



Full wwPDB EM Validation Report ⓘ

Oct 19, 2021 – 04:21 pm BST

PDB ID : 7PJS
EMDB ID : EMD-13458
Title : Structure of the 70S ribosome with tRNAs in the classical pre-translocation state and apramycin (C)
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.
Deposited on : 2021-08-24
Resolution : 2.35 Å (reported)
Based on initial models : 4AQY, 5LZD, 6YSS

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

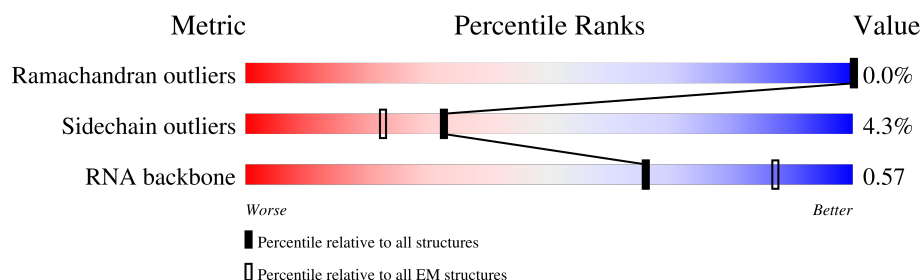
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	57	
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	




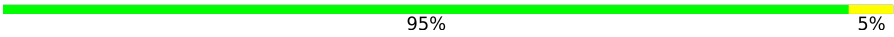
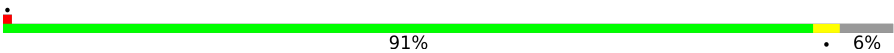


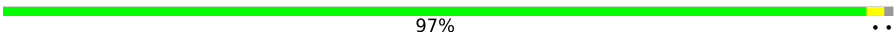



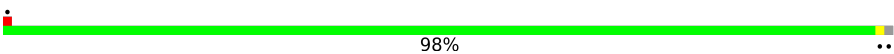

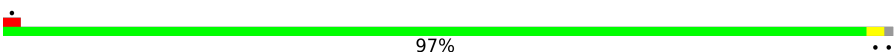

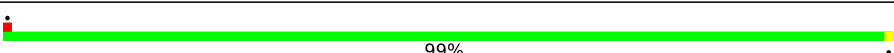
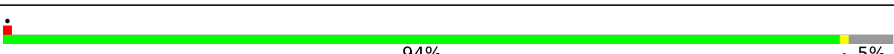
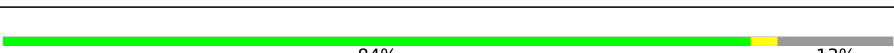
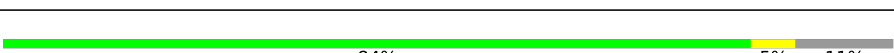

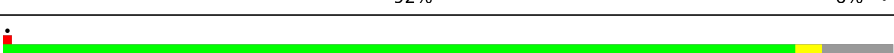



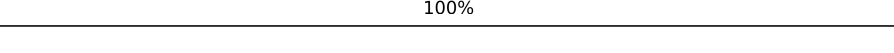
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Mol	Chain	Length	Quality of chain
9	B	120	
10	C	273	
11	D	209	
12	E	201	
13	F	179	
14	G	177	
15	H	149	
16	I	142	
17	J	142	
18	K	123	
19	L	144	
20	M	136	
21	N	127	
22	O	117	
23	P	115	
24	Q	118	
25	R	103	
26	S	110	
27	T	100	
28	U	104	
29	V	94	
30	W	85	
31	X	78	
32	Y	63	
33	Z	59	

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Mol	Chain	Length	Quality of chain
34	a	1542	
35	b	240	
36	c	233	
37	d	206	
38	e	167	
39	f	135	
40	g	179	
41	h	130	
42	i	130	
43	j	103	
44	k	129	
45	l	124	
46	m	118	
47	n	102	
48	o	89	
49	p	82	
50	q	84	
51	r	75	
52	s	92	
53	t	87	
54	u	71	
55	v	77	
56	w	76	
57	y	2	
58	z	33	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 147741 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	131	Total	C	N	O	0	0
			647	385	131	131		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2903	Total	C	N	O	P	0	0
			62338	27816	11471	20148	2903		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

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

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

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

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	141	Total	C	N	O	S	0	0
			693	411	141	141			

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

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

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

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

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

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

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	0	0
			33050	14748	6057	10705	1540		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

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

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

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

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

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

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace	
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	2	Total	C	N	O	S	0	0
			21	15	2	3	1		

- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	11	Total	C	N	O	P	0	0
			230	103	35	81	11		

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	0	1	Total	Mg	0
			1	1	
59	A	258	Total	Mg	0
			258	258	
59	B	4	Total	Mg	0
			4	4	
59	C	2	Total	Mg	0
			2	2	
59	D	1	Total	Mg	0
			1	1	
59	N	1	Total	Mg	0
			1	1	
59	O	1	Total	Mg	0
			1	1	
59	P	1	Total	Mg	0
			1	1	
59	a	92	Total	Mg	0
			92	92	

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Mol	Chain	Residues	Atoms		AltConf
59	m	1	Total	Mg	0
			1	1	
59	n	1	Total	Mg	0
			1	1	

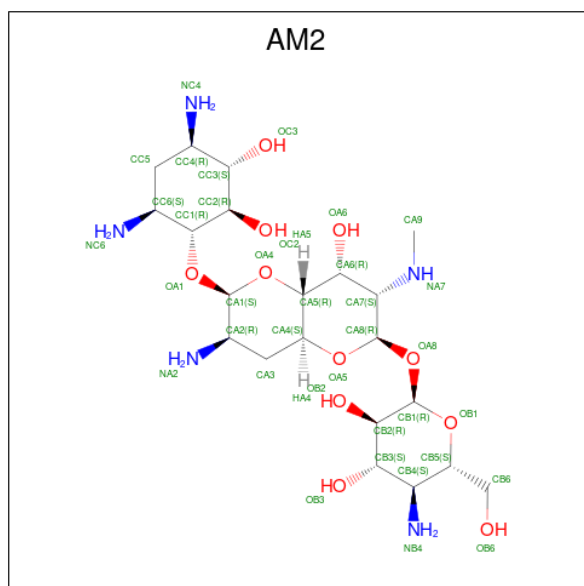
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	4	1	Total	Zn	0
			1	1	
60	6	1	Total	Zn	0
			1	1	

- Molecule 61 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
61	A	1	Total	Na	0
			1	1	
61	B	1	Total	Na	0
			1	1	

- Molecule 62 is APRAMYCIN (three-letter code: AM2) (formula: C₂₁H₄₁N₅O₁₁).



Mol	Chain	Residues	Atoms				AltConf
62	a	1	Total	C	N	O	0
			148	84	20	44	

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Mol	Chain	Residues	Atoms				AltConf
62	a	1	Total 148	C 84	N 20	O 44	0
62	a	1	Total 148	C 84	N 20	O 44	0
62	a	1	Total 148	C 84	N 20	O 44	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		AltConf
63	A	5	Total 5	O 5	0
63	a	15	Total 15	O 15	0
63	z	2	Total 2	O 2	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 50S ribosomal protein L32

Chain 0:  96%




- Molecule 2: 50S ribosomal protein L33

Chain 1:  85% 5% 9%



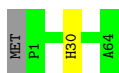
- Molecule 3: 50S ribosomal protein L34

Chain 2:  91% 9%



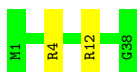
- Molecule 4: 50S ribosomal protein L35

Chain 3:  97%

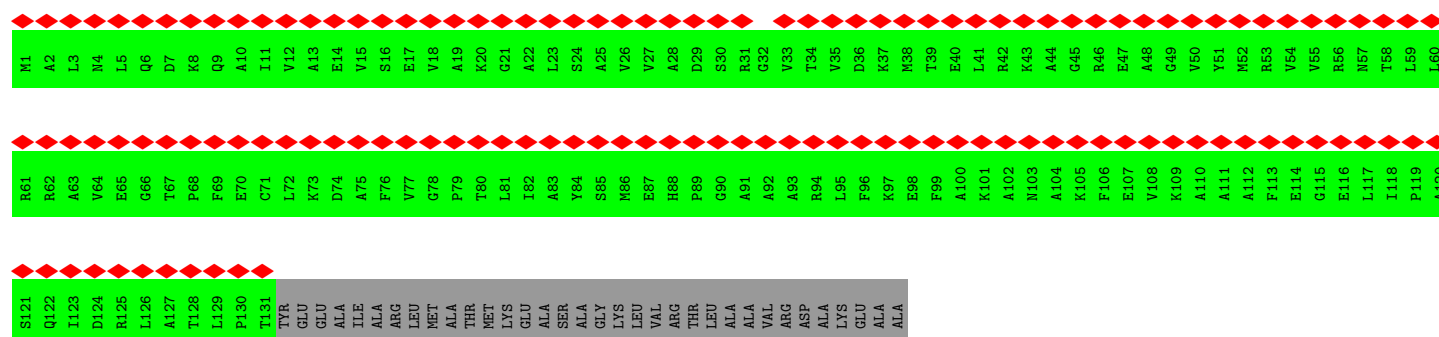
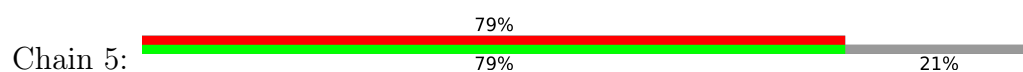


- Molecule 5: 50S ribosomal protein L36

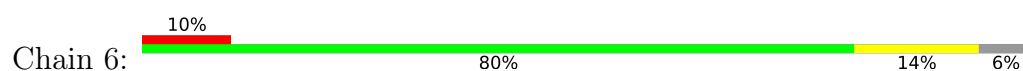
Chain 4:  95% 5%



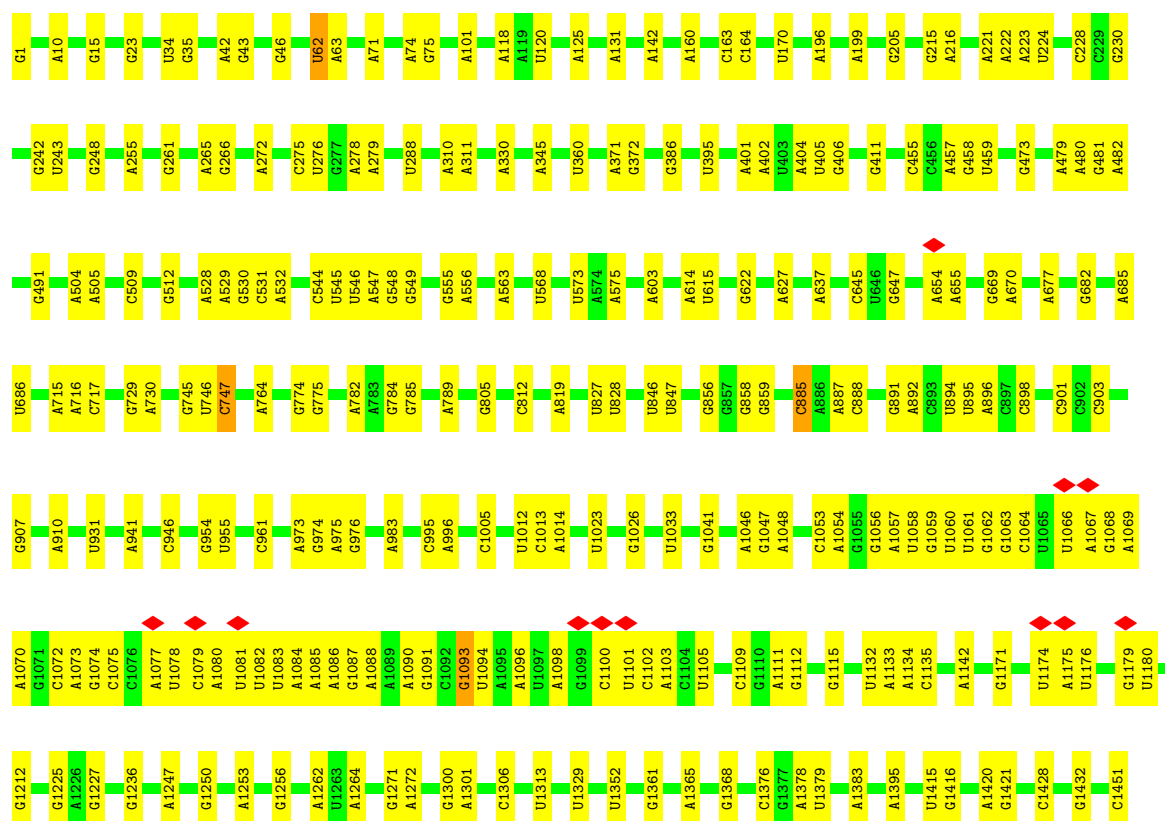
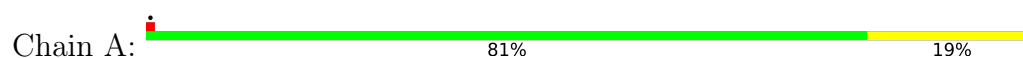
- Molecule 6: 50S ribosomal protein L10

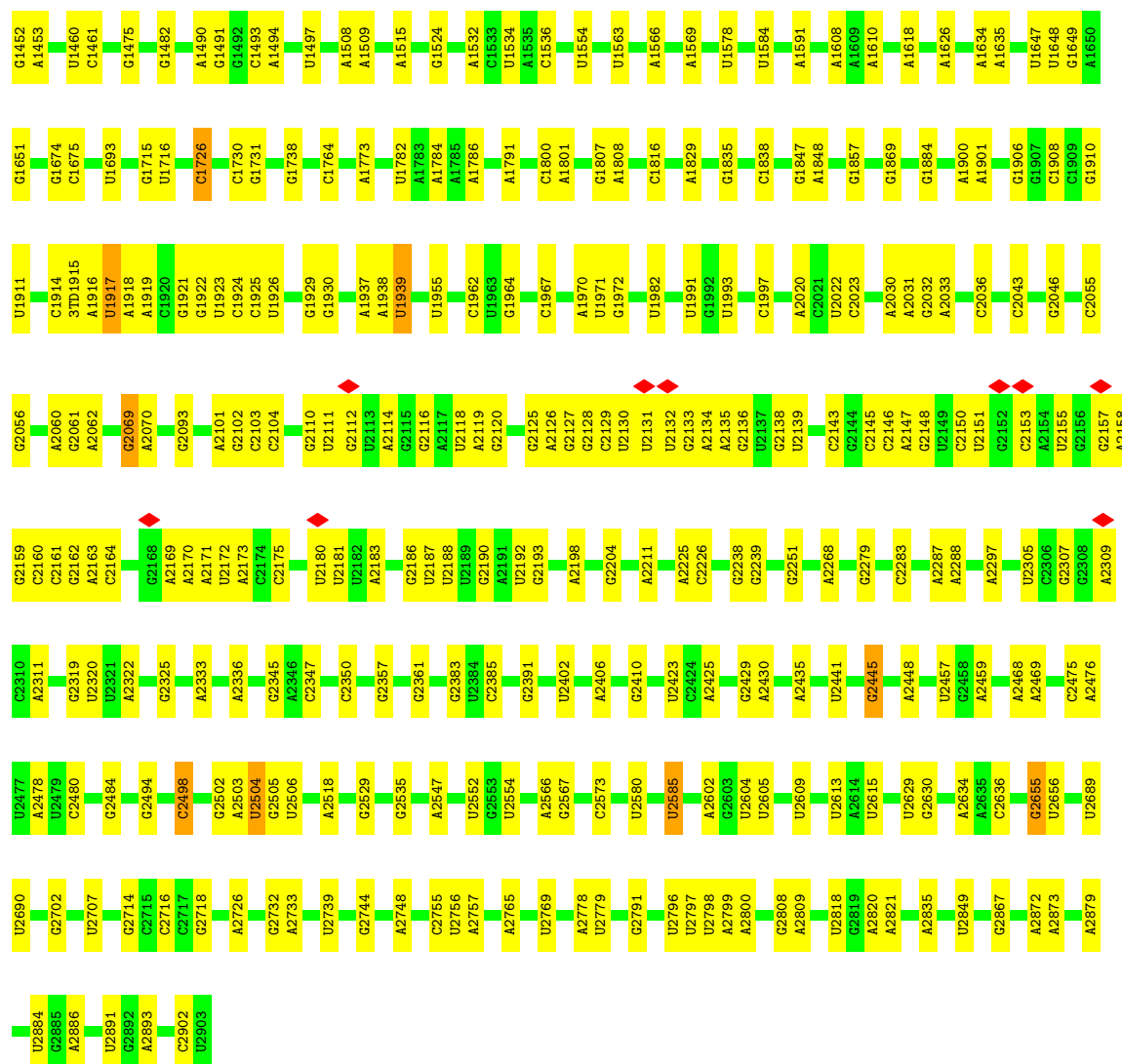


• Molecule 7: 50S ribosomal protein L31



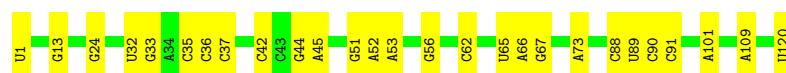
• Molecule 8: 23S ribosomal RNA





• Molecule 9: 5S ribosomal RNA

Chain B: 78% 22%



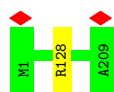
• Molecule 10: 50S ribosomal protein L2

Chain C: 98% ..



