,22,23	0.85	0	25,31,34	1.29	2 (8%)
12	4D4	l	81	12	9,11,12	1.91	3 (33%)	7,13,15	1.67	1 (14%)
33	PSU	A	516	33,55	18,21,22	1.38	3 (16%)	21,30,33	2.17	5 (23%)
33	5MC	A	1407	33	19,22,23	1.62	3 (15%)	26,32,35	1.30	3 (11%)
33	MA6	A	1519	33	19,26,27	1.00	1 (5%)	18,38,41	2.06	4 (22%)
1	2MG	a	1835	1	18,26,27	1.05	1 (5%)	16,38,41	1.43	5 (31%)
1	PSU	a	2605	1	18,21,22	1.52	5 (27%)	21,30,33	2.39	4 (19%)
1	6MZ	a	1618	1	17,25,26	0.92	0	15,36,39	2.50	4 (26%)
1	PSU	a	1917	1	18,21,22	1.44	3 (16%)	21,30,33	2.28	4 (19%)
1	PSU	a	2580	1	18,21,22	1.68	5 (27%)	21,30,33	2.41	6 (28%)
1	PSU	a	955	1	18,21,22	1.66	5 (27%)	21,30,33	2.20	5 (23%)
43	IAS	K	119	43	6,7,8	1.40	1 (16%)	3,8,10	0.94	0
33	G7M	A	527	33	20,26,27	1.15	2 (10%)	16,39,42	0.68	0
1	PSU	a	2457	1	18,21,22	1.65	5 (27%)	21,30,33	2.15	4 (19%)
1	PSU	a	2604	1	18,21,22	1.54	4 (22%)	21,30,33	1.98	5 (23%)
33	UR3	A	1498	33	19,22,23	0.90	0	26,32,35	1.97	5 (19%)
1	5MC	a	1962	1	19,22,23	1.34	3 (15%)	26,32,35	1.17	2 (7%)
1	PSU	a	746	55,1	18,21,22	1.57	5 (27%)	21,30,33	2.48	5 (23%)
32	8AN	Y	76	32,60,1	17,24,25	1.25	2 (11%)	13,35,38	1.09	1 (7%)
1	2MA	a	2503	55,58,1	17,25,26	1.02	1 (5%)	16,37,40	1.22	2 (12%)
1	OMU	a	2552	55,1	19,22,23	1.34	3 (15%)	25,31,34	1.72	5 (20%)
32	8AN	Z	76	32,60,55	17,24,25	1.18	2 (11%)	13,35,38	1.09	0
33	MA6	A	1518	33	19,26,27	0.86	0	18,38,41	2.03	3 (16%)
1	PSU	a	1911	1	18,21,22	1.47	3 (16%)	21,30,33	2.25	5 (23%)
1	G7M	a	2069	1	20,26,27	1.23	2 (10%)	16,39,42	0.89	1 (6%)
33	2MG	A	1516	33	18,26,27	0.96	1 (5%)	16,38,41	1.37	2 (12%)
4	MEQ	d	150	4	8,9,10	0.80	0	5,10,12	1.38	1 (20%)
33	5MC	A	967	33	19,22,23	1.41	3 (15%)	26,32,35	1.21	2 (7%)
33	2MG	A	1207	33	18,26,27	0.91	1 (5%)	16,38,41	1.21	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	D2T	L	89	44	8,9,10	2.01	3 (37%)	6,11,13	1.54	1 (16%)
1	OMG	a	2251	58,32,1	19,26,27	1.12	1 (5%)	21,38,41	1.05	2 (9%)
1	1MG	a	745	1	19,26,27	0.76	1 (5%)	18,39,42	1.18	2 (11%)