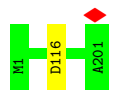
• Molecule 11: 50S ribosomal protein L3

Chain D: 100%



- Molecule 12: 50S ribosomal protein L4

Chain E: 100%



- Molecule 13: 50S ribosomal protein L5

Chain F: 95%



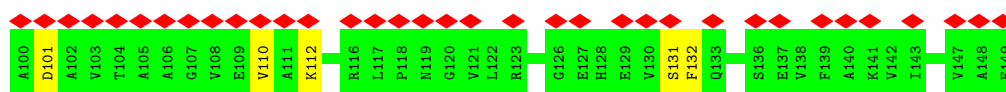
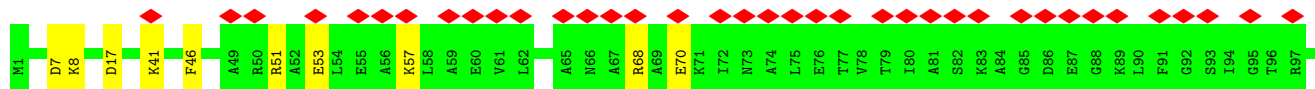
- Molecule 14: 50S ribosomal protein L6

Chain G: 95%



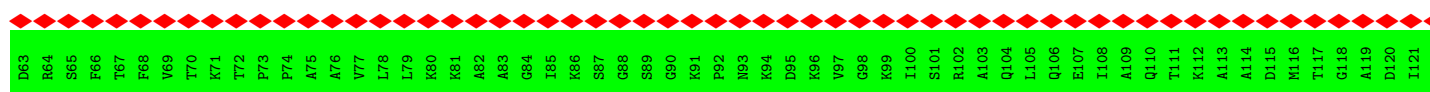
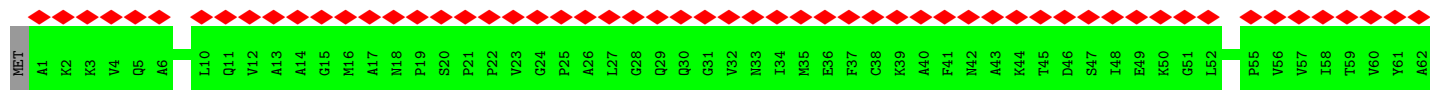
- Molecule 15: 50S ribosomal protein L9

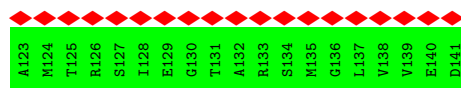
Chain H: 48%



- Molecule 16: 50S ribosomal protein L11

Chain I: 96%





- Molecule 17: 50S ribosomal protein L13

Chain J: 98%



- Molecule 18: 50S ribosomal protein L14

Chain K: 98%



- Molecule 19: 50S ribosomal protein L15

Chain L: 99%



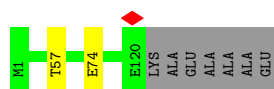
- Molecule 20: 50S ribosomal protein L16

Chain M: 97%



- Molecule 21: 50S ribosomal protein L17

Chain N: 93%



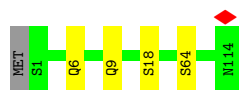
- Molecule 22: 50S ribosomal protein L18

Chain O: 97%



- Molecule 23: 50S ribosomal protein L19

Chain P:  96% ..



- Molecule 24: 50S ribosomal protein L20

Chain Q:  98% ..



- Molecule 25: 50S ribosomal protein L21

Chain R:  94% 6%



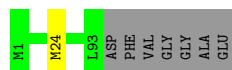
- Molecule 26: 50S ribosomal protein L22

Chain S:  100%



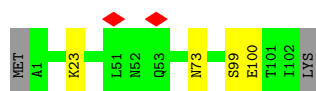
- Molecule 27: 50S ribosomal protein L23

Chain T:  92% 7%



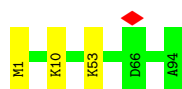
- Molecule 28: 50S ribosomal protein L24

Chain U:  94% ..

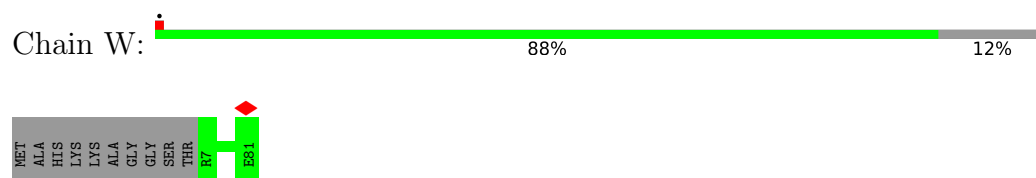


- Molecule 29: 50S ribosomal protein L25

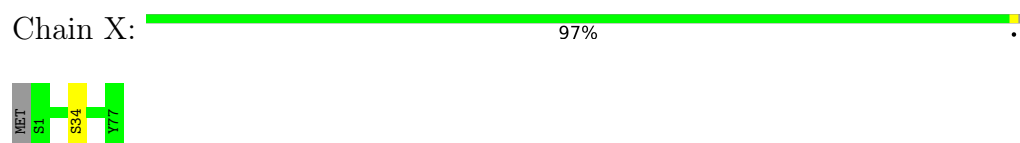
Chain V:  97% .



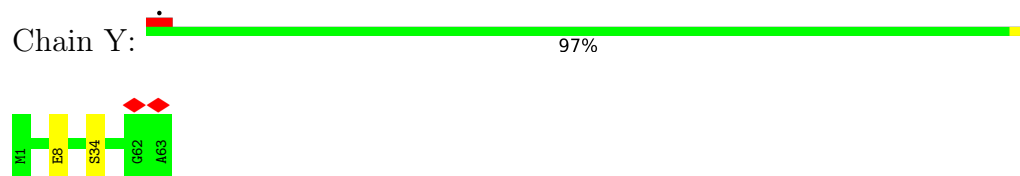
- Molecule 30: 50S ribosomal protein L27



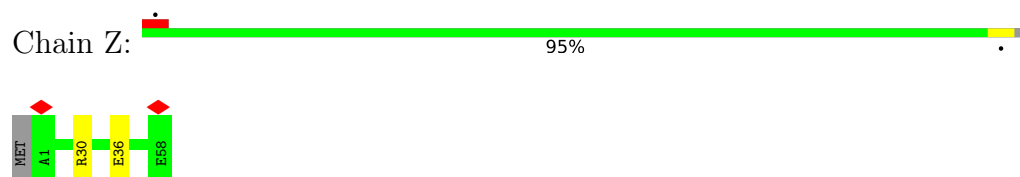
- Molecule 31: 50S ribosomal protein L28



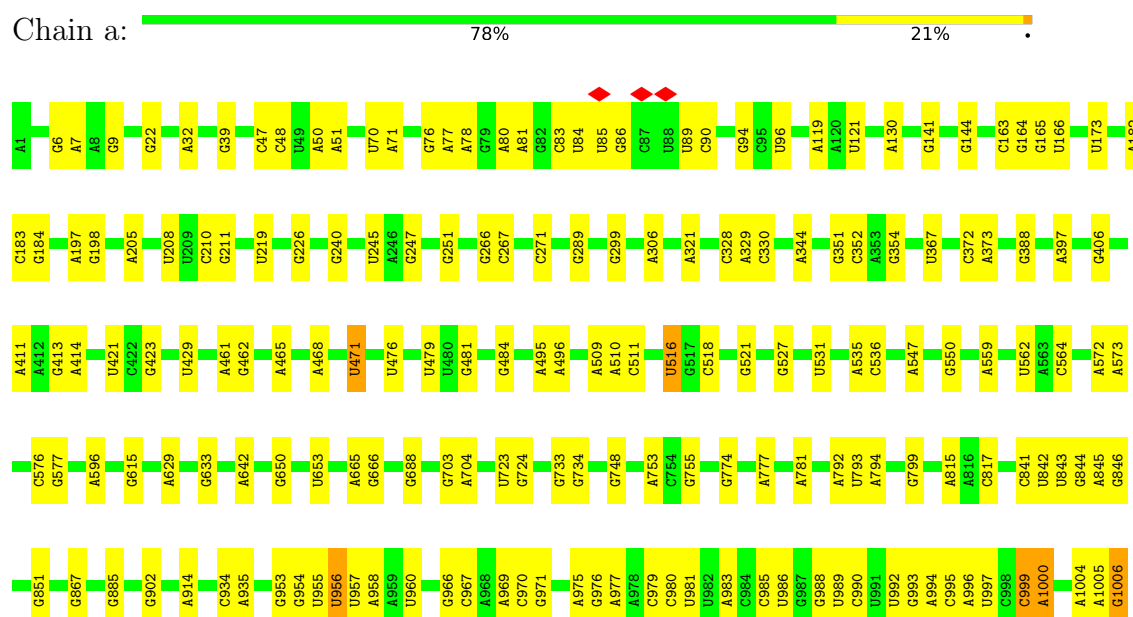
- Molecule 32: 50S ribosomal protein L29



- Molecule 33: 50S ribosomal protein L30

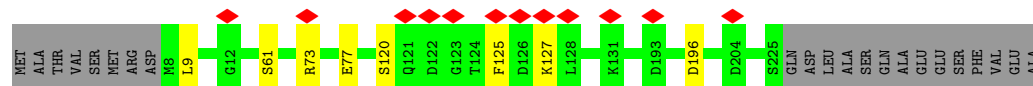
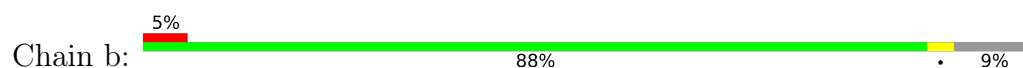


- Molecule 34: 16S ribosomal RNA

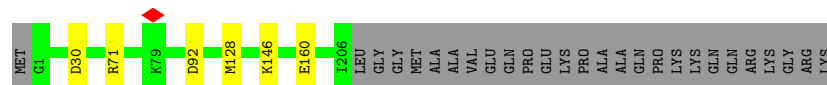
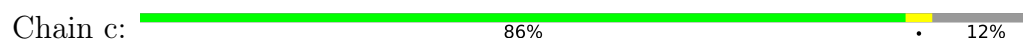




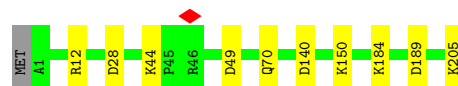
• Molecule 35: 30S ribosomal protein S2



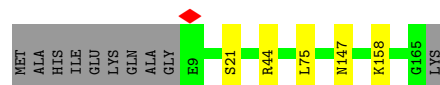
• Molecule 36: 30S ribosomal protein S3



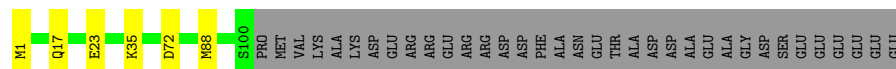
• Molecule 37: 30S ribosomal protein S4




• Molecule 38: 30S ribosomal protein S5



• Molecule 39: 30S ribosomal protein S6



- Molecule 40: 30S ribosomal protein S7

Chain g:  78% 7% 16%




- Molecule 41: 30S ribosomal protein S8

Chain h:  97% ..




- Molecule 42: 30S ribosomal protein S9

Chain i:  86% 12% .




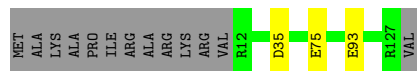
- Molecule 43: 30S ribosomal protein S10

Chain j:  88% 7% 5%



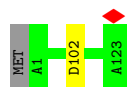
- Molecule 44: 30S ribosomal protein S11

Chain k:  88% . 10%




- Molecule 45: 30S ribosomal protein S12

Chain l:  98% ..



- Molecule 46: 30S ribosomal protein S13

Chain m:  88% 8% .



- Molecule 47: 30S ribosomal protein S14

Chain n:  97% ..



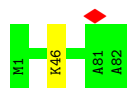
- Molecule 48: 30S ribosomal protein S15

Chain o:  94% ..



- Molecule 49: 30S ribosomal protein S16

Chain p:  99% .




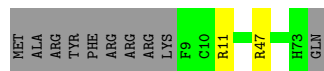
- Molecule 50: 30S ribosomal protein S17

Chain q:  94% . 5%




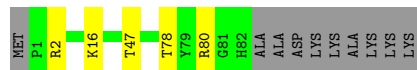
- Molecule 51: 30S ribosomal protein S18

Chain r:  84% . 13%




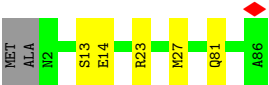
- Molecule 52: 30S ribosomal protein S19

Chain s:  84% 5% 11%

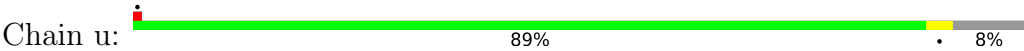


- Molecule 53: 30S ribosomal protein S20

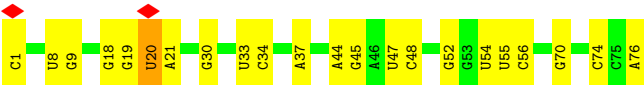
Chain t:  92% 6% .



• Molecule 54: 30S ribosomal protein S21



• Molecule 55: P-site tRNA(fMet)



• Molecule 56: P-site fMet-Phe-tRNA(Phe)



• Molecule 57: Dipeptide (FME-PHE)



• Molecule 58: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	537761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	21.985	Depositor
Minimum map value	-5.122	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6525, 0.6525, 0.6525	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, G7M, 6MZ, MA6, AM2, 4SU, OMU, MG, H2U, OMC, PSU, 3TD, FME, OMG, 2MG, 5MU, 1MG, 4OC, ZN, MIA, 2MA, NA, 5MC

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	0	0.31	0/450	0.65	1/599 (0.2%)
2	1	0.31	0/416	0.53	0/554
3	2	0.29	0/380	0.66	0/498
4	3	0.30	0/513	0.53	0/676
5	4	0.32	0/303	0.61	0/397
6	5	0.24	0/646	0.43	0/898
7	6	0.31	0/531	0.71	0/709
8	A	0.59	1/69266 (0.0%)	0.80	23/108055 (0.0%)
9	B	0.54	1/2873 (0.0%)	0.78	0/4478
10	C	0.34	0/2121	0.58	0/2852
11	D	0.33	0/1586	0.54	0/2134
12	E	0.31	0/1571	0.50	0/2113
13	F	0.31	0/1434	0.58	0/1926
14	G	0.29	0/1343	0.53	0/1816
15	H	0.32	0/1122	0.68	0/1515
16	I	0.25	0/692	0.45	0/960
17	J	0.33	0/1152	0.52	0/1551
18	K	0.33	0/947	0.60	0/1268
19	L	0.32	0/1054	0.60	0/1403
20	M	0.33	0/1093	0.58	0/1460
21	N	0.30	0/973	0.56	0/1301
22	O	0.31	0/902	0.60	0/1209
23	P	0.32	0/929	0.56	0/1242
24	Q	0.33	0/960	0.53	0/1278
25	R	0.34	0/829	0.59	0/1107
26	S	0.29	0/864	0.53	0/1156
27	T	0.31	0/744	0.55	0/994
28	U	0.31	0/787	0.52	0/1051
29	V	0.32	0/766	0.53	0/1025
30	W	0.32	0/582	0.54	0/769
31	X	0.33	0/635	0.59	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.30	0/510	0.58	0/677
33	Z	0.28	0/453	0.58	0/605
34	a	0.53	0/36725	0.83	25/57285 (0.0%)
35	b	0.29	0/1735	0.57	1/2338 (0.0%)
36	c	0.31	0/1651	0.55	0/2225
37	d	0.29	0/1665	0.55	0/2227
38	e	0.31	0/1154	0.55	0/1554
39	f	0.31	0/835	0.59	0/1128
40	g	0.28	0/1195	0.58	0/1602
41	h	0.30	0/989	0.50	0/1326
42	i	0.31	0/1034	0.64	0/1375
43	j	0.34	0/796	0.69	0/1077
44	k	0.31	0/885	0.63	0/1195
45	l	0.34	0/969	0.63	1/1300 (0.1%)
46	m	0.30	0/892	0.62	0/1193
47	n	0.28	0/811	0.55	0/1081
48	o	0.27	0/722	0.55	0/964
49	p	0.31	0/659	0.58	0/884
50	q	0.32	0/657	0.58	0/881
51	r	0.33	0/544	0.56	0/731
52	s	0.31	0/675	0.59	0/908
53	t	0.27	0/671	0.48	0/888
54	u	0.33	0/512	0.60	0/683
55	v	0.51	1/1745 (0.1%)	0.80	0/2716
56	w	0.36	0/1650	0.82	1/2569 (0.0%)
57	y	0.43	0/11	0.26	0/13
58	z	0.49	0/255	1.18	3/394 (0.8%)
All	All	0.51	3/158864 (0.0%)	0.76	55/237661 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1	U	OP3-P	-10.68	1.48	1.61
55	v	1	C	OP3-P	-10.66	1.48	1.61
8	A	1	G	OP3-P	-10.60	1.48	1.61

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	z	-1	C	OP2-P-O3'	-10.72	81.61	105.20
58	z	-1	C	OP1-P-O3'	-10.70	81.67	105.20
34	a	999	C	C2-N1-C1'	9.50	129.25	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	999	C	C6-N1-C1'	-7.77	111.47	120.80
8	A	2506	U	C2-N1-C1'	7.61	126.83	117.70
8	A	512	G	O4'-C1'-N9	7.60	114.28	108.20
8	A	2585	U	C2-N1-C1'	7.53	126.73	117.70
58	z	0	U	OP1-P-OP2	7.18	130.37	119.60
8	A	1313	U	C2-N1-C1'	7.04	126.14	117.70
1	0	45	ASP	CB-CG-OD1	6.86	124.47	118.30
34	a	1006	G	O4'-C1'-N9	6.74	113.59	108.20
34	a	1421	G	O5'-P-OP1	-6.70	99.67	105.70
34	a	999	C	N1-C2-O2	6.70	122.92	118.90
34	a	1000	A	OP1-P-OP2	-6.61	109.69	119.60
8	A	2585	U	N1-C2-O2	6.53	127.37	122.80
8	A	2506	U	N1-C2-O2	6.40	127.28	122.80
8	A	2585	U	N3-C2-O2	-6.33	117.77	122.20
8	A	528	A	C2-N3-C4	-5.75	107.73	110.60
34	a	1158	C	N1-C2-O2	5.67	122.30	118.90
34	a	1420	U	P-O3'-C3'	-5.67	112.90	119.70
34	a	471	U	N3-C2-O2	-5.64	118.25	122.20
8	A	901	C	C2-N1-C1'	5.60	124.96	118.80
56	w	74	C	O4'-C1'-N1	5.60	112.68	108.20
8	A	1914	C	C2-N1-C1'	5.57	124.93	118.80
34	a	970	C	C2-N1-C1'	5.56	124.92	118.80
34	a	1317	C	C2-N1-C1'	5.54	124.90	118.80
8	A	1313	U	N1-C2-O2	5.52	126.67	122.80
34	a	956	U	C2-N1-C1'	5.43	124.22	117.70
8	A	1726	C	C2-N1-C1'	5.42	124.76	118.80
34	a	979	C	N3-C2-O2	-5.40	118.12	121.90
8	A	2506	U	N3-C2-O2	-5.38	118.43	122.20
8	A	62	U	C2-N1-C1'	5.38	124.16	117.70
34	a	476	U	C2-N1-C1'	5.35	124.12	117.70
8	A	2506	U	C6-N1-C1'	-5.33	113.74	121.20
34	a	999	C	C5-C6-N1	5.32	123.66	121.00
34	a	1326	U	C2-N1-C1'	5.28	124.03	117.70
34	a	1327	C	C2-N1-C1'	5.27	124.60	118.80
8	A	1921	G	P-O3'-C3'	-5.26	113.38	119.70
34	a	471	U	N1-C2-O2	5.21	126.45	122.80
34	a	1432	G	C4-N9-C1'	5.20	133.25	126.50
8	A	1093	G	C3'-C2'-C1'	5.19	105.66	101.50
8	A	1675	C	N3-C2-O2	-5.18	118.27	121.90
34	a	1158	C	C2-N1-C1'	5.18	124.50	118.80
34	a	981	U	N3-C2-O2	-5.17	118.58	122.20
8	A	1914	C	N1-C2-O2	5.16	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	979	C	C2-N1-C1'	5.15	124.47	118.80
8	A	1675	C	C2-N1-C1'	5.14	124.46	118.80
34	a	1432	G	O4'-C1'-N9	5.14	112.31	108.20
8	A	2391	G	O4'-C1'-N9	5.13	112.31	108.20
34	a	481	G	C4-N9-C1'	5.11	133.15	126.50
45	l	102	ASP	CB-CG-OD1	5.10	122.89	118.30
34	a	1327	C	N3-C2-O2	-5.09	118.34	121.90
35	b	9	LEU	CA-CB-CG	5.05	126.92	115.30
8	A	885	C	O4'-C1'-N1	5.02	112.22	108.20
8	A	2655	G	P-O3'-C3'	5.01	125.72	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	54 (100%)	0	0	100	100
2	1	48/55 (87%)	48 (100%)	0	0	100	100
3	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
4	3	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
5	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
6	5	129/165 (78%)	116 (90%)	13 (10%)	0	100	100
7	6	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
10	C	269/273 (98%)	256 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
12	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
13	F	175/179 (98%)	161 (92%)	14 (8%)	0	100	100
14	G	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
15	H	147/149 (99%)	128 (87%)	19 (13%)	0	100	100
16	I	139/142 (98%)	130 (94%)	9 (6%)	0	100	100
17	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
18	K	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
19	L	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
20	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
21	N	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
22	O	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
23	P	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
24	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
25	R	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	15	15
26	S	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
27	T	91/100 (91%)	91 (100%)	0	0	100	100
28	U	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
29	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
30	W	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
31	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
32	Y	61/63 (97%)	61 (100%)	0	0	100	100
33	Z	56/59 (95%)	56 (100%)	0	0	100	100
35	b	216/240 (90%)	203 (94%)	13 (6%)	0	100	100
36	c	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
37	d	203/206 (98%)	190 (94%)	13 (6%)	0	100	100
38	e	155/167 (93%)	152 (98%)	3 (2%)	0	100	100
39	f	98/135 (73%)	94 (96%)	4 (4%)	0	100	100
40	g	149/179 (83%)	145 (97%)	4 (3%)	0	100	100
41	h	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
42	i	125/130 (96%)	122 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	j	96/103 (93%)	85 (88%)	11 (12%)	0	100	100
44	k	114/129 (88%)	106 (93%)	8 (7%)	0	100	100
45	l	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
46	m	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
47	n	99/102 (97%)	98 (99%)	1 (1%)	0	100	100
48	o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
49	p	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
50	q	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
51	r	63/75 (84%)	61 (97%)	2 (3%)	0	100	100
52	s	80/92 (87%)	79 (99%)	1 (1%)	0	100	100
53	t	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
54	u	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
All	All	5850/6220 (94%)	5602 (96%)	247 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	R	51	VAL

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	
1	0	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	42 (93%)	3 (7%)	16	17
3	2	38/38 (100%)	34 (90%)	4 (10%)	7	6
4	3	51/52 (98%)	50 (98%)	1 (2%)	55	66
5	4	34/34 (100%)	32 (94%)	2 (6%)	19	22
7	6	59/62 (95%)	49 (83%)	10 (17%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	C	216/218 (99%)	213 (99%)	3 (1%)	67	78
11	D	164/164 (100%)	163 (99%)	1 (1%)	86	93
12	E	165/165 (100%)	164 (99%)	1 (1%)	86	93
13	F	148/150 (99%)	141 (95%)	7 (5%)	26	31
14	G	137/138 (99%)	130 (95%)	7 (5%)	24	27
15	H	114/114 (100%)	99 (87%)	15 (13%)	4	4
17	J	116/116 (100%)	113 (97%)	3 (3%)	46	56
18	K	103/104 (99%)	101 (98%)	2 (2%)	57	68
19	L	102/103 (99%)	102 (100%)	0	100	100
20	M	109/109 (100%)	105 (96%)	4 (4%)	34	42
21	N	100/103 (97%)	98 (98%)	2 (2%)	55	66
22	O	86/87 (99%)	83 (96%)	3 (4%)	36	44
23	P	99/100 (99%)	95 (96%)	4 (4%)	31	39
24	Q	89/90 (99%)	88 (99%)	1 (1%)	73	84
25	R	84/84 (100%)	79 (94%)	5 (6%)	19	21
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	79 (99%)	1 (1%)	69	80
28	U	83/85 (98%)	79 (95%)	4 (5%)	25	30
29	V	78/78 (100%)	75 (96%)	3 (4%)	33	41
30	W	57/63 (90%)	57 (100%)	0	100	100
31	X	67/68 (98%)	66 (98%)	1 (2%)	65	76
32	Y	55/55 (100%)	53 (96%)	2 (4%)	35	43
33	Z	48/49 (98%)	46 (96%)	2 (4%)	30	36
35	b	180/198 (91%)	173 (96%)	7 (4%)	32	40
36	c	170/190 (90%)	164 (96%)	6 (4%)	36	44
37	d	172/173 (99%)	162 (94%)	10 (6%)	20	22
38	e	114/126 (90%)	109 (96%)	5 (4%)	28	34
39	f	87/116 (75%)	81 (93%)	6 (7%)	15	15
40	g	124/147 (84%)	112 (90%)	12 (10%)	8	7
41	h	104/105 (99%)	101 (97%)	3 (3%)	42	52
42	i	105/107 (98%)	90 (86%)	15 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	j	86/90 (96%)	79 (92%)	7 (8%)	11	11
44	k	89/99 (90%)	86 (97%)	3 (3%)	37	46
45	l	103/104 (99%)	103 (100%)	0	100	100
46	m	92/96 (96%)	82 (89%)	10 (11%)	6	6
47	n	79/84 (94%)	77 (98%)	2 (2%)	47	58
48	o	76/77 (99%)	72 (95%)	4 (5%)	22	26
49	p	65/65 (100%)	64 (98%)	1 (2%)	65	76
50	q	74/78 (95%)	73 (99%)	1 (1%)	67	78
51	r	56/65 (86%)	54 (96%)	2 (4%)	35	43
52	s	72/79 (91%)	67 (93%)	5 (7%)	15	15
53	t	65/66 (98%)	60 (92%)	5 (8%)	13	12
54	u	46/61 (75%)	44 (96%)	2 (4%)	29	35
57	y	1/1 (100%)	0	1 (100%)	0	0
All	All	4627/4830 (96%)	4429 (96%)	198 (4%)	33	35

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	7	LYS
2	1	27	ARG
2	1	52	LYS
3	2	15	SER
3	2	24	THR
3	2	25	LYS
3	2	41	ARG
4	3	30	HIS
5	4	4	ARG
5	4	12	ARG
7	6	3	LYS
7	6	4	ASP
7	6	10	GLU
7	6	39	LYS
7	6	47	LYS
7	6	49	ARG
7	6	50	ASP
7	6	59	ARG
7	6	62	LYS

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Mol	Chain	Res	Type
7	6	66	ILE
10	C	86	ARG
10	C	259	ASN
10	C	263	ASP
11	D	128	ARG
12	E	116	ASP
13	F	13	LYS
13	F	46	LYS
13	F	48	LEU
13	F	77	LYS
13	F	132	ARG
13	F	146	ASP
13	F	174	PHE
14	G	41	GLU
14	G	47	ASN
14	G	94	ARG
14	G	151	ARG
14	G	152	ARG
14	G	165	ASP
14	G	175	LYS
15	H	7	ASP
15	H	8	LYS
15	H	17	ASP
15	H	41	LYS
15	H	46	PHE
15	H	51	ARG
15	H	53	GLU
15	H	57	LYS
15	H	68	ARG
15	H	70	GLU
15	H	101	ASP
15	H	110	VAL
15	H	112	LYS
15	H	131	SER
15	H	132	PHE
17	J	1	MET
17	J	71	ASP
17	J	129	GLU
18	K	40	LYS
18	K	49	ARG
20	M	6	ARG
20	M	58	LYS

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Mol	Chain	Res	Type
20	M	110	GLU
20	M	127	LYS
21	N	57	THR
21	N	74	GLU
22	O	46	GLU
22	O	88	LYS
22	O	89	ASP
23	P	6	GLN
23	P	9	GLN
23	P	18	SER
23	P	64	SER
24	Q	12	ARG
25	R	1	MET
25	R	43	ASN
25	R	60	LYS
25	R	70	GLU
25	R	73	LYS
27	T	24	MET
28	U	23	LYS
28	U	73	ASN
28	U	99	SER
28	U	100	GLU
29	V	1	MET
29	V	10	LYS
29	V	53	LYS
31	X	34	SER
32	Y	8	GLU
32	Y	34	SER
33	Z	30	ARG
33	Z	36	GLU
35	b	61	SER
35	b	73	ARG
35	b	77	GLU
35	b	120	SER
35	b	125	PHE
35	b	127	LYS
35	b	196	ASP
36	c	30	ASP
36	c	71	ARG
36	c	92	ASP
36	c	128	MET
36	c	146	LYS

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Mol	Chain	Res	Type
36	c	160	GLU
37	d	12	ARG
37	d	28	ASP
37	d	44	LYS
37	d	49	ASP
37	d	70	GLN
37	d	140	ASP
37	d	150	LYS
37	d	184	LYS
37	d	189	ASP
37	d	205	LYS
38	e	21	SER
38	e	44	ARG
38	e	75	LEU
38	e	147	ASN
38	e	158	LYS
39	f	1	MET
39	f	17	GLN
39	f	23	GLU
39	f	35	LYS
39	f	72	ASP
39	f	88	MET
40	g	3	ARG
40	g	4	ARG
40	g	36	SER
40	g	42	VAL
40	g	48	THR
40	g	51	GLN
40	g	52	ARG
40	g	55	LYS
40	g	56	SER
40	g	110	ARG
40	g	114	SER
40	g	119	LEU
41	h	37	ASN
41	h	42	GLU
41	h	49	LYS
42	i	11	ARG
42	i	13	SER
42	i	26	LYS
42	i	28	VAL
42	i	55	ASP