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
33	2MG	A	966	33	-	0/5/27/28	0/3/3/3
1	5MU	a	1939	1	-	0/7/25/26	0/2/2/2
1	5MU	a	747	1	-	0/7/25/26	0/2/2/2
33	4OC	A	1402	33	-	0/9/29/30	0/2/2/2
1	3TD	a	1915	1	-	0/7/25/26	0/2/2/2
1	6MZ	a	2030	1	-	2/5/27/28	0/3/3/3
1	PSU	a	2504	58,1	-	0/7/25/26	0/2/2/2
1	H2U	a	2449	1	-	0/7/38/39	0/2/2/2
1	2MG	a	2445	1	-	0/5/27/28	0/3/3/3
1	OMC	a	2498	55,1	-	0/9/27/28	0/2/2/2
12	4D4	l	81	12	-	1/11/12/14	-
33	PSU	A	516	33,55	-	0/7/25/26	0/2/2/2
33	5MC	A	1407	33	-	0/7/25/26	0/2/2/2
33	MA6	A	1519	33	-	1/7/29/30	0/3/3/3
1	2MG	a	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	a	2605	1	-	0/7/25/26	0/2/2/2
1	6MZ	a	1618	1	-	0/5/27/28	0/3/3/3
1	PSU	a	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	a	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	a	955	1	-	0/7/25/26	0/2/2/2
43	IAS	K	119	43	-	0/7/7/8	-
33	G7M	A	527	33	-	1/3/25/26	0/3/3/3
1	PSU	a	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	a	2604	1	-	0/7/25/26	0/2/2/2
33	UR3	A	1498	33	-	0/7/25/26	0/2/2/2
1	5MC	a	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	a	746	55,1	-	3/7/25/26	0/2/2/2
32	8AN	Y	76	32,60,1	-	0/3/25/26	0/3/3/3
1	2MA	a	2503	55,58,1	-	1/3/25/26	0/3/3/3
1	OMU	a	2552	55,1	-	0/9/27/28	0/2/2/2
32	8AN	Z	76	32,60,55	-	1/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	MA6	A	1518	33	-	0/7/29/30	0/3/3/3
1	PSU	a	1911	1	-	0/7/25/26	0/2/2/2
1	G7M	a	2069	1	-	1/3/25/26	0/3/3/3
33	2MG	A	1516	33	-	0/5/27/28	0/3/3/3
4	MEQ	d	150	4	-	5/8/9/11	-
33	5MC	A	967	33	-	0/7/25/26	0/2/2/2
33	2MG	A	1207	33	-	0/5/27/28	0/3/3/3
44	D2T	L	89	44	-	4/7/12/14	-
1	OMG	a	2251	58,32,1	-	0/5/27/28	0/3/3/3
1	1MG	a	745	1	-	0/3/25/26	0/3/3/3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	1407	5MC	C5-C4	5.75	1.48	1.44
33	A	967	5MC	C5-C4	4.77	1.47	1.44
1	a	1962	5MC	C5-C4	4.24	1.47	1.44
1	a	2251	OMG	C6-N1	-3.75	1.32	1.37
32	Y	76	8AN	C3'-N3'	-3.73	1.41	1.47
1	a	2457	PSU	C4-N3	-3.72	1.31	1.38
44	L	89	D2T	CB-CG	3.69	1.58	1.52
1	a	2504	PSU	C4-N3	-3.62	1.32	1.38
1	a	2445	2MG	C6-N1	-3.61	1.32	1.37
1	a	2552	OMU	C4-N3	-3.55	1.32	1.38
1	a	2580	PSU	C4-N3	-3.54	1.32	1.38
1	a	2069	G7M	C6-N1	-3.51	1.32	1.37
1	a	2504	PSU	C6-C5	3.43	1.39	1.35
1	a	2604	PSU	C4-N3	-3.42	1.32	1.38
1	a	746	PSU	C4-N3	-3.41	1.32	1.38
1	a	1915	3TD	C4-N3	-3.38	1.33	1.40
1	a	955	PSU	C4-N3	-3.35	1.32	1.38
33	A	527	G7M	C5-C4	3.34	1.45	1.39
1	a	1939	5MU	C4-N3	-3.31	1.32	1.38
32	Z	76	8AN	C3'-N3'	-3.27	1.42	1.47
1	a	955	PSU	C2-N1	-3.20	1.32	1.36
1	a	2605	PSU	C4-N3	-3.20	1.32	1.38
1	a	1915	3TD	C10-N3	3.19	1.52	1.47
1	a	1917	PSU	C4-N3	-3.16	1.32	1.38
33	A	516	PSU	C6-C5	3.16	1.38	1.35
1	a	1911	PSU	C4-N3	-3.12	1.33	1.38
1	a	1835	2MG	C6-N1	-3.11	1.33	1.37
1	a	2504	PSU	C2-N1	-3.06	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1939	5MU	C2-N3	-3.05	1.32	1.38
1	a	747	5MU	C4-N3	-3.05	1.33	1.38
44	L	89	D2T	CB-SB	3.03	1.85	1.82
1	a	2580	PSU	C2-N3	-3.02	1.32	1.37
1	a	2069	G7M	C5-C4	3.01	1.45	1.39
1	a	1917	PSU	C6-C5	3.00	1.38	1.35
33	A	1407	5MC	C6-C5	2.99	1.39	1.34
12	l	81	4D4	CZ-NE	2.95	1.39	1.33
1	a	2457	PSU	C2-N3	-2.94	1.32	1.37
1	a	2604	PSU	C2-N3	-2.94	1.32	1.37
1	a	2449	H2U	C2-N3	-2.93	1.32	1.38
1	a	1939	5MU	C6-N1	-2.90	1.33	1.38
1	a	2580	PSU	C2-N1	-2.79	1.33	1.36
33	A	516	PSU	C4-N3	-2.79	1.33	1.38
1	a	1911	PSU	C6-C5	2.79	1.38	1.35
1	a	1915	3TD	C6-C5	2.75	1.38	1.35
1	a	747	5MU	C2-N3	-2.75	1.33	1.38
33	A	967	5MC	C6-N1	-2.75	1.33	1.38
1	a	1962	5MC	C6-N1	-2.73	1.33	1.38
1	a	955	PSU	C2-N3	-2.73	1.33	1.37
1	a	747	5MU	C6-N1	-2.72	1.33	1.38
33	A	966	2MG	C6-N1	-2.72	1.33	1.37
1	a	747	5MU	C6-C5	2.71	1.39	1.34
1	a	746	PSU	C2-N3	-2.71	1.33	1.37
1	a	2449	H2U	C4-N3	-2.70	1.33	1.37
33	A	1207	2MG	C6-N1	-2.70	1.33	1.37
1	a	2552	OMU	C2-N3	-2.65	1.33	1.38
1	a	2605	PSU	C2-N3	-2.65	1.33	1.37
33	A	1516	2MG	C6-N1	-2.64	1.33	1.37
12	l	81	4D4	CZ-NH2	2.61	1.41	1.32
1	a	2605	PSU	C6-C5	2.59	1.38	1.35
33	A	527	G7M	C6-N1	-2.57	1.33	1.37
1	a	1915	3TD	C2-N1	-2.55	1.34	1.37
12	l	81	4D4	CD-NE	-2.53	1.40	1.46
1	a	2552	OMU	C5-C4	-2.52	1.38	1.43
1	a	2580	PSU	C6-C5	2.52	1.38	1.35
1	a	746	PSU	C6-C5	2.52	1.38	1.35
1	a	2504	PSU	C2-N3	-2.51	1.33	1.37
1	a	2604	PSU	C6-C5	2.50	1.38	1.35
1	a	1962	5MC	C6-C5	2.49	1.38	1.34
1	a	2504	PSU	C6-N1	-2.49	1.32	1.36
1	a	955	PSU	C6-C5	2.48	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	2457	PSU	C2-N1	-2.46	1.33	1.36
32	Y	76	8AN	C8-N7	-2.45	1.30	1.34
1	a	2457	PSU	C6-C5	2.45	1.38	1.35
1	a	2457	PSU	O4'-C1'	-2.45	1.40	1.43
1	a	2605	PSU	C2-N1	-2.45	1.33	1.36
1	a	1911	PSU	C2-N3	-2.44	1.33	1.37
33	A	1519	MA6	C6-C5	2.43	1.48	1.44
1	a	2445	2MG	C2-N1	-2.42	1.32	1.36
43	K	119	IAS	CB-CG	2.38	1.56	1.50
1	a	746	PSU	O4'-C1'	-2.37	1.40	1.43
1	a	2604	PSU	C2-N1	-2.37	1.33	1.36
1	a	746	PSU	C2-N1	-2.36	1.33	1.36
1	a	2503	2MA	C6-N1	-2.32	1.33	1.37
1	a	747	5MU	C4-C5	2.29	1.48	1.44
1	a	1939	5MU	C4-C5	2.29	1.48	1.44
1	a	955	PSU	C6-N1	-2.28	1.32	1.36
1	a	1917	PSU	C2-N3	-2.28	1.33	1.37
33	A	967	5MC	C6-C5	2.27	1.38	1.34
1	a	2580	PSU	C6-N1	-2.18	1.32	1.36
33	A	1407	5MC	C6-N1	-2.18	1.34	1.38
1	a	2605	PSU	C6-N1	-2.18	1.32	1.36
1	a	1915	3TD	C2-N3	-2.15	1.34	1.38
44	L	89	D2T	CB-CA	2.14	1.55	1.54
32	Z	76	8AN	C8-N7	-2.11	1.30	1.34
1	a	2030	6MZ	C6-C5	2.06	1.48	1.44
33	A	516	PSU	C2-N3	-2.05	1.34	1.37
1	a	745	1MG	C2-N1	2.02	1.40	1.37
1	a	2449	H2U	C2-N1	-2.00	1.32	1.35

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1915	3TD	N1-C2-N3	8.23	122.11	116.13
1	a	746	PSU	N1-C2-N3	8.04	123.65	115.17
33	A	1498	UR3	C4-N3-C2	-7.85	118.26	124.58
1	a	2605	PSU	N1-C2-N3	7.65	123.24	115.17
1	a	1618	6MZ	C2-N1-C6	7.54	122.46	116.60
1	a	2504	PSU	N1-C2-N3	7.37	122.94	115.17
1	a	1917	PSU	N1-C2-N3	6.96	122.51	115.17
1	a	2030	6MZ	C2-N1-C6	6.95	122.00	116.60
1	a	2580	PSU	N1-C2-N3	6.89	122.44	115.17
1	a	1911	PSU	N1-C2-N3	6.89	122.44	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	516	PSU	N1-C2-N3	6.68	122.22	115.17
33	A	1518	MA6	C2-N1-C6	6.36	123.08	116.84
1	a	2457	PSU	N1-C2-N3	6.32	121.84	115.17
1	a	1939	5MU	N3-C2-N1	6.25	123.03	114.89
1	a	747	5MU	N3-C2-N1	6.13	122.87	114.89
1	a	2604	PSU	N1-C2-N3	6.11	121.61	115.17
33	A	1519	MA6	C2-N1-C6	5.87	122.59	116.84
1	a	955	PSU	N1-C2-N3	5.76	121.25	115.17
1	a	1939	5MU	C4-N3-C2	-5.56	120.06	127.34
1	a	746	PSU	C4-N3-C2	-5.36	118.99	126.37
1	a	747	5MU	C4-N3-C2	-5.12	120.63	127.34
1	a	955	PSU	O2-C2-N1	-4.92	117.72	122.79
1	a	1917	PSU	C4-N3-C2	-4.91	119.61	126.37
1	a	2457	PSU	C4-N3-C2	-4.71	119.88	126.37
1	a	2605	PSU	C4-N3-C2	-4.63	120.00	126.37
1	a	1911	PSU	C4-N3-C2	-4.61	120.03	126.37
1	a	2580	PSU	C4-N3-C2	-4.58	120.06	126.37
1	a	2498	OMC	O2-C2-N3	-4.44	115.33	122.33
1	a	955	PSU	C4-N3-C2	-4.42	120.28	126.37
1	a	2552	OMU	C4-N3-C2	-4.38	121.18	126.61
33	A	516	PSU	C4-N3-C2	-4.36	120.36	126.37
33	A	1518	MA6	N3-C2-N1	-4.28	122.86	128.67
1	a	2030	6MZ	N3-C2-N1	-4.28	122.87	128.67
1	a	2552	OMU	N3-C2-N1	4.21	120.37	114.89
1	a	1618	6MZ	N3-C2-N1	-4.16	123.02	128.67
1	a	1962	5MC	C5-C6-N1	-4.14	118.82	123.31
1	a	1915	3TD	C4-N3-C2	-4.06	120.32	124.61
1	a	2604	PSU	C4-N3-C2	-4.03	120.82	126.37
12	l	81	4D4	CG-CD-NE	-4.00	100.91	111.88
1	a	1939	5MU	O2-C2-N1	-3.94	117.67	122.80
33	A	1519	MA6	N3-C2-N1	-3.89	123.39	128.67
1	a	2580	PSU	O2-C2-N1	-3.81	118.86	122.79
33	A	1407	5MC	C5-C6-N1	-3.77	119.21	123.31
33	A	516	PSU	O2-C2-N1	-3.77	118.90	122.79
33	A	967	5MC	C5-C6-N1	-3.76	119.23	123.31
1	a	1939	5MU	C5-C4-N3	3.72	118.56	115.32
1	a	1939	5MU	C5-C6-N1	-3.72	119.28	123.31
1	a	746	PSU	O2-C2-N1	-3.71	118.96	122.79
1	a	2552	OMU	C5-C4-N3	3.70	119.98	114.80
1	a	2580	PSU	C3'-C2'-C1'	3.68	106.04	101.69
1	a	2504	PSU	C4-N3-C2	-3.65	121.34	126.37
1	a	2030	6MZ	C4-C5-N7	-3.65	105.48	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1911	PSU	O2-C2-N1	-3.64	119.03	122.79
33	A	1498	UR3	C5-C4-N3	3.63	119.81	115.04
1	a	1917	PSU	O2-C2-N1	-3.60	119.08	122.79
1	a	747	5MU	C5-C4-N3	3.57	118.43	115.32
1	a	2504	PSU	O2-C2-N1	-3.56	119.11	122.79
1	a	2605	PSU	O2-C2-N1	-3.53	119.15	122.79
1	a	745	1MG	C8-N7-C5	3.49	108.50	102.55
1	a	747	5MU	O2-C2-N1	-3.43	118.33	122.80
33	A	1519	MA6	C4-C5-N7	-3.42	105.72	109.34
1	a	1939	5MU	O4-C4-C5	-3.36	121.08	124.92
1	a	2030	6MZ	C9-N6-C6	-3.32	119.77	122.85
1	a	2457	PSU	O2-C2-N1	-3.22	119.47	122.79
33	A	1407	5MC	C5-C4-N3	-3.14	118.54	121.75
33	A	1516	2MG	C8-N7-C5	3.13	107.87	102.55
1	a	955	PSU	C6-C5-C4	-3.02	116.14	118.17
1	a	2251	OMG	C8-N7-C5	2.99	107.64	102.55
32	Y	76	8AN	C5-C6-N6	2.98	124.85	120.31
1	a	747	5MU	C5-C6-N1	-2.94	120.12	123.31
33	A	1519	MA6	C1'-N9-C4	-2.94	121.48	126.64
1	a	1835	2MG	C8-N7-C5	2.90	107.48	102.55
1	a	1618	6MZ	C4-C5-N7	-2.88	106.30	109.34
1	a	2503	2MA	C5-C6-N1	2.87	119.47	114.12
1	a	2503	2MA	C8-N7-C5	2.85	107.40	102.55
1	a	1917	PSU	C5-C6-N1	-2.83	118.21	122.14
1	a	1915	3TD	C1'-C5-C4	2.78	121.83	117.61
1	a	2457	PSU	C5-C6-N1	-2.78	118.28	122.14
33	A	1207	2MG	C8-N7-C5	2.77	107.27	102.55
1	a	2552	OMU	O4-C4-C5	-2.74	120.44	125.16
1	a	1939	5MU	C5M-C5-C4	2.74	121.70	118.78
33	A	1407	5MC	O2-C2-N3	-2.71	118.06	122.33
1	a	2504	PSU	C6-N1-C2	-2.70	120.19	122.69
1	a	1911	PSU	C5-C6-N1	-2.70	118.39	122.14
33	A	966	2MG	C8-N7-C5	2.69	107.13	102.55
1	a	1939	5MU	C5M-C5-C6	-2.67	119.24	122.85
1	a	1911	PSU	C3'-C2'-C1'	2.66	104.83	101.69
1	a	746	PSU	C5-C6-N1	-2.64	118.47	122.14
1	a	747	5MU	O4-C4-C5	-2.61	121.93	124.92
1	a	2604	PSU	O2-C2-N1	-2.60	120.10	122.79
1	a	2069	G7M	O6-C6-N1	-2.57	117.57	120.62
44	L	89	D2T	OD1-CG-CB	-2.57	117.06	122.44
33	A	1498	UR3	C3U-N3-C2	2.56	121.79	117.33
1	a	2580	PSU	C5-C6-N1	-2.53	118.63	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	746	PSU	O2-C2-N3	-2.52	117.38	121.86
1	a	2449	H2U	C5-C4-N3	2.52	119.37	116.69
33	A	967	5MC	C5-C4-N3	-2.48	119.21	121.75
1	a	2251	OMG	C5-C6-N1	2.46	118.77	114.07
1	a	745	1MG	C5-C6-N1	2.43	117.47	113.96
1	a	2580	PSU	O2'-C2'-C1'	-2.43	105.45	111.21
1	a	2504	PSU	C6-C5-C4	-2.42	116.54	118.17
1	a	2498	OMC	O2-C2-N1	2.41	123.61	118.90
33	A	1518	MA6	C4-C5-N7	-2.40	106.80	109.34
1	a	2605	PSU	O2-C2-N3	-2.39	117.61	121.86
4	d	150	MEQ	OE1-CD-CG	-2.37	117.73	122.02
33	A	1516	2MG	C5-C6-N1	2.36	118.57	114.07
33	A	966	2MG	N1-C2-N2	2.33	118.94	116.56
1	a	1835	2MG	N1-C2-N2	2.29	118.90	116.56
1	a	955	PSU	C5-C6-N1	-2.29	118.96	122.14
33	A	966	2MG	C5-C6-N1	2.29	118.44	114.07
1	a	1835	2MG	N2-C2-N3	-2.28	117.61	120.51
33	A	1207	2MG	C5-C6-N1	2.28	118.41	114.07
1	a	1962	5MC	C5-C4-N3	-2.27	119.43	121.75
1	a	2445	2MG	C8-N7-C5	2.25	106.38	102.55
33	A	1498	UR3	C6-N1-C2	-2.25	119.96	121.80
1	a	747	5MU	C5M-C5-C4	2.24	121.17	118.78
1	a	2504	PSU	O2-C2-N3	-2.23	117.91	121.86
1	a	2604	PSU	C5-C6-N1	-2.20	119.09	122.14
1	a	1915	3TD	C5-C6-N1	-2.15	119.16	122.14
33	A	516	PSU	C5-C6-N1	-2.13	119.18	122.14
33	A	516	PSU	O4'-C1'-C2'	2.13	108.10	105.15
1	a	2445	2MG	C5-C6-N1	2.13	118.13	114.07
1	a	1835	2MG	C5-C6-N1	2.11	118.10	114.07
33	A	966	2MG	O6-C6-C5	-2.11	120.14	124.32
33	A	1402	4OC	C6-C5-C4	2.10	119.53	117.00
1	a	2552	OMU	O2-C2-N1	-2.07	120.10	122.80
1	a	1618	6MZ	C9-N6-C6	-2.06	120.94	122.85
1	a	747	5MU	C6-N1-C2	-2.05	119.26	121.30
1	a	1835	2MG	O6-C6-C5	-2.04	120.28	124.32
33	A	1498	UR3	C1'-N1-C2	2.02	120.35	117.04
33	A	966	2MG	N2-C2-N3	-2.02	117.94	120.51
1	a	2449	H2U	N3-C2-N1	2.02	118.68	116.65
1	a	2604	PSU	O2-C2-N3	-2.01	118.29	121.86

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	d	150	MEQ	C-CA-CB-CG
32	Z	76	8AN	C4'-C5'-O5'-P
44	L	89	D2T	CA-CB-CG-OD1
44	L	89	D2T	CA-CB-CG-OD2
1	a	746	PSU	O4'-C1'-C5-C6
4	d	150	MEQ	NE2-CD-CG-CB
4	d	150	MEQ	OE1-CD-CG-CB
1	a	2030	6MZ	O4'-C4'-C5'-O5'
1	a	2030	6MZ	C3'-C4'-C5'-O5'
33	A	1519	MA6	O4'-C4'-C5'-O5'
1	a	746	PSU	O4'-C1'-C5-C4
4	d	150	MEQ	CA-CB-CG-CD
44	L	89	D2T	SB-CB-CG-OD2
4	d	150	MEQ	OE1-CD-NE2-CE
44	L	89	D2T	CG-CB-SB-CB1
1	a	746	PSU	C2'-C1'-C5-C6
1	a	2503	2MA	C4'-C5'-O5'-P
12	l	81	4D4	O-C-CA-CB
33	A	527	G7M	C4'-C5'-O5'-P
1	a	2069	G7M	C4'-C5'-O5'-P