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Mol	Chain	Res	Type
42	i	58	GLU
42	i	65	THR
42	i	71	ILE
42	i	79	ARG
42	i	84	ARG
42	i	96	GLU
42	i	98	ARG
42	i	104	THR
42	i	105	ARG
42	i	128	LYS
43	j	20	GLN
43	j	24	GLU
43	j	35	GLN
43	j	46	LYS
43	j	78	GLU
43	j	82	LYS
43	j	88	MET
44	k	35	ASP
44	k	75	GLU
44	k	93	GLU
46	m	2	ARG
46	m	15	VAL
46	m	26	LYS
46	m	30	LYS
46	m	42	VAL
46	m	49	GLU
46	m	53	ASP
46	m	59	VAL
46	m	77	LYS
46	m	113	LYS
47	n	25	GLU
47	n	45	VAL
48	o	13	GLU
48	o	17	ASP
48	o	57	ARG
48	o	87	ARG
49	p	46	LYS
50	q	41	THR
51	r	11	ARG
51	r	47	ARG
52	s	2	ARG
52	s	16	LYS

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Mol	Chain	Res	Type
52	s	47	THR
52	s	78	THR
52	s	80	ARG
53	t	13	SER
53	t	14	GLU
53	t	23	ARG
53	t	27	MET
53	t	81	GLN
54	u	6	ARG
54	u	12	ASP
57	y	102	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
32	Y	15	ASN
32	Y	36	GLN
32	Y	45	GLN
36	c	99	GLN
39	f	3	HIS
47	n	49	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	312 (20%)	0
55	v	76/77 (98%)	18 (23%)	0
56	w	74/76 (97%)	18 (24%)	0
58	z	10/33 (30%)	1 (10%)	0
8	A	2898/2903 (99%)	517 (17%)	37 (1%)
9	B	119/120 (99%)	23 (19%)	4 (3%)
All	All	4713/4751 (99%)	889 (18%)	41 (0%)

All (889) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	15	G
8	A	23	G
8	A	34	U

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Mol	Chain	Res	Type
8	A	35	G
8	A	42	A
8	A	43	G
8	A	46	G
8	A	62	U
8	A	63	A
8	A	71	A
8	A	74	A
8	A	75	G
8	A	101	A
8	A	118	A
8	A	120	U
8	A	125	A
8	A	131	A
8	A	142	A
8	A	160	A
8	A	163	C
8	A	164	C
8	A	170	U
8	A	196	A
8	A	199	A
8	A	205	G
8	A	215	G
8	A	216	A
8	A	221	A
8	A	222	A
8	A	223	A
8	A	224	U
8	A	228	C
8	A	230	G
8	A	242	G
8	A	243	U
8	A	248	G
8	A	255	A
8	A	261	G
8	A	265	A
8	A	266	G
8	A	272	A
8	A	275	C
8	A	276	U
8	A	278	A
8	A	279	A

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Mol	Chain	Res	Type
8	A	288	U
8	A	311	A
8	A	330	A
8	A	345	A
8	A	360	U
8	A	371	A
8	A	372	G
8	A	386	G
8	A	395	U
8	A	401	A
8	A	402	A
8	A	404	A
8	A	405	U
8	A	406	G
8	A	411	G
8	A	455	C
8	A	457	A
8	A	458	G
8	A	459	U
8	A	473	G
8	A	480	A
8	A	481	G
8	A	482	A
8	A	491	G
8	A	504	A
8	A	505	A
8	A	509	C
8	A	529	A
8	A	530	G
8	A	531	C
8	A	532	A
8	A	544	C
8	A	545	U
8	A	546	U
8	A	547	A
8	A	548	G
8	A	549	G
8	A	556	A
8	A	563	A
8	A	568	U
8	A	573	U
8	A	575	A

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Mol	Chain	Res	Type
8	A	603	A
8	A	614	A
8	A	615	U
8	A	622	G
8	A	627	A
8	A	637	A
8	A	645	C
8	A	647	G
8	A	654	A
8	A	655	A
8	A	669	G
8	A	670	A
8	A	677	A
8	A	682	G
8	A	685	A
8	A	686	U
8	A	715	A
8	A	716	A
8	A	717	C
8	A	729	G
8	A	730	A
8	A	747	5MC
8	A	764	A
8	A	775	G
8	A	782	A
8	A	784	G
8	A	785	G
8	A	789	A
8	A	805	G
8	A	812	C
8	A	819	A
8	A	827	U
8	A	828	U
8	A	846	U
8	A	847	U
8	A	856	G
8	A	858	G
8	A	859	G
8	A	885	C
8	A	887	A
8	A	888	C
8	A	891	G

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Mol	Chain	Res	Type
8	A	892	A
8	A	894	U
8	A	895	U
8	A	896	A
8	A	898	C
8	A	903	C
8	A	907	G
8	A	910	A
8	A	931	U
8	A	941	A
8	A	946	C
8	A	961	C
8	A	973	A
8	A	974	G
8	A	975	A
8	A	983	A
8	A	995	C
8	A	996	A
8	A	1005	C
8	A	1012	U
8	A	1013	C
8	A	1026	G
8	A	1033	U
8	A	1041	G
8	A	1046	A
8	A	1047	G
8	A	1048	A
8	A	1053	C
8	A	1054	A
8	A	1056	G
8	A	1057	A
8	A	1058	U
8	A	1059	G
8	A	1060	U
8	A	1061	U
8	A	1062	G
8	A	1063	G
8	A	1064	C
8	A	1066	U
8	A	1067	A
8	A	1068	G
8	A	1069	A

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Mol	Chain	Res	Type
8	A	1070	A
8	A	1072	C
8	A	1073	A
8	A	1074	G
8	A	1075	C
8	A	1077	A
8	A	1078	U
8	A	1079	C
8	A	1080	A
8	A	1081	U
8	A	1082	U
8	A	1083	U
8	A	1084	A
8	A	1085	A
8	A	1086	A
8	A	1087	G
8	A	1088	A
8	A	1090	A
8	A	1091	G
8	A	1093	G
8	A	1094	U
8	A	1096	A
8	A	1098	A
8	A	1100	C
8	A	1101	U
8	A	1102	C
8	A	1103	A
8	A	1105	U
8	A	1109	C
8	A	1111	A
8	A	1112	G
8	A	1115	G
8	A	1132	U
8	A	1133	A
8	A	1134	A
8	A	1135	C
8	A	1142	A
8	A	1171	G
8	A	1174	U
8	A	1175	A
8	A	1176	U
8	A	1179	G

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Mol	Chain	Res	Type
8	A	1180	U
8	A	1212	G
8	A	1225	G
8	A	1227	G
8	A	1236	G
8	A	1247	A
8	A	1250	G
8	A	1253	A
8	A	1256	G
8	A	1262	A
8	A	1264	A
8	A	1271	G
8	A	1272	A
8	A	1300	G
8	A	1301	A
8	A	1306	C
8	A	1329	U
8	A	1352	U
8	A	1365	A
8	A	1368	G
8	A	1376	C
8	A	1378	A
8	A	1379	U
8	A	1383	A
8	A	1395	A
8	A	1415	U
8	A	1416	G
8	A	1420	A
8	A	1421	G
8	A	1428	C
8	A	1432	G
8	A	1452	G
8	A	1453	A
8	A	1460	U
8	A	1461	C
8	A	1475	G
8	A	1482	G
8	A	1490	A
8	A	1491	G
8	A	1493	C
8	A	1494	A
8	A	1497	U

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Mol	Chain	Res	Type
8	A	1508	A
8	A	1509	A
8	A	1515	A
8	A	1524	G
8	A	1532	A
8	A	1534	U
8	A	1536	C
8	A	1554	U
8	A	1563	U
8	A	1566	A
8	A	1569	A
8	A	1578	U
8	A	1584	U
8	A	1591	A
8	A	1608	A
8	A	1610	A
8	A	1626	A
8	A	1634	A
8	A	1635	A
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1651	G
8	A	1674	G
8	A	1693	U
8	A	1715	G
8	A	1716	U
8	A	1726	C
8	A	1730	C
8	A	1731	G
8	A	1738	G
8	A	1764	C
8	A	1773	A
8	A	1782	U
8	A	1784	A
8	A	1786	A
8	A	1791	A
8	A	1800	C
8	A	1801	A
8	A	1807	G
8	A	1808	A
8	A	1816	C

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Mol	Chain	Res	Type
8	A	1829	A
8	A	1838	C
8	A	1847	G
8	A	1848	A
8	A	1857	G
8	A	1869	G
8	A	1884	G
8	A	1900	A
8	A	1901	A
8	A	1906	G
8	A	1908	C
8	A	1910	G
8	A	1916	A
8	A	1917	PSU
8	A	1918	A
8	A	1919	A
8	A	1922	G
8	A	1923	U
8	A	1924	C
8	A	1925	C
8	A	1926	U
8	A	1929	G
8	A	1930	G
8	A	1937	A
8	A	1938	A
8	A	1939	5MU
8	A	1955	U
8	A	1964	G
8	A	1967	C
8	A	1970	A
8	A	1971	U
8	A	1972	G
8	A	1982	U
8	A	1991	U
8	A	1993	U
8	A	1997	C
8	A	2020	A
8	A	2022	U
8	A	2023	C
8	A	2031	A
8	A	2032	G
8	A	2033	A

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Mol	Chain	Res	Type
8	A	2036	C
8	A	2043	C
8	A	2046	G
8	A	2055	C
8	A	2056	G
8	A	2060	A
8	A	2061	G
8	A	2062	A
8	A	2069	G7M
8	A	2070	A
8	A	2093	G
8	A	2101	A
8	A	2102	G
8	A	2103	C
8	A	2104	C
8	A	2110	G
8	A	2111	U
8	A	2112	G
8	A	2114	A
8	A	2116	G
8	A	2118	U
8	A	2119	A
8	A	2120	G
8	A	2125	G
8	A	2126	A
8	A	2127	G
8	A	2128	G
8	A	2129	C
8	A	2130	U
8	A	2131	U
8	A	2132	U
8	A	2133	G
8	A	2134	A
8	A	2135	A
8	A	2136	G
8	A	2138	G
8	A	2139	U
8	A	2143	C
8	A	2145	C
8	A	2146	C
8	A	2147	A
8	A	2148	G

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Mol	Chain	Res	Type
8	A	2150	C
8	A	2151	U
8	A	2153	C
8	A	2155	U
8	A	2157	G
8	A	2159	G
8	A	2160	C
8	A	2161	C
8	A	2162	G
8	A	2163	A
8	A	2164	C
8	A	2169	A
8	A	2170	A
8	A	2171	A
8	A	2172	U
8	A	2173	A
8	A	2175	C
8	A	2180	U
8	A	2181	U
8	A	2183	A
8	A	2186	G
8	A	2187	U
8	A	2188	U
8	A	2190	G
8	A	2193	G
8	A	2198	A
8	A	2204	G
8	A	2211	A
8	A	2225	A
8	A	2226	C
8	A	2238	G
8	A	2239	G
8	A	2268	A
8	A	2279	G
8	A	2283	C
8	A	2287	A
8	A	2288	A
8	A	2297	A
8	A	2305	U
8	A	2307	G
8	A	2309	A
8	A	2311	A

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Mol	Chain	Res	Type
8	A	2320	U
8	A	2322	A
8	A	2325	G
8	A	2333	A
8	A	2336	A
8	A	2345	G
8	A	2347	C
8	A	2350	C
8	A	2357	G
8	A	2361	G
8	A	2383	G
8	A	2385	C
8	A	2402	U
8	A	2406	A
8	A	2410	G
8	A	2423	U
8	A	2425	A
8	A	2429	G
8	A	2430	A
8	A	2435	A
8	A	2441	U
8	A	2445	2MG
8	A	2448	A
8	A	2459	A
8	A	2469	A
8	A	2475	C
8	A	2476	A
8	A	2478	A
8	A	2480	C
8	A	2484	G
8	A	2494	G
8	A	2498	OMC
8	A	2502	G
8	A	2504	PSU
8	A	2505	G
8	A	2518	A
8	A	2529	G
8	A	2535	G
8	A	2547	A
8	A	2554	U
8	A	2566	A
8	A	2567	G

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Mol	Chain	Res	Type
8	A	2573	C
8	A	2585	U
8	A	2602	A
8	A	2609	U
8	A	2613	U
8	A	2615	U
8	A	2629	U
8	A	2630	G
8	A	2634	A
8	A	2636	C
8	A	2656	U
8	A	2689	U
8	A	2690	U
8	A	2702	G
8	A	2707	U
8	A	2714	G
8	A	2716	C
8	A	2718	G
8	A	2726	A
8	A	2732	G
8	A	2733	A
8	A	2739	U
8	A	2744	G
8	A	2748	A
8	A	2755	C
8	A	2757	A
8	A	2765	A
8	A	2769	U
8	A	2778	A
8	A	2779	U
8	A	2791	G
8	A	2796	U
8	A	2797	U
8	A	2798	U
8	A	2799	A
8	A	2800	A
8	A	2809	A
8	A	2818	U
8	A	2820	A
8	A	2821	A
8	A	2835	A
8	A	2849	U

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Mol	Chain	Res	Type
8	A	2867	G
8	A	2872	A
8	A	2873	A
8	A	2879	A
8	A	2884	U
8	A	2886	A
8	A	2891	U
8	A	2893	A
8	A	2902	C
9	B	13	G
9	B	24	G
9	B	32	U
9	B	33	G
9	B	35	C
9	B	37	C
9	B	42	C
9	B	44	G
9	B	45	A
9	B	51	G
9	B	53	A
9	B	56	G
9	B	62	C
9	B	65	U
9	B	67	G
9	B	73	A
9	B	88	C
9	B	89	U
9	B	90	C
9	B	91	C
9	B	101	A
9	B	109	A
9	B	120	U
34	a	6	G
34	a	7	A
34	a	9	G
34	a	22	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	50	A
34	a	51	A

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Mol	Chain	Res	Type
34	a	70	U
34	a	71	A
34	a	76	G
34	a	77	A
34	a	78	A
34	a	80	A
34	a	81	A
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	89	U
34	a	90	C
34	a	94	G
34	a	96	U
34	a	119	A
34	a	121	U
34	a	130	A
34	a	141	G
34	a	144	G
34	a	163	C
34	a	164	G
34	a	165	G
34	a	166	U
34	a	173	U
34	a	182	A
34	a	183	C
34	a	184	G
34	a	197	A
34	a	198	G
34	a	205	A
34	a	208	U
34	a	210	C
34	a	211	G
34	a	219	U
34	a	226	G
34	a	240	G
34	a	245	U
34	a	247	G
34	a	251	G
34	a	266	G
34	a	267	C

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Mol	Chain	Res	Type
34	a	271	C
34	a	289	G
34	a	299	G
34	a	306	A
34	a	321	A
34	a	328	C
34	a	329	A
34	a	330	C
34	a	344	A
34	a	351	G
34	a	352	C
34	a	354	G
34	a	367	U
34	a	372	C
34	a	373	A
34	a	388	G
34	a	397	A
34	a	406	G
34	a	411	A
34	a	413	G
34	a	414	A
34	a	421	U
34	a	423	G
34	a	429	U
34	a	461	A
34	a	462	G
34	a	465	A
34	a	468	A
34	a	471	U
34	a	479	U
34	a	484	G
34	a	495	A
34	a	496	A
34	a	509	A
34	a	510	A
34	a	511	C
34	a	516	PSU
34	a	518	C
34	a	521	G
34	a	531	U
34	a	535	A
34	a	536	C

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Mol	Chain	Res	Type
34	a	547	A
34	a	550	G
34	a	559	A
34	a	562	U
34	a	564	C
34	a	572	A
34	a	573	A
34	a	576	C
34	a	577	G
34	a	596	A
34	a	615	G
34	a	629	A
34	a	633	G
34	a	642	A
34	a	650	G
34	a	653	U
34	a	665	A
34	a	666	G
34	a	688	G
34	a	703	G
34	a	704	A
34	a	723	U
34	a	724	G
34	a	733	G
34	a	734	G
34	a	748	G
34	a	753	A
34	a	755	G
34	a	774	G
34	a	777	A
34	a	781	A
34	a	792	A
34	a	793	U
34	a	794	A
34	a	799	G
34	a	815	A
34	a	817	C
34	a	841	C
34	a	842	U
34	a	843	U
34	a	844	G
34	a	845	A

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Mol	Chain	Res	Type
34	a	846	G
34	a	851	G
34	a	867	G
34	a	885	G
34	a	902	G
34	a	914	A
34	a	934	C
34	a	935	A
34	a	953	G
34	a	954	G
34	a	955	U
34	a	956	U
34	a	957	U
34	a	958	A
34	a	960	U
34	a	969	A
34	a	971	G
34	a	975	A
34	a	976	G
34	a	977	A
34	a	980	C
34	a	983	A
34	a	985	C
34	a	986	U
34	a	988	G
34	a	989	U
34	a	990	C
34	a	992	U
34	a	993	G
34	a	994	A
34	a	995	C
34	a	996	A
34	a	997	U
34	a	999	C
34	a	1000	A
34	a	1004	A
34	a	1005	A
34	a	1006	G
34	a	1007	U
34	a	1011	C
34	a	1014	A
34	a	1015	G

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Mol	Chain	Res	Type
34	a	1020	G
34	a	1022	A
34	a	1023	U
34	a	1024	G
34	a	1027	C
34	a	1028	C
34	a	1029	U
34	a	1031	C
34	a	1032	G
34	a	1035	A
34	a	1036	A
34	a	1037	C
34	a	1040	U
34	a	1042	A
34	a	1043	G
34	a	1044	A
34	a	1065	U
34	a	1085	U
34	a	1094	G
34	a	1101	A
34	a	1104	G
34	a	1124	G
34	a	1125	U
34	a	1132	C
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1139	G
34	a	1159	U
34	a	1160	G
34	a	1167	A
34	a	1168	U
34	a	1183	U
34	a	1184	G
34	a	1196	A
34	a	1197	A
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1215	G
34	a	1227	A
34	a	1229	A

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Mol	Chain	Res	Type
34	a	1230	C
34	a	1236	A
34	a	1238	A
34	a	1239	A
34	a	1242	G
34	a	1243	C
34	a	1248	A
34	a	1250	A
34	a	1254	A
34	a	1255	G
34	a	1257	A
34	a	1258	G
34	a	1260	G
34	a	1261	A
34	a	1272	G
34	a	1275	A
34	a	1280	A
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1294	G
34	a	1297	G
34	a	1298	U
34	a	1299	A
34	a	1300	G
34	a	1302	C
34	a	1305	G
34	a	1306	A
34	a	1307	U
34	a	1309	G
34	a	1310	G
34	a	1311	A
34	a	1312	G
34	a	1314	C
34	a	1315	U
34	a	1316	G
34	a	1317	C
34	a	1323	G
34	a	1324	A
34	a	1335	U
34	a	1336	C
34	a	1344	C

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Mol	Chain	Res	Type
34	a	1345	U
34	a	1346	A
34	a	1347	G
34	a	1350	A
34	a	1353	G
34	a	1355	G
34	a	1356	G
34	a	1357	A
34	a	1362	A
34	a	1363	A
34	a	1370	G
34	a	1371	G
34	a	1372	U
34	a	1374	A
34	a	1378	C
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1397	C
34	a	1398	A
34	a	1419	G
34	a	1421	G
34	a	1422	G
34	a	1429	A
34	a	1432	G
34	a	1433	A
34	a	1440	U
34	a	1441	A
34	a	1442	G
34	a	1446	A
34	a	1451	U
34	a	1452	C
34	a	1472	U
34	a	1473	G
34	a	1475	G
34	a	1487	G
34	a	1492	A
34	a	1494	G
34	a	1497	G
34	a	1499	A
34	a	1506	U
34	a	1517	G

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Mol	Chain	Res	Type
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1538	C
34	a	1539	C
34	a	1540	U
55	v	9	G
55	v	18	G
55	v	19	G
55	v	20	H2U
55	v	21	A
55	v	30	G
55	v	33	U
55	v	34	C
55	v	37	A
55	v	44	A
55	v	45	G
55	v	47	U
55	v	48	C
55	v	52	G
55	v	56	C
55	v	70	G
55	v	74	C
55	v	76	A
56	w	10	G
56	w	13	C
56	w	16	U
56	w	17	C
56	w	18	G
56	w	19	G
56	w	20	U
56	w	21	A
56	w	45	U
56	w	46	G7M
56	w	47	U
56	w	48	C
56	w	49	C
56	w	59	U
56	w	60	U
56	w	67	C

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Mol	Chain	Res	Type
56	w	68	C
56	w	74	C
58	z	0	U

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	242	G
8	A	310	A
8	A	458	G
8	A	479	A
8	A	481	G
8	A	504	A
8	A	545	U
8	A	555	G
8	A	715	A
8	A	774	G
8	A	784	G
8	A	887	A
8	A	954	G
8	A	976	G
8	A	1014	A
8	A	1023	U
8	A	1062	G
8	A	1082	U
8	A	1090	A
8	A	1093	G
8	A	1361	G
8	A	1432	G
8	A	1451	C
8	A	1490	A
8	A	1715	G
8	A	1730	C
8	A	1847	G
8	A	2150	C
8	A	2158	A
8	A	2192	U
8	A	2287	A
8	A	2319	G
8	A	2468	A
8	A	2655	G
8	A	2756	U

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Mol	Chain	Res	Type
8	A	2796	U
8	A	2808	G
9	B	36	C
9	B	44	G
9	B	52	A
9	B	66	A

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

46 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$
8	5MU	A	1939	8	15,22,23	2.90	3 (20%)	16,32,35	2.92	2 (12%)
55	4SU	v	8	55	14,21,22	3.35	5 (35%)	15,30,33	1.25	2 (13%)
34	MA6	a	1519	34	19,26,27	1.00	1 (5%)	18,38,41	2.76	2 (11%)
34	G7M	a	527	34	20,26,27	3.43	7 (35%)	20,39,42	2.29	4 (20%)
57	FME	y	101	57	8,9,10	0.88	0	7,9,11	1.81	2 (28%)
55	PSU	v	55	55	17,21,22	0.99	1 (5%)	20,30,33	3.20	7 (35%)
8	PSU	A	2504	8	17,21,22	1.06	2 (11%)	20,30,33	3.13	6 (30%)
8	PSU	A	955	8	17,21,22	1.10	3 (17%)	20,30,33	3.02	6 (30%)
8	PSU	A	1917	8	17,21,22	1.04	2 (11%)	20,30,33	3.09	6 (30%)
8	PSU	A	2604	8	17,21,22	1.06	2 (11%)	20,30,33	3.02	6 (30%)
8	6MZ	A	1618	8	18,25,26	2.14	3 (16%)	16,36,39	1.85	3 (18%)
8	PSU	A	2457	8	17,21,22	1.11	3 (17%)	20,30,33	2.96	6 (30%)
55	5MU	v	54	55	15,22,23	2.86	3 (20%)	16,32,35	2.83	2 (12%)
8	G7M	A	2069	8	20,26,27	3.41	8 (40%)	20,39,42	2.72	7 (35%)
34	2MG	a	1516	34	19,26,27	4.79	8 (42%)	21,38,41	2.36	8 (38%)
8	5MC	A	1962	8	15,22,23	3.18	5 (33%)	19,32,35	1.19	2 (10%)
8	PSU	A	1911	8	17,21,22	1.07	3 (17%)	20,30,33	3.04	6 (30%)
34	2MG	a	966	34	19,26,27	4.75	8 (42%)	21,38,41	2.12	8 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	G7M	w	46	56	20,26,27	3.50	8 (40%)	20,39,42	2.52	5 (25%)
8	6MZ	A	2030	8	18,25,26	2.05	3 (16%)	16,36,39	2.30	3 (18%)
34	5MC	a	967	34	15,22,23	3.16	5 (33%)	19,32,35	1.24	3 (15%)
56	PSU	w	55	56	17,21,22	1.15	3 (17%)	20,30,33	3.07	7 (35%)
56	PSU	w	32	56	17,21,22	1.00	1 (5%)	20,30,33	3.15	7 (35%)
8	OMG	A	2251	8,55,59	18,26,27	3.49	7 (38%)	20,38,41	1.81	4 (20%)
8	5MC	A	747	8	15,22,23	3.12	5 (33%)	19,32,35	1.33	3 (15%)
56	5MU	w	54	56	15,22,23	2.85	3 (20%)	16,32,35	2.76	2 (12%)
8	OMC	A	2498	8,59	15,22,23	3.44	5 (33%)	17,31,34	1.27	1 (5%)
8	3TD	A	1915	8	17,22,23	3.68	6 (35%)	19,32,35	1.80	4 (21%)
55	H2U	v	20	55	18,21,22	3.08	5 (27%)	21,30,33	1.98	5 (23%)
8	PSU	A	2605	8	17,21,22	1.07	2 (11%)	20,30,33	3.04	5 (25%)
56	PSU	w	39	56	17,21,22	0.99	2 (11%)	20,30,33	3.06	6 (30%)
8	2MA	A	2503	8,59	17,25,26	3.75	5 (29%)	19,37,40	1.86	4 (21%)
34	PSU	a	516	34,59	17,21,22	0.97	1 (5%)	20,30,33	3.10	6 (30%)
8	2MG	A	1835	8	19,26,27	4.77	7 (36%)	21,38,41	2.14	8 (38%)
8	PSU	A	2580	8	17,21,22	1.16	3 (17%)	20,30,33	3.15	8 (40%)
8	OMU	A	2552	8,59	14,22,23	3.26	5 (35%)	14,31,34	0.73	0
34	4OC	a	1402	34	16,23,24	3.19	6 (37%)	17,32,35	1.30	1 (5%)
34	5MC	a	1407	34	15,22,23	3.14	5 (33%)	19,32,35	1.23	2 (10%)
8	PSU	A	746	8,59	17,21,22	1.09	2 (11%)	20,30,33	3.19	7 (35%)
34	MA6	a	1518	34	19,26,27	1.00	1 (5%)	18,38,41	2.71	2 (11%)
8	2MG	A	2445	8	19,26,27	4.72	8 (42%)	21,38,41	2.22	8 (38%)
34	2MG	a	1207	34	19,26,27	4.82	8 (42%)	21,38,41	2.15	8 (38%)
34	UR3	a	1498	34	14,22,23	2.79	4 (28%)	15,32,35	0.69	0
56	4SU	w	8	56	14,21,22	3.34	5 (35%)	15,30,33	1.25	2 (13%)
8	1MG	A	745	8	18,26,27	3.54	5 (27%)	19,39,42	2.26	2 (10%)
56	MIA	w	37	56	24,31,32	2.51	4 (16%)	26,44,47	3.11	9 (34%)

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
8	5MU	A	1939	8	-	4/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	4SU	v	8	55	-	0/5/25/26	0/2/2/2
34	MA6	a	1519	34	-	1/7/29/30	0/3/3/3
34	G7M	a	527	34	-	1/3/25/26	0/3/3/3
57	FME	y	101	57	-	5/7/9/11	-
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
8	PSU	A	2504	8	-	2/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	2/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	0/5/27/28	0/3/3/3
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	0/5/25/26	0/2/2/2
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
8	5MC	A	1962	8	-	2/5/25/26	0/2/2/2
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
34	2MG	a	966	34	-	0/5/27/28	0/3/3/3
56	G7M	w	46	56	-	0/3/25/26	0/3/3/3
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3
34	5MC	a	967	34	-	0/5/25/26	0/2/2/2
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
8	OMG	A	2251	8,55,59	-	1/5/27/28	0/3/3/3
8	5MC	A	747	8	-	0/5/25/26	0/2/2/2
56	5MU	w	54	56	-	0/5/25/26	0/2/2/2
8	OMC	A	2498	8,59	-	2/7/27/28	0/2/2/2
8	3TD	A	1915	8	-	2/7/25/26	0/2/2/2
55	H2U	v	20	55	-	3/7/38/39	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2
8	2MA	A	2503	8,59	-	2/3/25/26	0/3/3/3
34	PSU	a	516	34,59	-	0/7/25/26	0/2/2/2
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
8	OMU	A	2552	8,59	-	1/7/27/28	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
34	5MC	a	1407	34	-	0/5/25/26	0/2/2/2
8	PSU	A	746	8,59	-	3/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	UR3	a	1498	34	-	0/5/25/26	0/2/2/2
56	4SU	w	8	56	-	0/5/25/26	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
56	MIA	w	37	56	-	2/11/33/34	0/3/3/3