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 354 ligands modelled in this entry, 333 are monoatomic - leaving 21 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	$\# Z  > 2$
56	SPD	A	1693	-	9,9,9	0.17	0	8,8,8	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	SPD	a	6210	-	9,9,9	0.32	0	8,8,8	0.63	0
56	SPD	a	6213	-	9,9,9	0.28	0	8,8,8	0.60	0
56	SPD	a	6205	-	9,9,9	0.35	0	8,8,8	0.82	0
56	SPD	a	6218	-	9,9,9	0.34	0	8,8,8	0.69	0
56	SPD	a	6214	-	9,9,9	0.32	0	8,8,8	0.62	0
56	SPD	a	6221	-	9,9,9	0.67	0	8,8,8	0.70	0
56	SPD	a	6211	-	9,9,9	0.31	0	8,8,8	0.73	0
56	SPD	a	6207	-	9,9,9	0.28	0	8,8,8	0.67	0
57	SPM	a	6219	-	13,13,13	0.40	0	12,12,12	0.76	0
60	MET	Z	101	32	6,7,8	0.44	0	2,7,9	0.18	0
56	SPD	a	6215	-	9,9,9	0.45	0	8,8,8	0.94	0
56	SPD	a	6216	-	9,9,9	0.31	0	8,8,8	0.73	0
56	SPD	a	6208	-	9,9,9	0.35	0	8,8,8	0.72	0
56	SPD	a	6212	-	9,9,9	0.26	0	8,8,8	0.85	0
56	SPD	a	6209	-	9,9,9	0.29	0	8,8,8	0.62	0
56	SPD	a	6206	-	9,9,9	0.33	0	8,8,8	0.87	0
61	PAR	A	1601	-	44,45,45	0.56	0	63,67,67	0.84	1 (1%)
56	SPD	a	6217	-	9,9,9	0.38	0	8,8,8	0.96	0
60	MET	Y	101	32	6,7,8	0.87	0	2,7,9	0.50	0
56	SPD	a	6220	-	9,9,9	0.33	0	8,8,8	0.74	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
56	SPD	A	1693	-	-	1/7/7/7	-
56	SPD	a	6210	-	-	3/7/7/7	-
56	SPD	a	6213	-	-	5/7/7/7	-
56	SPD	a	6205	-	-	2/7/7/7	-
56	SPD	a	6218	-	-	3/7/7/7	-
56	SPD	a	6214	-	-	3/7/7/7	-
56	SPD	a	6221	-	-	1/7/7/7	-
56	SPD	a	6211	-	-	3/7/7/7	-
56	SPD	a	6207	-	-	4/7/7/7	-
57	SPM	a	6219	-	-	2/11/11/11	-
60	MET	Z	101	32	-	1/5/6/8	-
56	SPD	a	6215	-	-	3/7/7/7	-
56	SPD	a	6216	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SPD	a	6208	-	-	2/7/7/7	-
56	SPD	a	6212	-	-	2/7/7/7	-
56	SPD	a	6209	-	-	1/7/7/7	-
56	SPD	a	6206	-	-	1/7/7/7	-
61	PAR	A	1601	-	-	3/18/94/94	0/4/4/4
56	SPD	a	6217	-	-	1/7/7/7	-
60	MET	Y	101	32	-	1/5/6/8	-
56	SPD	a	6220	-	-	4/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	A	1601	PAR	C53-C43-C33	-2.31	107.58	114.84

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	a	6220	SPD	C8-C7-N6-C5
60	Z	101	MET	O-C-CA-CB
61	A	1601	PAR	O54-C54-C64-N64
57	a	6219	SPM	C2-C3-C4-N5
56	a	6208	SPD	C3-C4-C5-N6
56	a	6215	SPD	C3-C4-C5-N6
56	a	6213	SPD	C3-C4-C5-N6
60	Y	101	MET	CA-CB-CG-SD
56	a	6220	SPD	N6-C7-C8-C9
56	a	6217	SPD	N6-C7-C8-C9
56	a	6218	SPD	N6-C7-C8-C9
56	a	6210	SPD	C2-C3-C4-C5
56	a	6207	SPD	C2-C3-C4-C5
56	a	6210	SPD	C8-C7-N6-C5
56	a	6220	SPD	C4-C5-N6-C7
56	a	6212	SPD	C8-C7-N6-C5
56	a	6214	SPD	C8-C7-N6-C5
56	a	6221	SPD	C4-C5-N6-C7
56	a	6212	SPD	N1-C2-C3-C4
56	a	6215	SPD	C8-C7-N6-C5
56	a	6207	SPD	C3-C4-C5-N6

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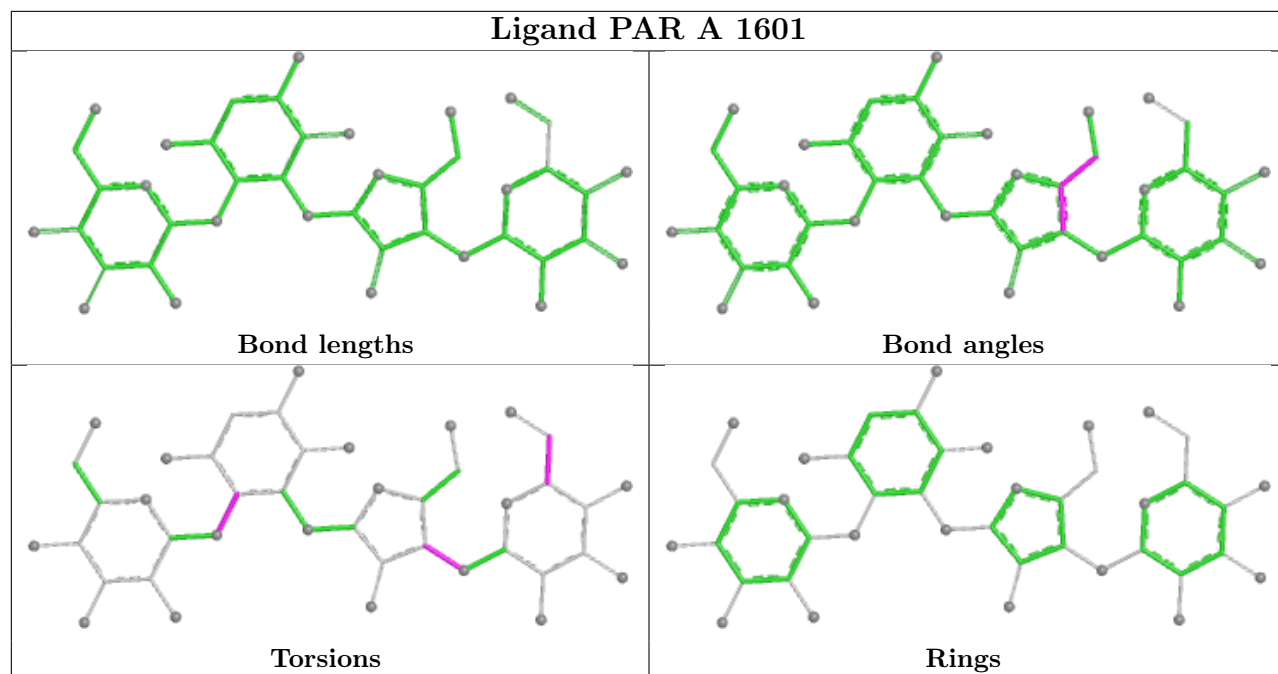
*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
56	a	6218	SPD	C2-C3-C4-C5
56	a	6214	SPD	C3-C4-C5-N6
56	a	6207	SPD	C8-C7-N6-C5
56	a	6211	SPD	C8-C7-N6-C5
56	a	6220	SPD	C2-C3-C4-C5
56	a	6206	SPD	C3-C4-C5-N6
56	a	6208	SPD	C7-C8-C9-N10
56	a	6210	SPD	C4-C5-N6-C7
57	a	6219	SPM	N5-C6-C7-C8
56	a	6205	SPD	N1-C2-C3-C4
56	a	6211	SPD	C2-C3-C4-C5
56	a	6211	SPD	N1-C2-C3-C4
56	a	6207	SPD	N1-C2-C3-C4
56	a	6209	SPD	C2-C3-C4-C5
56	a	6213	SPD	N6-C7-C8-C9
56	a	6213	SPD	C4-C5-N6-C7
56	a	6213	SPD	C2-C3-C4-C5
61	A	1601	PAR	C52-C42-O11-C11
56	a	6213	SPD	N1-C2-C3-C4
56	a	6205	SPD	C7-C8-C9-N10
56	a	6215	SPD	C4-C5-N6-C7
56	A	1693	SPD	C4-C5-N6-C7
61	A	1601	PAR	C23-C33-O33-C14
56	a	6214	SPD	N1-C2-C3-C4
56	a	6218	SPD	C4-C5-N6-C7

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

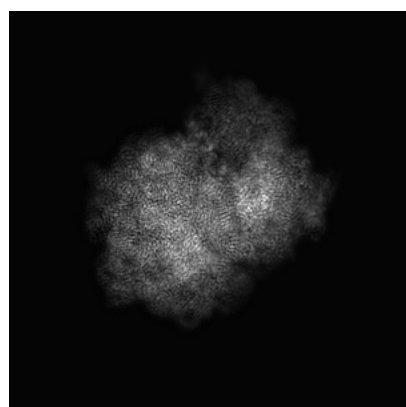
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28254. These allow visual inspection of the internal detail of the map and identification of artifacts.

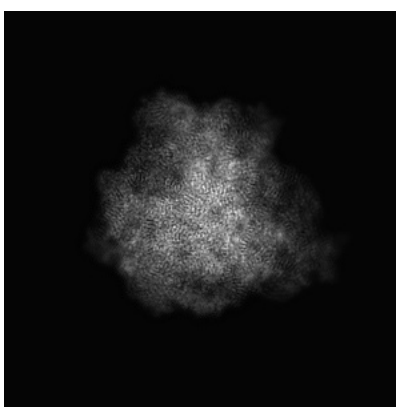
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

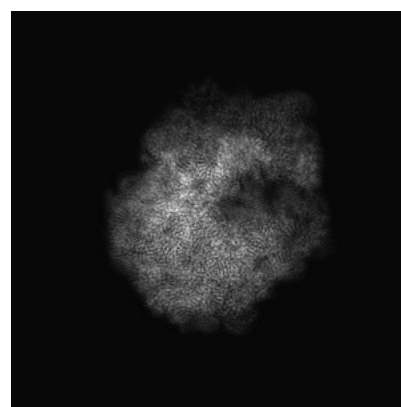
#### 6.1.1 Primary map



X



Y

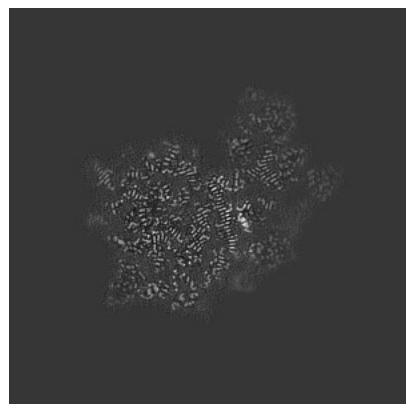


Z

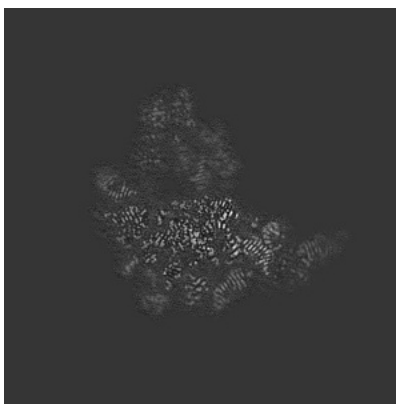
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

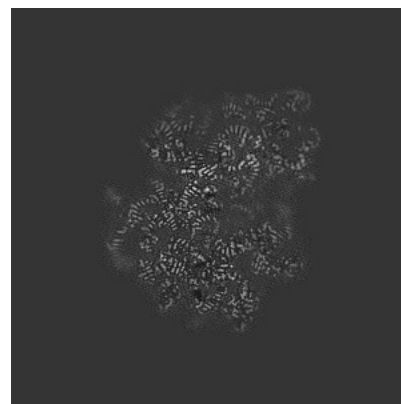
#### 6.2.1 Primary map



X Index: 228



Y Index: 228

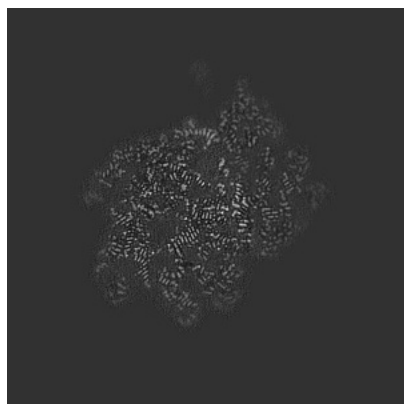


Z Index: 228

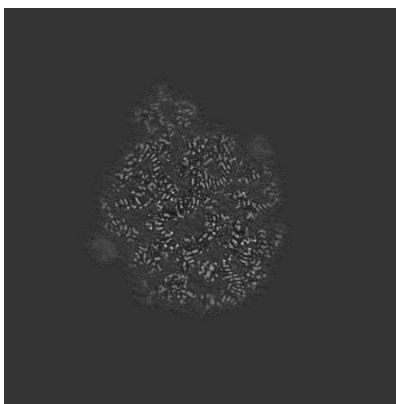
The images above show central slices of the map in three orthogonal directions.

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

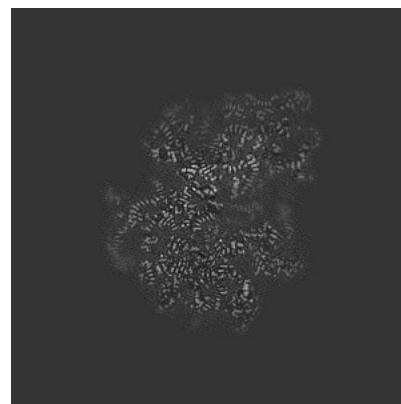
### 6.3.1 Primary map



X Index: 199



Y Index: 188

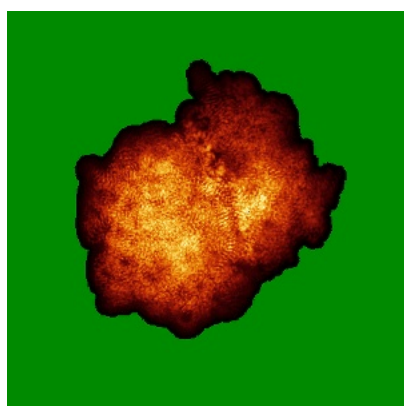


Z Index: 227

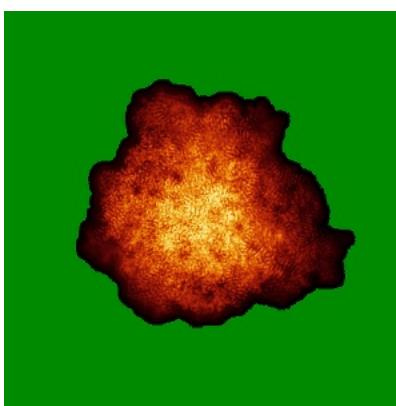
The images above show the largest variance slices of the map in three orthogonal directions.