All (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1207	2MG	C2-N2	15.71	1.47	1.34
34	a	1516	2MG	C2-N2	15.65	1.47	1.34
8	A	1835	2MG	C2-N2	15.52	1.47	1.34
34	a	966	2MG	C2-N2	15.37	1.47	1.34
8	A	2445	2MG	C2-N2	15.30	1.47	1.34
55	v	20	H2U	C2-N1	9.43	1.49	1.35
55	v	54	5MU	C4-C5	9.39	1.61	1.41
8	A	1939	5MU	C4-C5	9.21	1.61	1.41
56	w	54	5MU	C4-C5	9.21	1.61	1.41
8	A	2503	2MA	C4-N3	8.81	1.49	1.35
8	A	1835	2MG	C4-N3	8.78	1.49	1.35
34	a	966	2MG	C4-N3	8.76	1.49	1.35
34	a	1207	2MG	C4-N3	8.75	1.49	1.35
34	a	527	G7M	C4-N3	8.73	1.49	1.35
8	A	745	1MG	C4-N3	8.67	1.49	1.35
56	w	46	G7M	C4-N3	8.63	1.49	1.35
8	A	2498	OMC	C6-N1	8.59	1.46	1.35
34	a	1516	2MG	C4-N3	8.58	1.49	1.35
8	A	2069	G7M	C4-N3	8.52	1.49	1.35
8	A	2445	2MG	C4-N3	8.50	1.49	1.35
8	A	2251	OMG	C4-N3	8.42	1.48	1.35
8	A	1915	3TD	C6-C5	7.88	1.50	1.38
8	A	2503	2MA	C6-C5	7.72	1.53	1.41
8	A	1618	6MZ	C6-N6	7.62	1.47	1.35
34	a	1402	4OC	C6-N1	7.61	1.45	1.35
56	w	46	G7M	C6-C5	7.60	1.54	1.41
8	A	1962	5MC	C4-N3	7.45	1.45	1.35
34	a	1498	UR3	C6-N1	7.43	1.45	1.35
34	a	967	5MC	C4-N3	7.42	1.45	1.35
55	v	8	4SU	C5-C4	7.37	1.46	1.38
34	a	527	G7M	C6-C5	7.33	1.54	1.41
56	w	8	4SU	C5-C4	7.30	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	747	5MC	C4-N3	7.28	1.45	1.35
34	a	1407	5MC	C4-N3	7.26	1.45	1.35
8	A	2030	6MZ	C6-N6	7.21	1.46	1.35
8	A	2069	G7M	C6-C5	7.19	1.53	1.41
56	w	37	MIA	C13-C14	7.19	1.53	1.32
56	w	37	MIA	C2-S10	7.01	1.81	1.75
34	a	1207	2MG	C6-C5	6.98	1.53	1.41
8	A	2445	2MG	C6-C5	6.96	1.53	1.41
34	a	1516	2MG	C6-C5	6.93	1.53	1.41
8	A	1915	3TD	C5-C1'	-6.84	1.46	1.52
8	A	2251	OMG	C6-C5	6.82	1.53	1.41
8	A	2503	2MA	C2-N3	6.80	1.46	1.34
8	A	1835	2MG	C6-C5	6.79	1.53	1.41
8	A	2552	OMU	C6-N1	6.77	1.44	1.35
34	a	966	2MG	C6-C5	6.73	1.53	1.41
8	A	745	1MG	C2-N3	6.67	1.44	1.34
8	A	2552	OMU	C4-N3	6.63	1.44	1.33
8	A	745	1MG	C2-N2	6.55	1.47	1.33
8	A	745	1MG	C6-C5	6.53	1.51	1.41
55	v	20	H2U	C2-N3	6.49	1.49	1.38
8	A	2498	OMC	C4-N3	6.22	1.45	1.35
56	w	46	G7M	C6-N1	6.05	1.43	1.33
8	A	1915	3TD	C4-N3	6.01	1.47	1.38
8	A	2069	G7M	C6-N1	5.83	1.43	1.33
34	a	527	G7M	C6-N1	5.70	1.43	1.33
8	A	2503	2MA	C2-N1	5.69	1.44	1.34
34	a	1516	2MG	C6-N1	5.65	1.42	1.33
55	v	8	4SU	C6-N1	5.61	1.42	1.35
56	w	37	MIA	C6-N6	5.61	1.44	1.34
8	A	2251	OMG	C6-N1	5.60	1.42	1.33
34	a	966	2MG	C6-N1	5.59	1.42	1.33
56	w	8	4SU	C6-N1	5.58	1.42	1.35
8	A	2552	OMU	C2-N3	5.57	1.49	1.38
8	A	1915	3TD	C2-N1	5.56	1.49	1.38
8	A	1835	2MG	C6-N1	5.55	1.42	1.33
8	A	2445	2MG	C6-N1	5.51	1.42	1.33
34	a	1207	2MG	C6-N1	5.51	1.42	1.33
8	A	2251	OMG	C2-N2	5.49	1.44	1.33
34	a	967	5MC	C2-N3	5.46	1.49	1.38
8	A	1962	5MC	C2-N3	5.40	1.48	1.38
8	A	1939	5MU	C4-N3	-5.36	1.23	1.33
8	A	747	5MC	C2-N3	5.33	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C6-N1	5.31	1.45	1.34
34	a	1407	5MC	C2-N3	5.30	1.48	1.38
56	w	46	G7M	C2-N2	5.25	1.44	1.33
8	A	1962	5MC	C5-C4	5.22	1.49	1.41
34	a	527	G7M	C2-N2	5.17	1.44	1.33
8	A	2498	OMC	C6-C5	5.17	1.49	1.38
34	a	1407	5MC	C5-C4	5.13	1.49	1.41
56	w	46	G7M	C2-N1	5.12	1.44	1.35
8	A	2498	OMC	C2-N3	5.09	1.48	1.38
34	a	1498	UR3	C6-C5	5.06	1.49	1.38
8	A	2069	G7M	C2-N2	5.06	1.44	1.33
56	w	54	5MU	C4-N3	-5.04	1.24	1.33
8	A	747	5MC	C5-C4	5.01	1.49	1.41
34	a	967	5MC	C5-C4	4.98	1.49	1.41
34	a	1402	4OC	C4-N3	4.98	1.44	1.34
55	v	20	H2U	C4-N3	4.97	1.46	1.37
34	a	1402	4OC	C6-C5	4.97	1.49	1.38
34	a	967	5MC	C4-N4	4.95	1.46	1.34
55	v	8	4SU	C2-N3	4.91	1.47	1.38
8	A	747	5MC	C4-N4	4.90	1.46	1.34
55	v	54	5MU	C4-N3	-4.89	1.24	1.33
8	A	1962	5MC	C4-N4	4.89	1.46	1.34
34	a	1407	5MC	C4-N4	4.89	1.46	1.34
56	w	8	4SU	C4-S4	-4.85	1.58	1.67
8	A	2069	G7M	C2-N1	4.84	1.44	1.35
55	v	8	4SU	C4-S4	-4.83	1.58	1.67
56	w	8	4SU	C6-C5	4.82	1.48	1.38
34	a	1402	4OC	C2-N3	4.82	1.47	1.38
56	w	8	4SU	C2-N3	4.79	1.47	1.38
55	v	8	4SU	C6-C5	4.77	1.48	1.38
34	a	527	G7M	C2-N1	4.76	1.43	1.35
8	A	2251	OMG	C2-N1	4.72	1.43	1.35
8	A	2552	OMU	C6-C5	4.46	1.47	1.38
8	A	1915	3TD	C4-C5	4.42	1.50	1.41
34	a	1498	UR3	C4-N3	4.25	1.44	1.38
34	a	1402	4OC	C5-C4	4.09	1.48	1.39
8	A	2503	2MA	C6-N1	4.08	1.43	1.35
34	a	966	2MG	C2-N3	3.77	1.46	1.34
34	a	1207	2MG	C2-N3	3.76	1.46	1.34
34	a	1402	4OC	C4-N4	3.72	1.44	1.36
8	A	1835	2MG	C2-N3	3.71	1.45	1.34
34	a	1516	2MG	C2-N3	3.66	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1407	5MC	C6-C5	3.59	1.50	1.40
8	A	2445	2MG	C2-N3	3.58	1.45	1.34
34	a	967	5MC	C6-C5	3.47	1.49	1.40
8	A	1962	5MC	C6-C5	3.47	1.49	1.40
8	A	747	5MC	C6-C5	3.46	1.49	1.40
8	A	745	1MG	C6-N1	3.31	1.43	1.38
8	A	2030	6MZ	C5-C4	-3.08	1.32	1.40
8	A	2445	2MG	O6-C6	-3.06	1.16	1.24
56	w	55	PSU	C4-N3	3.06	1.38	1.33
8	A	1835	2MG	O6-C6	-3.06	1.16	1.24
34	a	966	2MG	O6-C6	-2.99	1.17	1.24
34	a	966	2MG	C2-N1	2.97	1.43	1.34
34	a	1207	2MG	O6-C6	-2.97	1.17	1.24
34	a	1516	2MG	C2-N1	2.96	1.43	1.34
34	a	1207	2MG	C2-N1	2.96	1.43	1.34
34	a	1516	2MG	O6-C6	-2.95	1.17	1.24
8	A	1618	6MZ	C5-C4	-2.94	1.33	1.40
55	v	55	PSU	C4-N3	2.94	1.38	1.33
8	A	1835	2MG	C2-N1	2.93	1.43	1.34
8	A	2445	2MG	C2-N1	2.91	1.43	1.34
56	w	37	MIA	C5-C4	-2.85	1.33	1.40
56	w	32	PSU	C4-N3	2.80	1.37	1.33
34	a	516	PSU	C4-N3	2.80	1.37	1.33
8	A	1917	PSU	C4-N3	2.78	1.37	1.33
8	A	2504	PSU	C4-N3	2.72	1.37	1.33
34	a	1518	MA6	C5-C4	-2.70	1.33	1.40
8	A	746	PSU	C4-N3	2.69	1.37	1.33
34	a	1519	MA6	C5-C4	-2.64	1.33	1.40
8	A	1911	PSU	C4-N3	2.63	1.37	1.33
56	w	46	G7M	C2-N3	2.62	1.46	1.34
8	A	2580	PSU	O4'-C1'	-2.60	1.40	1.44
8	A	2580	PSU	C4-N3	2.59	1.37	1.33
8	A	2457	PSU	C4-N3	2.59	1.37	1.33
8	A	1618	6MZ	C2-N3	2.58	1.36	1.32
34	a	527	G7M	C2-N3	2.58	1.46	1.34
8	A	2604	PSU	C4-N3	2.57	1.37	1.33
8	A	1939	5MU	O4-C4	-2.56	1.18	1.24
8	A	2498	OMC	C4-N4	2.55	1.42	1.35
8	A	955	PSU	C4-N3	2.55	1.37	1.33
8	A	2069	G7M	O6-C6	-2.52	1.18	1.24
8	A	2605	PSU	C4-N3	2.52	1.37	1.33
34	a	527	G7M	O6-C6	-2.51	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1498	UR3	O4-C4	-2.50	1.18	1.24
8	A	2251	OMG	O6-C6	-2.48	1.18	1.24
56	w	54	5MU	O4-C4	-2.48	1.18	1.24
56	w	55	PSU	C5-C1'	-2.47	1.50	1.52
56	w	39	PSU	C4-N3	2.45	1.37	1.33
8	A	2552	OMU	O4-C4	-2.44	1.18	1.24
8	A	2069	G7M	C2-N3	2.44	1.46	1.34
55	v	54	5MU	O4-C4	-2.38	1.18	1.24
8	A	2069	G7M	C5-C4	-2.37	1.36	1.39
8	A	2251	OMG	C2-N3	2.36	1.45	1.34
8	A	2030	6MZ	C2-N3	2.35	1.35	1.32
8	A	955	PSU	C5-C1'	-2.33	1.50	1.52
56	w	46	G7M	O6-C6	-2.32	1.18	1.24
55	v	20	H2U	O4-C4	-2.31	1.18	1.23
55	v	20	H2U	O2-C2	-2.27	1.18	1.23
8	A	1911	PSU	C5-C1'	-2.20	1.50	1.52
8	A	2580	PSU	C5-C1'	-2.19	1.50	1.52
8	A	2457	PSU	C5-C1'	-2.18	1.50	1.52
8	A	746	PSU	O4'-C1'	-2.17	1.41	1.44
34	a	1516	2MG	C5-C4	-2.15	1.35	1.40
56	w	55	PSU	O4'-C1'	-2.14	1.41	1.44
8	A	2457	PSU	O4'-C1'	-2.14	1.41	1.44
8	A	1917	PSU	O4'-C1'	-2.13	1.41	1.44
8	A	2604	PSU	C5-C1'	-2.13	1.50	1.52
8	A	2445	2MG	C5-C4	-2.08	1.35	1.40
8	A	2605	PSU	C5-C1'	-2.08	1.50	1.52
56	w	39	PSU	O4'-C1'	-2.06	1.41	1.44
56	w	46	G7M	C5-C4	-2.05	1.36	1.39
8	A	955	PSU	O4'-C1'	-2.05	1.41	1.44
8	A	2504	PSU	O4'-C1'	-2.04	1.41	1.44
8	A	1911	PSU	O4'-C1'	-2.03	1.41	1.44
34	a	966	2MG	C5-C4	-2.01	1.35	1.40
34	a	1207	2MG	C5-C4	-2.00	1.35	1.40