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

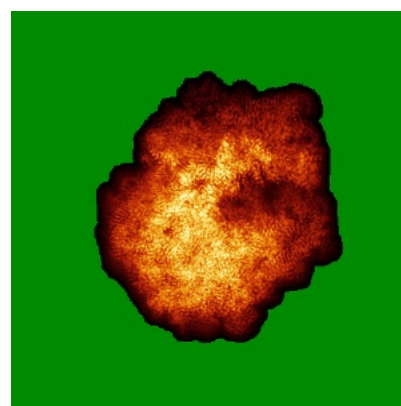
### 6.4.1 Primary map



X



Y

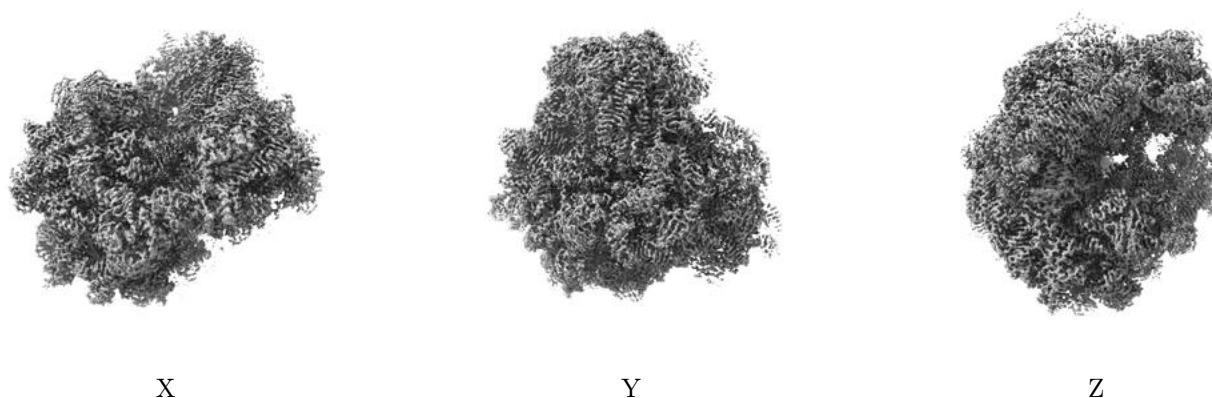


Z

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 0.0151. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

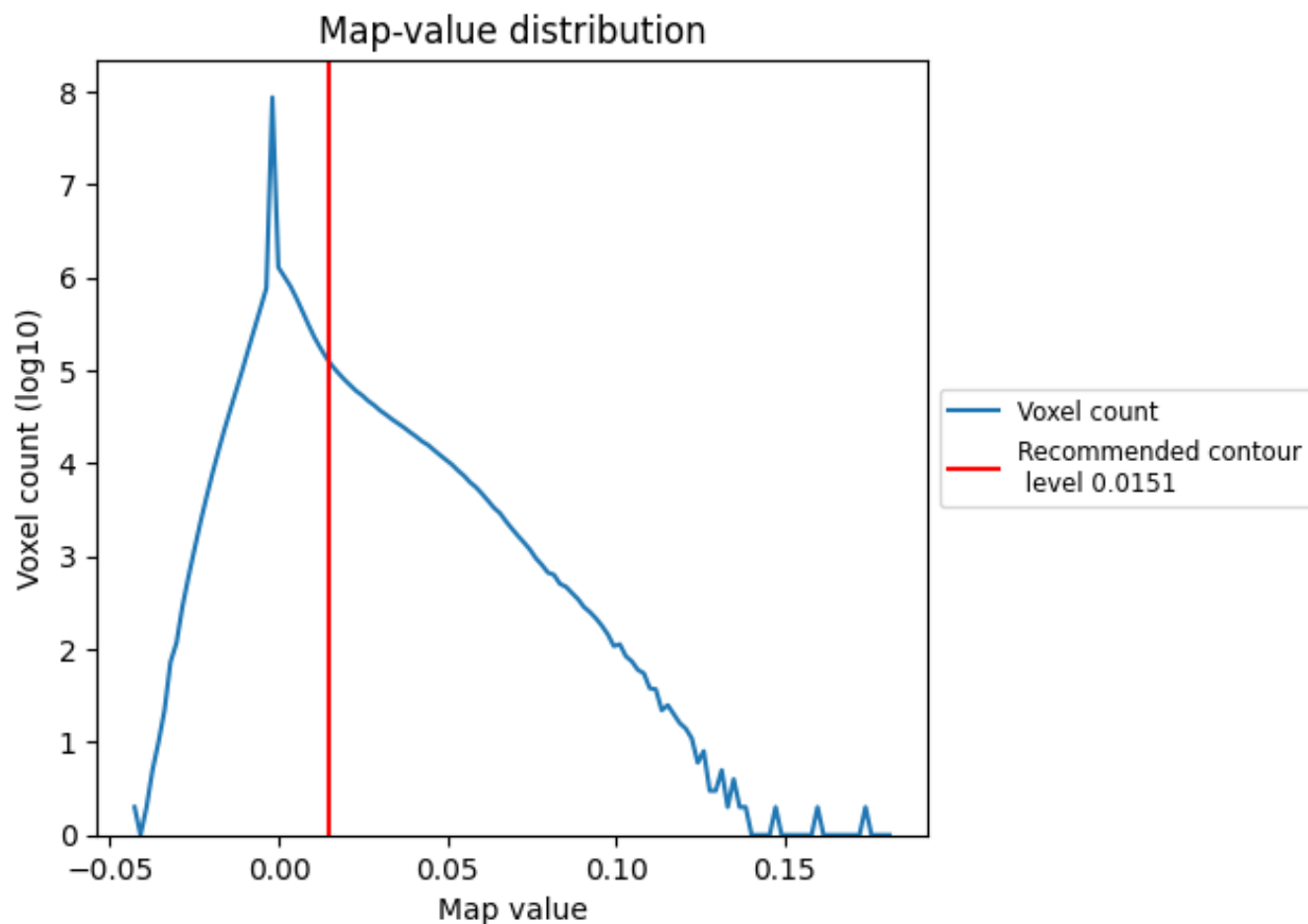
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

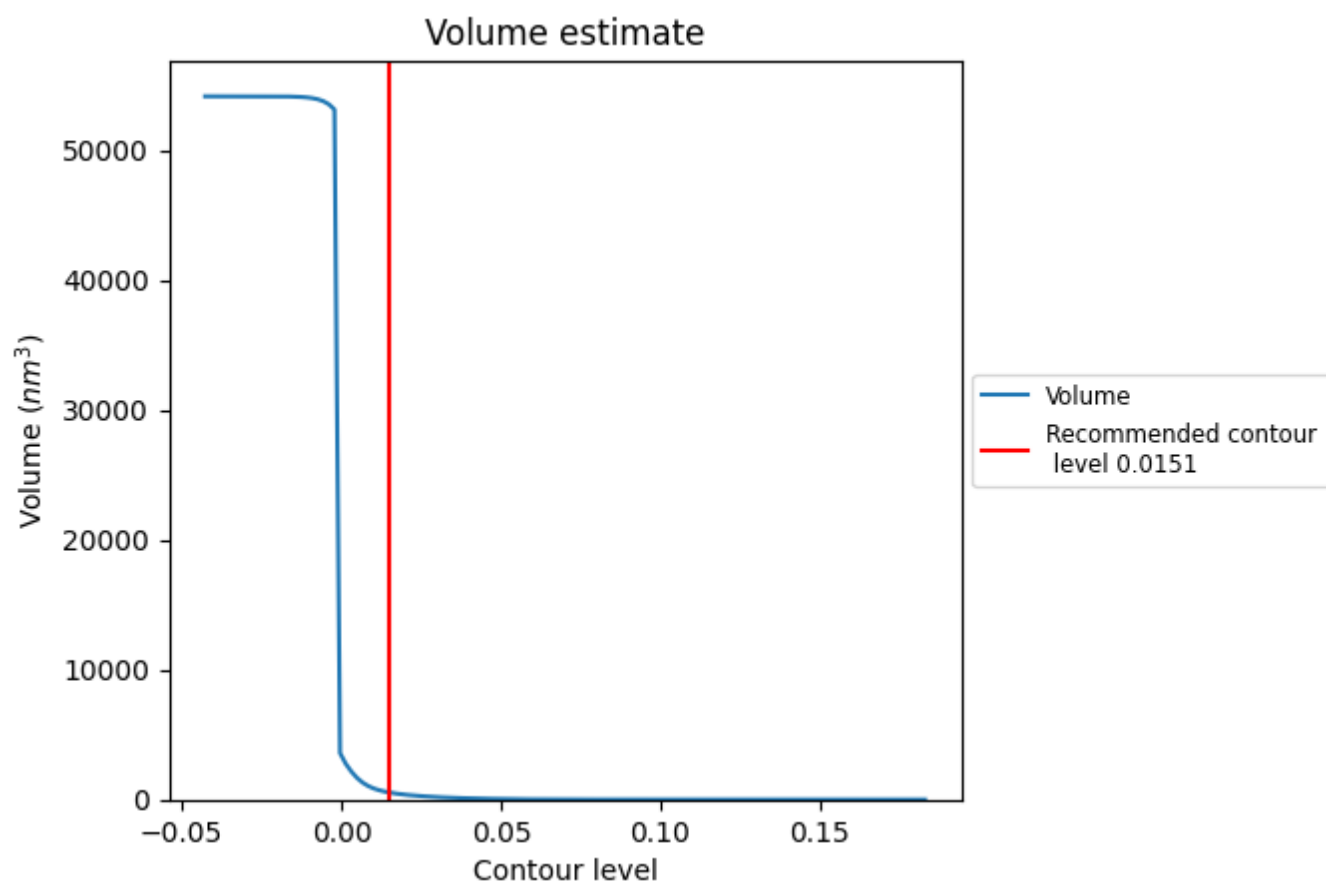
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

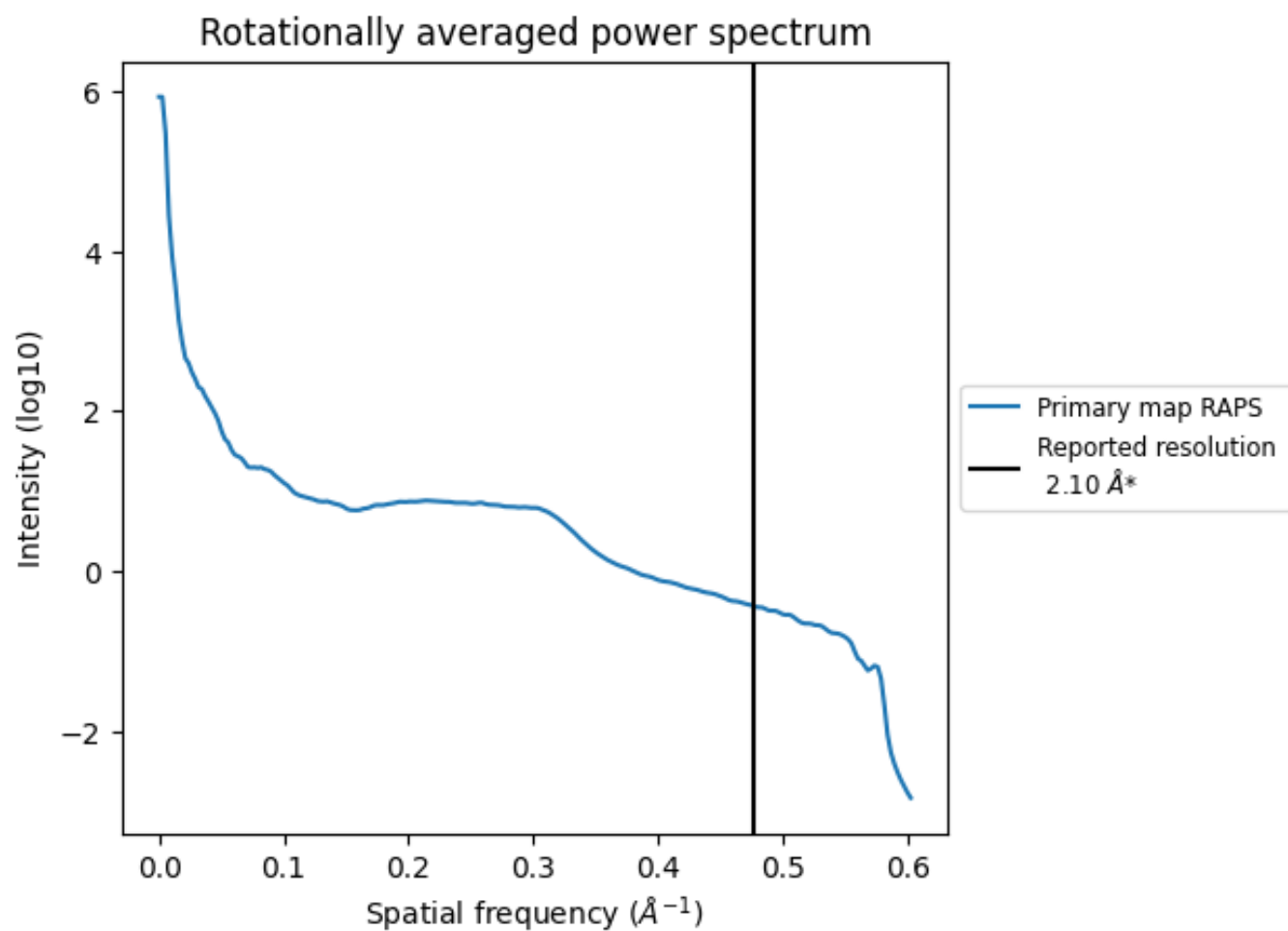
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 544 nm<sup>3</sup>; this corresponds to an approximate mass of 491 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.476 Å<sup>-1</sup>



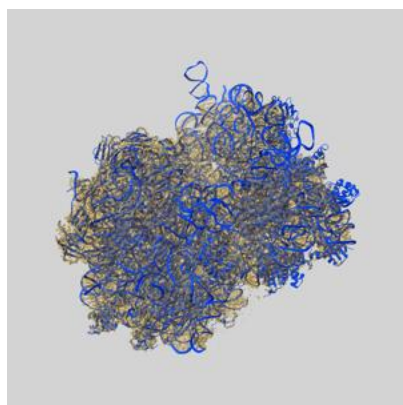
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

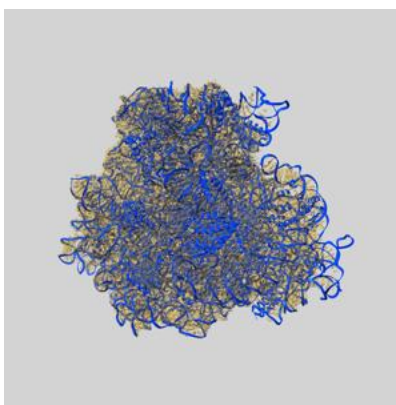
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28254 and PDB model 8EMM. Per-residue inclusion information can be found in section [3](#) on page [19](#).

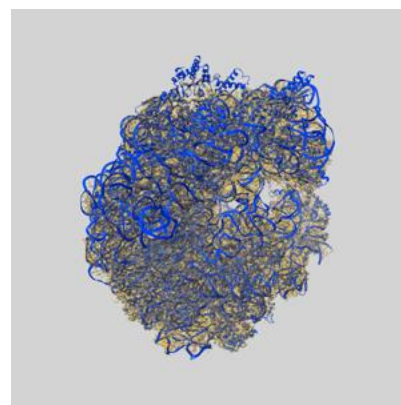
### 9.1 Map-model overlay [i](#)