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	516	PSU	N1-C2-N3	-10.66	119.96	128.43
55	v	55	PSU	N1-C2-N3	-10.56	120.03	128.43
56	w	32	PSU	N1-C2-N3	-10.44	120.13	128.43
8	A	746	PSU	N1-C2-N3	-10.40	120.16	128.43
56	w	39	PSU	N1-C2-N3	-10.33	120.22	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1917	PSU	N1-C2-N3	-10.24	120.29	128.43
8	A	2504	PSU	N1-C2-N3	-10.21	120.32	128.43
8	A	2605	PSU	N1-C2-N3	-10.18	120.34	128.43
8	A	1911	PSU	N1-C2-N3	-10.12	120.38	128.43
8	A	2580	PSU	N1-C2-N3	-10.04	120.45	128.43
34	a	1519	MA6	N1-C6-N6	-10.03	106.50	117.06
8	A	2457	PSU	N1-C2-N3	-10.01	120.47	128.43
8	A	2604	PSU	N1-C2-N3	-9.99	120.49	128.43
8	A	955	PSU	N1-C2-N3	-9.91	120.55	128.43
34	a	1518	MA6	N1-C6-N6	-9.73	106.81	117.06
56	w	55	PSU	N1-C2-N3	-9.69	120.73	128.43
8	A	1939	5MU	C5-C6-N1	-9.47	111.99	122.19
56	w	37	MIA	C12-C13-C14	-9.05	109.52	127.14
56	w	37	MIA	C11-S10-C2	8.78	108.82	102.27
55	v	54	5MU	C5-C6-N1	-8.58	112.95	122.19
8	A	745	1MG	C1'-N9-C4	-8.30	112.06	126.64
56	w	54	5MU	C5-C6-N1	-8.30	113.25	122.19
56	w	46	G7M	C1'-N9-C4	-7.95	112.67	126.64
8	A	2069	G7M	C1'-N9-C4	-7.75	113.03	126.64
55	v	54	5MU	C4-N3-C2	7.08	121.12	115.14
56	w	54	5MU	C4-N3-C2	7.01	121.06	115.14
55	v	20	H2U	C4-N3-C2	-6.66	120.27	125.79
8	A	1939	5MU	C4-N3-C2	6.34	120.50	115.14
34	a	527	G7M	C1'-N9-C4	-6.20	115.74	126.64
8	A	2030	6MZ	C9-N6-C6	-5.88	117.81	122.87
8	A	2503	2MA	C2-N3-C4	5.80	120.23	115.52
8	A	1917	PSU	C4-N3-C2	5.79	120.03	115.14
56	w	55	PSU	C4-N3-C2	5.78	120.02	115.14
34	a	516	PSU	C4-N3-C2	5.73	119.98	115.14
8	A	2030	6MZ	N3-C2-N1	-5.70	119.76	128.68
34	a	1518	MA6	N3-C2-N1	-5.69	119.79	128.68
34	a	1516	2MG	C1'-N9-C4	-5.63	116.75	126.64
56	w	32	PSU	C4-N3-C2	5.63	119.90	115.14
55	v	55	PSU	C4-N3-C2	5.58	119.86	115.14
34	a	1519	MA6	N3-C2-N1	-5.57	119.98	128.68
8	A	2069	G7M	N3-C2-N1	-5.51	119.87	127.22
8	A	2580	PSU	C4-N3-C2	5.45	119.75	115.14
56	w	55	PSU	C5-C4-N3	-5.44	118.35	125.36
8	A	746	PSU	C4-N3-C2	5.43	119.72	115.14
56	w	39	PSU	C4-N3-C2	5.42	119.72	115.14
8	A	1618	6MZ	N3-C2-N1	-5.40	120.23	128.68
8	A	2504	PSU	C4-N3-C2	5.39	119.69	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1911	PSU	C4-N3-C2	5.36	119.67	115.14
8	A	2251	OMG	N3-C2-N1	-5.29	120.16	127.22
8	A	2605	PSU	C4-N3-C2	5.20	119.53	115.14
34	a	527	G7M	N3-C2-N1	-5.11	120.40	127.22
8	A	955	PSU	C4-N3-C2	5.10	119.45	115.14
56	w	46	G7M	N3-C2-N1	-5.07	120.46	127.22
8	A	2457	PSU	C4-N3-C2	4.94	119.31	115.14
8	A	2604	PSU	C4-N3-C2	4.94	119.31	115.14
8	A	1915	3TD	C5-C1'-C2'	-4.67	106.99	115.32
56	w	37	MIA	C15-C14-C13	-4.65	109.22	122.65
8	A	2580	PSU	C5-C4-N3	-4.61	119.43	125.36
34	a	527	G7M	C2-N3-C4	4.60	120.61	115.36
56	w	37	MIA	C16-C14-C13	-4.60	109.35	122.65
8	A	1917	PSU	C5-C4-N3	-4.60	119.44	125.36
34	a	1402	4OC	CM4-N4-C4	-4.56	119.05	122.97
8	A	1835	2MG	C2-N3-C4	4.49	120.38	115.28
8	A	2445	2MG	C1'-N9-C4	-4.49	118.75	126.64
34	a	1207	2MG	C1'-N9-C4	-4.46	118.80	126.64
8	A	2069	G7M	C2-N3-C4	4.42	120.41	115.36
34	a	1516	2MG	C2-N3-C4	4.36	120.23	115.28
8	A	1911	PSU	C5-C4-N3	-4.33	119.78	125.36
8	A	2445	2MG	C2-N3-C4	4.33	120.19	115.28
8	A	955	PSU	C5-C4-N3	-4.29	119.83	125.36
34	a	1207	2MG	C2-N3-C4	4.27	120.12	115.28
8	A	746	PSU	C5-C4-N3	-4.26	119.88	125.36
8	A	2498	OMC	C2-N3-C4	4.24	120.64	116.34
8	A	2504	PSU	C5-C4-N3	-4.22	119.92	125.36
34	a	516	PSU	C5-C4-N3	-4.18	119.97	125.36
8	A	745	1MG	C2-N3-C4	4.18	120.13	115.36
56	w	32	PSU	C5-C4-N3	-4.17	119.99	125.36
8	A	2504	PSU	C5-C1'-C2'	-4.16	107.90	115.32
8	A	2457	PSU	C5-C4-N3	-4.16	120.01	125.36
8	A	2605	PSU	C5-C4-N3	-4.15	120.01	125.36
34	a	966	2MG	CM2-N2-C2	-4.14	118.59	123.59
8	A	746	PSU	C5-C1'-C2'	-4.14	107.93	115.32
34	a	966	2MG	C2-N3-C4	4.12	119.95	115.28
56	w	46	G7M	C2-N3-C4	4.11	120.05	115.36
55	v	55	PSU	C5-C4-N3	-4.09	120.09	125.36
8	A	2604	PSU	C5-C4-N3	-4.07	120.12	125.36
8	A	2251	OMG	C2-N3-C4	4.06	119.99	115.36
34	a	1516	2MG	N3-C2-N1	-3.98	119.94	126.23
34	a	966	2MG	C1'-N9-C4	-3.98	119.66	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2445	2MG	CM2-N2-C2	-3.94	118.83	123.59
8	A	2445	2MG	N2-C2-N1	3.89	120.70	116.96
8	A	1835	2MG	C1'-N9-C4	-3.86	119.85	126.64
8	A	1835	2MG	N3-C2-N1	-3.83	120.18	126.23
8	A	1618	6MZ	C9-N6-C6	-3.81	119.59	122.87
34	a	1207	2MG	N3-C2-N1	-3.76	120.28	126.23
8	A	2457	PSU	C5-C6-N1	-3.76	119.81	124.44
8	A	2445	2MG	N3-C2-N1	-3.75	120.29	126.23
34	a	1516	2MG	N2-C2-N1	3.75	120.57	116.96
56	w	39	PSU	C5-C4-N3	-3.75	120.53	125.36
8	A	2605	PSU	C5-C6-N1	-3.74	119.85	124.44
8	A	2604	PSU	C5-C6-N1	-3.67	119.93	124.44
8	A	1835	2MG	CM2-N2-C2	-3.66	119.18	123.59
34	a	1516	2MG	CM2-N2-C2	-3.63	119.21	123.59
8	A	2030	6MZ	C1'-N9-C4	-3.62	120.28	126.64
56	w	37	MIA	N3-C2-N1	-3.61	120.34	126.98
34	a	1407	5MC	C2-N3-C4	3.58	120.34	116.02
34	a	966	2MG	N3-C2-N1	-3.58	120.57	126.23
8	A	955	PSU	C5-C6-N1	-3.53	120.11	124.44
8	A	747	5MC	C2-N3-C4	3.49	120.23	116.02
8	A	1911	PSU	C5-C6-N1	-3.48	120.17	124.44
8	A	2580	PSU	C5-C6-N1	-3.45	120.20	124.44
8	A	746	PSU	C5-C6-N1	-3.43	120.22	124.44
34	a	1207	2MG	CM2-N2-C2	-3.43	119.45	123.59
8	A	1962	5MC	C2-N3-C4	3.39	120.11	116.02
56	w	37	MIA	C2-N3-C4	3.35	119.95	115.32
8	A	1915	3TD	O4'-C1'-C5	3.31	115.06	109.93
34	a	967	5MC	C2-N3-C4	3.27	119.97	116.02
56	w	8	4SU	C2-N3-C4	3.27	119.89	115.15
56	w	39	PSU	C5-C6-N1	-3.25	120.45	124.44
8	A	1835	2MG	N2-C2-N1	3.24	120.07	116.96
55	v	8	4SU	C2-N3-C4	3.23	119.83	115.15
55	v	20	H2U	N3-C2-N1	3.23	120.07	116.65
56	w	55	PSU	C5-C6-N1	-3.22	120.48	124.44
8	A	2457	PSU	C6-N1-C2	3.21	120.66	115.36
8	A	2605	PSU	C6-N1-C2	3.21	120.66	115.36
57	y	101	FME	CA-N-CN	3.21	127.75	122.82
8	A	2504	PSU	C5-C6-N1	-3.20	120.51	124.44
8	A	2604	PSU	C6-N1-C2	3.19	120.63	115.36
8	A	746	PSU	C6-N1-C2	3.18	120.61	115.36
8	A	2503	2MA	N3-C2-N1	-3.16	119.90	125.72
8	A	955	PSU	C5-C1'-C2'	-3.14	109.71	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	v	55	PSU	C6-N1-C2	3.14	120.54	115.36
56	w	39	PSU	C6-N1-C2	3.14	120.53	115.36
57	y	101	FME	C-CA-N	3.11	115.35	109.73
56	w	32	PSU	C6-N1-C2	3.10	120.47	115.36
55	v	8	4SU	C5-C4-N3	-3.09	119.70	123.83
8	A	955	PSU	C6-N1-C2	3.08	120.44	115.36
8	A	1911	PSU	C6-N1-C2	3.06	120.41	115.36
8	A	2504	PSU	C6-N1-C2	3.04	120.38	115.36
34	a	1207	2MG	N2-C2-N3	3.03	119.87	116.96
55	v	55	PSU	C5-C6-N1	-3.01	120.74	124.44
34	a	1207	2MG	N2-C2-N1	3.01	119.85	116.96
8	A	2580	PSU	C5-C1'-C2'	3.00	120.67	115.32
8	A	2580	PSU	C6-N1-C2	3.00	120.30	115.36
56	w	8	4SU	C5-C4-N3	-2.99	119.83	123.83
8	A	1915	3TD	C5-C6-N1	-2.99	120.77	124.44
56	w	32	PSU	C5-C6-N1	-2.99	120.77	124.44
8	A	1917	PSU	C6-N1-C2	2.96	120.25	115.36
55	v	55	PSU	C5-C1'-C2'	-2.96	110.04	115.32
34	a	516	PSU	C6-N1-C2	2.94	120.21	115.36
34	a	966	2MG	N2-C2-N1	2.94	119.78	116.96
8	A	1835	2MG	N2-C2-N3	2.91	119.75	116.96
8	A	1917	PSU	C5-C6-N1	-2.90	120.88	124.44
55	v	20	H2U	C5-C6-N1	2.83	120.95	111.61
55	v	55	PSU	O4'-C1'-C5	2.81	114.28	109.93
8	A	2604	PSU	C5-C1'-C2'	-2.81	110.31	115.32
34	a	966	2MG	N2-C2-N3	2.79	119.64	116.96
56	w	55	PSU	C6-N1-C2	2.78	119.94	115.36
8	A	1915	3TD	C6-N1-C2	2.69	119.81	115.36
56	w	39	PSU	C5-C1'-C2'	-2.67	110.55	115.32
55	v	20	H2U	C5-C4-N3	2.67	119.65	116.65
8	A	2503	2MA	C5-C6-N1	-2.66	120.27	123.06
56	w	32	PSU	O4'-C1'-C5	2.66	114.05	109.93
34	a	1516	2MG	N2-C2-N3	2.63	119.49	116.96
8	A	2580	PSU	O4'-C1'-C2'	2.54	108.78	104.66
8	A	2445	2MG	C5-C6-N1	-2.50	120.02	123.43
55	v	20	H2U	O2-C2-N1	-2.47	120.00	123.11
34	a	516	PSU	C5-C6-N1	-2.47	121.40	124.44
8	A	1835	2MG	C5-C6-N1	-2.42	120.12	123.43
8	A	747	5MC	C5-C6-N1	-2.42	119.59	122.19
56	w	37	MIA	C16-C14-C15	-2.41	109.27	114.60
8	A	1911	PSU	C5-C1'-C2'	-2.41	111.02	115.32
56	w	37	MIA	S10-C2-N1	2.40	124.31	116.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1207	2MG	C5-C6-N1	-2.39	120.16	123.43
8	A	2069	G7M	O3'-C3'-C2'	2.39	119.57	111.82
56	w	46	G7M	C5-C6-N1	-2.39	120.16	123.43
34	a	1516	2MG	C6-N1-C2	2.39	119.45	115.18
8	A	2251	OMG	C5-C6-N1	-2.37	120.20	123.43
8	A	746	PSU	O4'-C1'-C5	2.35	113.57	109.93
8	A	2445	2MG	C6-N1-C2	2.33	119.36	115.18
34	a	1516	2MG	C5-C6-N1	-2.33	120.24	123.43
34	a	966	2MG	C5-C6-N1	-2.33	120.25	123.43
34	a	1207	2MG	C6-N1-C2	2.32	119.34	115.18
8	A	1835	2MG	C6-N1-C2	2.32	119.33	115.18
8	A	2069	G7M	C5-C6-N1	-2.32	120.26	123.43
8	A	2069	G7M	C6-N1-C2	2.30	119.59	115.93
34	a	527	G7M	C5-C6-N1	-2.29	120.31	123.43
8	A	1618	6MZ	C1'-N9-C4	-2.24	122.71	126.64
8	A	1962	5MC	C5-C6-N1	-2.21	119.81	122.19
8	A	2251	OMG	C6-N1-C2	2.21	119.44	115.93
56	w	37	MIA	C12-N6-C6	-2.19	119.30	122.55
56	w	32	PSU	C5-C1'-C2'	-2.17	111.45	115.32
8	A	2580	PSU	O4'-C1'-C5	-2.17	106.57	109.93
34	a	966	2MG	C6-N1-C2	2.14	119.00	115.18
8	A	2445	2MG	N2-C2-N3	2.13	119.01	116.96
8	A	747	5MC	N4-C4-N3	2.12	120.03	117.03
34	a	967	5MC	C5-C6-N1	-2.12	119.91	122.19
34	a	516	PSU	O4'-C1'-C2'	2.09	108.04	104.66
56	w	55	PSU	C5-C1'-C2'	-2.07	111.62	115.32
34	a	967	5MC	N4-C4-N3	2.07	119.96	117.03
8	A	2069	G7M	N2-C2-N1	2.06	120.46	117.25
34	a	1407	5MC	C5-C6-N1	-2.06	119.98	122.19
8	A	1917	PSU	O4'-C1'-C2'	2.06	107.99	104.66
56	w	46	G7M	C6-N1-C2	2.05	119.18	115.93
8	A	2457	PSU	O4'-C1'-C2'	2.04	107.97	104.66
8	A	2503	2MA	C1'-N9-C4	-2.02	123.08	126.64
56	w	55	PSU	O4'-C1'-C2'	2.02	107.94	104.66

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	20	H2U	O4'-C4'-C5'-O5'
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
8	A	746	PSU	O4'-C1'-C5-C4
8	A	746	PSU	O4'-C1'-C5-C6
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1939	5MU	C2'-C1'-N1-C6
8	A	1939	5MU	O4'-C1'-N1-C6
8	A	1962	5MC	O4'-C1'-N1-C6
8	A	1962	5MC	C2'-C1'-N1-C6
8	A	2251	OMG	C1'-C2'-O2'-CM2
8	A	2445	2MG	C3'-C4'-C5'-O5'
8	A	2498	OMC	O4'-C4'-C5'-O5'
8	A	2552	OMU	C1'-C2'-O2'-CM2
56	w	32	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C6
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
56	w	39	PSU	O4'-C1'-C5-C4
57	y	101	FME	CB-CA-N-CN
57	y	101	FME	N-CA-CB-CG
57	y	101	FME	C-CA-CB-CG
8	A	1939	5MU	O4'-C4'-C5'-O5'
8	A	2030	6MZ	O4'-C4'-C5'-O5'
8	A	2030	6MZ	C3'-C4'-C5'-O5'
8	A	2503	2MA	O4'-C4'-C5'-O5'
8	A	2503	2MA	C3'-C4'-C5'-O5'
8	A	2498	OMC	C3'-C4'-C5'-O5'
8	A	2445	2MG	O4'-C4'-C5'-O5'
8	A	746	PSU	C2'-C1'-C5-C6
8	A	1939	5MU	C3'-C4'-C5'-O5'
55	v	20	H2U	C4'-C5'-O5'-P
8	A	1835	2MG	O4'-C4'-C5'-O5'
8	A	1915	3TD	O4'-C1'-C5-C6
56	w	39	PSU	O4'-C1'-C5-C6
8	A	2504	PSU	O4'-C4'-C5'-O5'
34	a	1402	4OC	O4'-C4'-C5'-O5'
57	y	101	FME	CA-CB-CG-SD
57	y	101	FME	CB-CG-SD-CE
8	A	1835	2MG	C3'-C4'-C5'-O5'
56	w	39	PSU	C2'-C1'-C5-C6
34	a	527	G7M	C4'-C5'-O5'-P
8	A	1917	PSU	C2'-C1'-C5-C6
8	A	1917	PSU	C4'-C5'-O5'-P
8	A	2504	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	v	20	H2U	C2'-C1'-N1-C6
8	A	2069	G7M	O4'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
34	a	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 371 ligands modelled in this entry, 367 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
62	AM2	a	1685	-	40,40,40	1.67	7 (17%)	53,60,60	1.08	5 (9%)
62	AM2	a	1684	-	40,40,40	1.62	8 (20%)	53,60,60	1.10	3 (5%)
62	AM2	a	1689	-	40,40,40	1.64	8 (20%)	53,60,60	1.09	4 (7%)
62	AM2	a	1682	-	40,40,40	1.61	9 (22%)	53,60,60	1.05	3 (5%)

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
62	AM2	a	1685	-	-	4/12/84/84	0/4/4/4
62	AM2	a	1684	-	-	4/12/84/84	0/4/4/4

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	AM2	a	1689	-	-	3/12/84/84	0/4/4/4
62	AM2	a	1682	-	-	1/12/84/84	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	a	1685	AM2	OA4-CA1	4.60	1.53	1.41
62	a	1689	AM2	OA4-CA1	4.58	1.53	1.41
62	a	1684	AM2	OA4-CA1	4.49	1.53	1.41
62	a	1682	AM2	OA4-CA1	4.32	1.52	1.41
62	a	1685	AM2	OA4-CA5	3.77	1.49	1.44
62	a	1685	AM2	OA5-CA8	3.76	1.51	1.41
62	a	1689	AM2	OA4-CA5	3.73	1.49	1.44
62	a	1685	AM2	OB1-CB1	3.69	1.51	1.41
62	a	1684	AM2	OA4-CA5	3.62	1.49	1.44
62	a	1689	AM2	OA5-CA8	3.52	1.50	1.41
62	a	1684	AM2	OA5-CA8	3.49	1.50	1.41
62	a	1689	AM2	OB1-CB1	3.49	1.50	1.41
62	a	1684	AM2	OB1-CB1	3.48	1.50	1.41
62	a	1682	AM2	OB1-CB1	3.43	1.50	1.41
62	a	1685	AM2	OA5-CA4	3.41	1.52	1.44
62	a	1682	AM2	OA5-CA8	3.34	1.50	1.41
62	a	1682	AM2	OA4-CA5	3.15	1.48	1.44
62	a	1689	AM2	OA5-CA4	3.14	1.52	1.44
62	a	1684	AM2	OA5-CA4	3.09	1.51	1.44
62	a	1682	AM2	OA5-CA4	2.92	1.51	1.44
62	a	1682	AM2	CB3-CB4	-2.90	1.49	1.53
62	a	1684	AM2	CB3-CB4	-2.79	1.50	1.53
62	a	1685	AM2	CB3-CB4	-2.63	1.50	1.53
62	a	1689	AM2	CB3-CB4	-2.58	1.50	1.53
62	a	1682	AM2	OA1-CA1	-2.47	1.34	1.41
62	a	1684	AM2	OA1-CA1	-2.37	1.35	1.41
62	a	1682	AM2	OA8-CA8	-2.32	1.35	1.41
62	a	1689	AM2	OA1-CA1	-2.31	1.35	1.41
62	a	1685	AM2	OA1-CA1	-2.27	1.35	1.41
62	a	1689	AM2	OA8-CA8	-2.15	1.35	1.41
62	a	1682	AM2	OA8-CB1	-2.09	1.35	1.41
62	a	1684	AM2	OA8-CA8	-2.01	1.36	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	a	1684	AM2	CA9-NA7-CA7	-3.48	109.32	114.38
62	a	1682	AM2	CA9-NA7-CA7	-3.46	109.35	114.38
62	a	1684	AM2	CA1-OA1-CC1	-3.28	109.83	117.96
62	a	1689	AM2	CA9-NA7-CA7	-3.19	109.74	114.38
62	a	1689	AM2	CA1-OA1-CC1	-3.08	110.35	117.96
62	a	1682	AM2	CA1-OA1-CC1	-2.97	110.61	117.96
62	a	1685	AM2	CA1-OA1-CC1	-2.96	110.64	117.96
62	a	1685	AM2	OA4-CA5-CA4	2.76	113.07	108.88
62	a	1682	AM2	CB1-OA8-CA8	-2.68	109.64	114.42
62	a	1684	AM2	CB1-OA8-CA8	-2.61	109.75	114.42
62	a	1685	AM2	CB1-OA8-CA8	-2.55	109.86	114.42
62	a	1689	AM2	CB1-OA8-CA8	-2.55	109.87	114.42
62	a	1685	AM2	CC5-CC4-CC3	2.34	113.57	110.04
62	a	1685	AM2	CC3-CC2-CC1	2.29	114.92	109.68
62	a	1689	AM2	OA4-CA5-CA4	2.29	112.35	108.88

There are no chirality outliers.