X



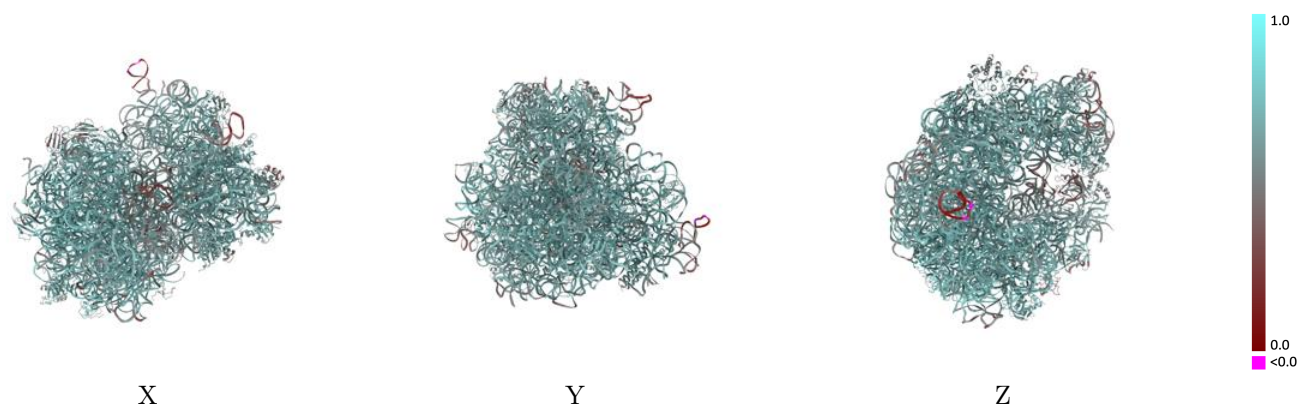
Y



Z

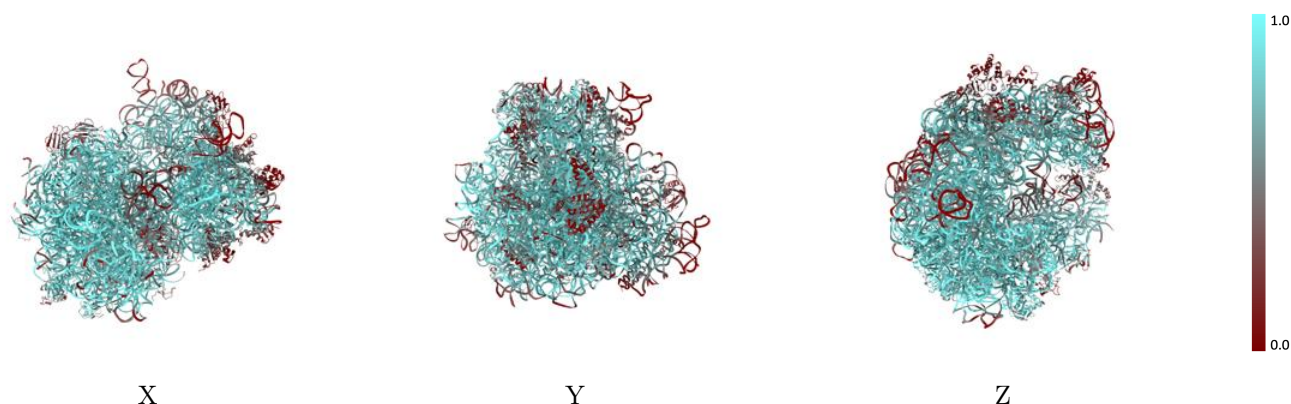
The images above show the 3D surface view of the map at the recommended contour level 0.0151 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



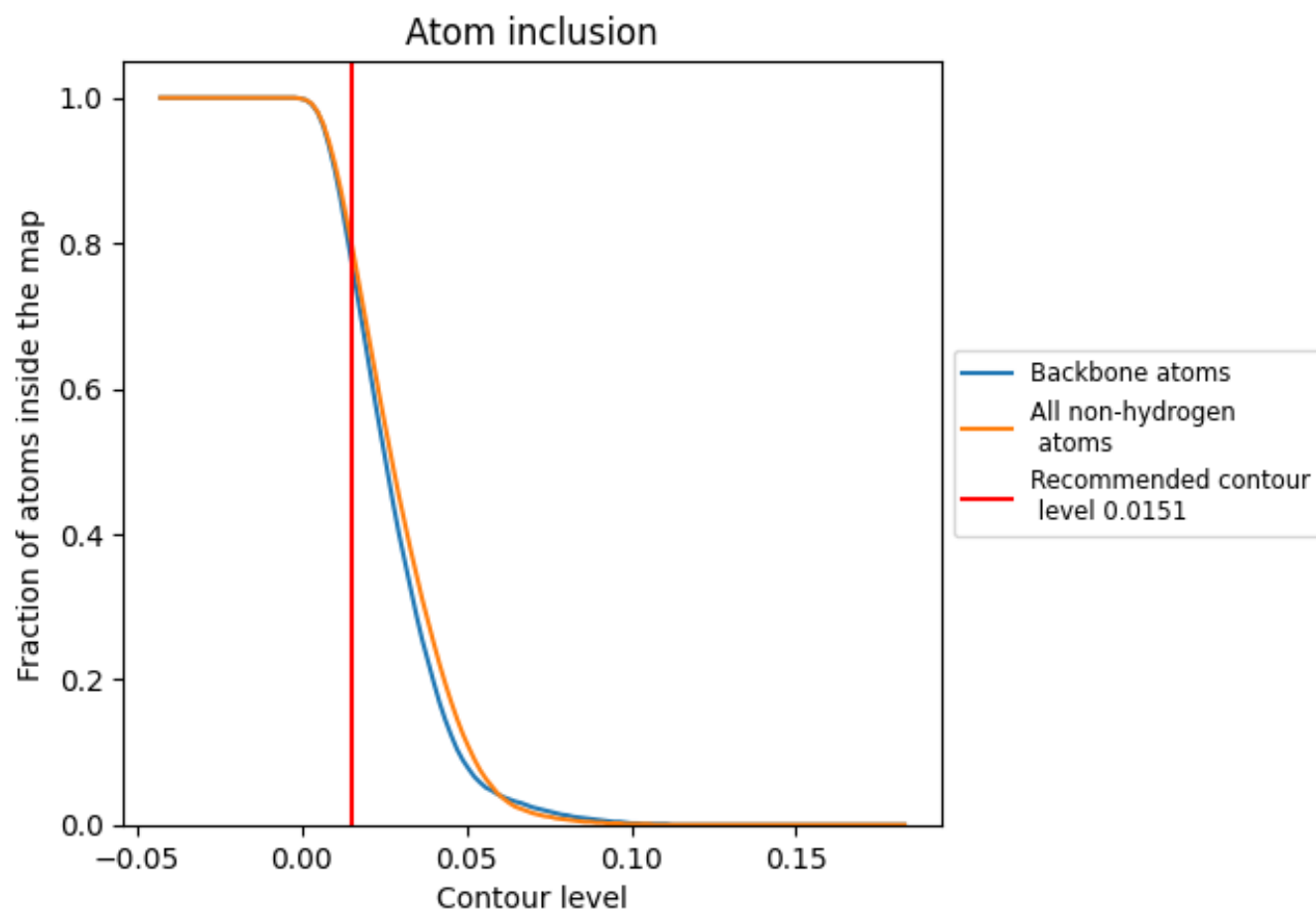
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0151).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ











































The table lists the average atom inclusion at the recommended contour level (0.0151) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8030	 0.6780
0	 0.7680	 0.6840
1	 0.9610	 0.7610
2	 0.9670	 0.7630
3	 0.8940	 0.7060
4	 0.4360	 0.4880
A	 0.7930	 0.6540
B	 0.1610	 0.5710
C	 0.5780	 0.6590
D	 0.3150	 0.6240
E	 0.6570	 0.6810
F	 0.4910	 0.6250
G	 0.3930	 0.6110
H	 0.6710	 0.6900
I	 0.5490	 0.6470
J	 0.4000	 0.5940
K	 0.6000	 0.6650
L	 0.7020	 0.7010
M	 0.8010	 0.6190
N	 0.7230	 0.6560
O	 0.7620	 0.6610
P	 0.5640	 0.6510
Q	 0.4270	 0.6300
R	 0.5870	 0.6700
S	 0.7040	 0.6320
T	 0.5020	 0.6370
U	 0.2990	 0.5950
X	 0.8730	 0.5770
Y	 0.4840	 0.5220
Z	 0.6930	 0.5880
a	 0.9150	 0.7090
b	 0.8310	 0.6470
c	 0.9340	 0.7410
d	 0.8920	 0.7340
e	 0.7800	 0.6890



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Chain	Atom inclusion	Q-score
f	 0.4520	 0.5340
g	 0.4070	 0.5250
h	 0.4230	 0.5470
i	 0.9070	 0.7290
j	 0.9000	 0.7150
k	 0.8580	 0.7100
l	 0.8970	 0.7250
m	 0.9620	 0.7530
n	 0.7080	 0.6360
o	 0.8660	 0.7070
p	 0.9270	 0.7510
q	 0.8030	 0.6910
r	 0.8850	 0.7320
s	 0.7840	 0.6760
t	 0.6580	 0.6270
u	 0.7330	 0.6560
v	 0.8620	 0.7260
w	 0.8770	 0.7170
x	 0.6140	 0.6090
y	 0.8380	 0.7060
z	 0.8630	 0.7160