All (12) torsion outliers are listed below:

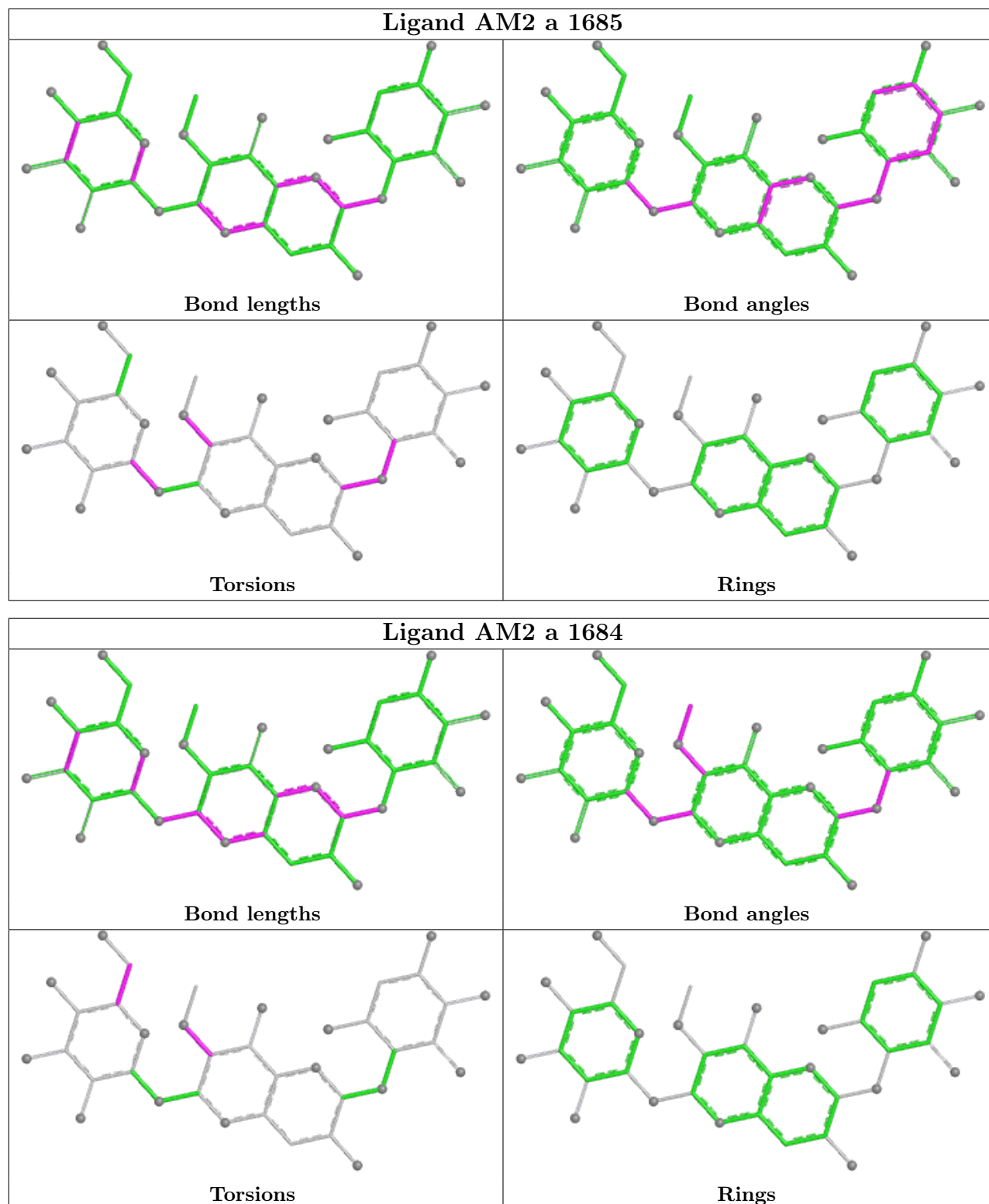
Mol	Chain	Res	Type	Atoms
62	a	1684	AM2	CA6-CA7-NA7-CA9
62	a	1684	AM2	CA8-CA7-NA7-CA9
62	a	1685	AM2	CA8-CA7-NA7-CA9
62	a	1684	AM2	OB1-CB5-CB6-OB6
62	a	1684	AM2	CB4-CB5-CB6-OB6
62	a	1685	AM2	OB1-CB1-OA8-CA8
62	a	1685	AM2	CC2-CC1-OA1-CA1
62	a	1689	AM2	OB1-CB5-CB6-OB6
62	a	1682	AM2	OB1-CB5-CB6-OB6
62	a	1685	AM2	OA4-CA1-OA1-CC1
62	a	1689	AM2	CA6-CA7-NA7-CA9
62	a	1689	AM2	CA8-CA7-NA7-CA9

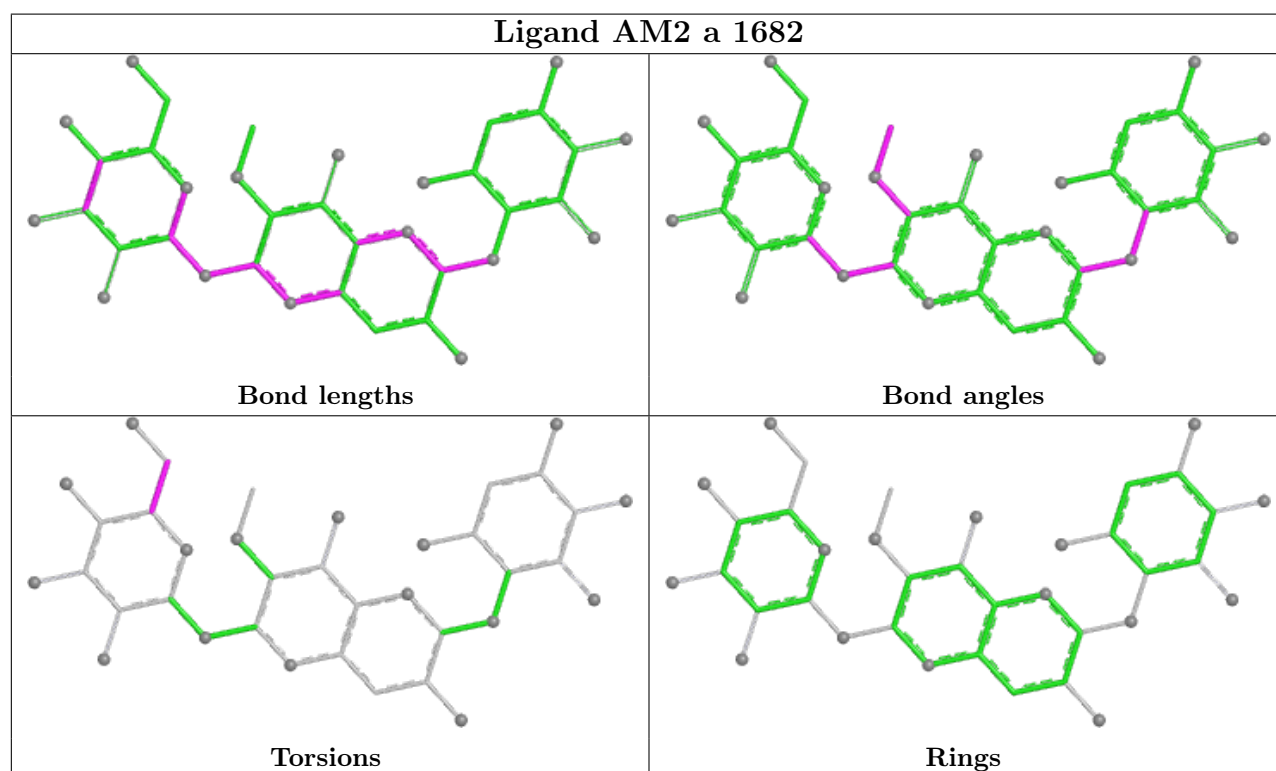
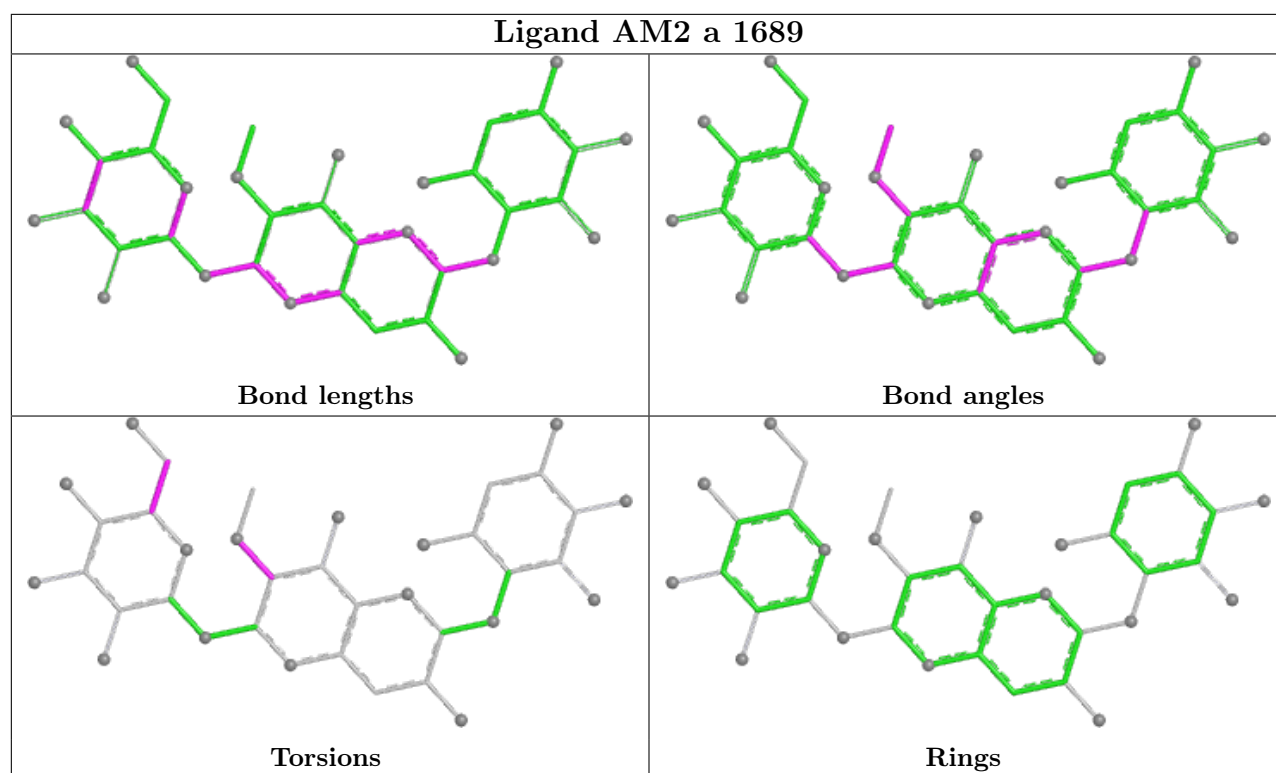
There are no ring outliers.

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 ⓘ

There are no chain breaks in this entry.

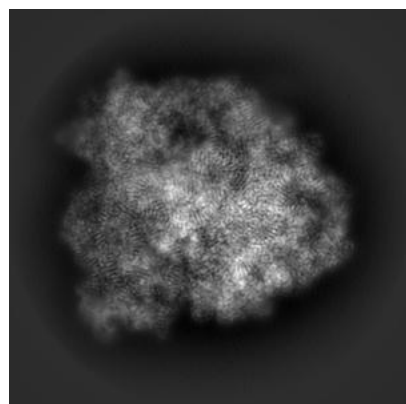
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13458. These allow visual inspection of the internal detail of the map and identification of artifacts.

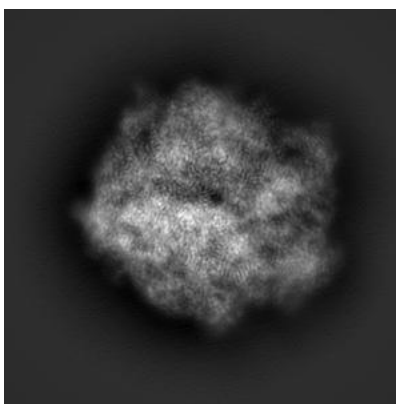
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

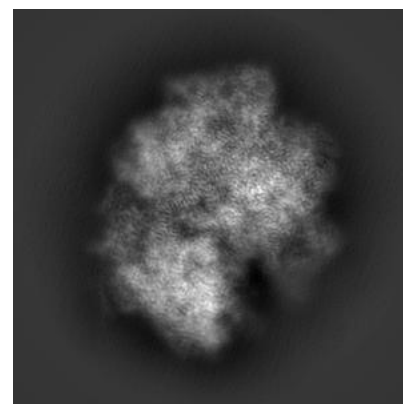
6.1.1 Primary map



X

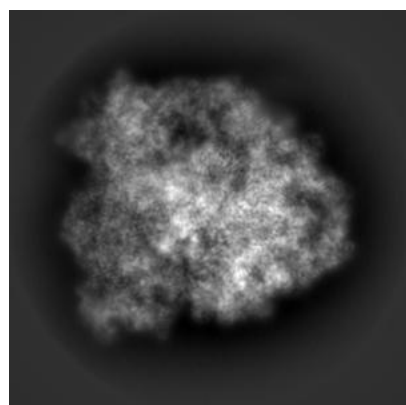


Y

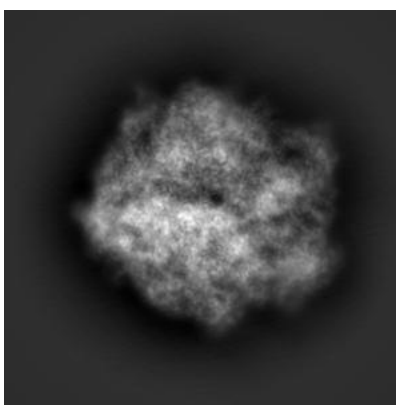


Z

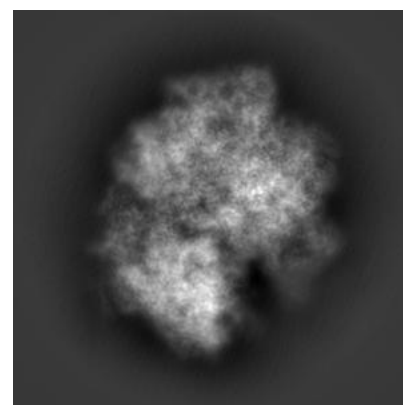
6.1.2 Raw map



X



Y

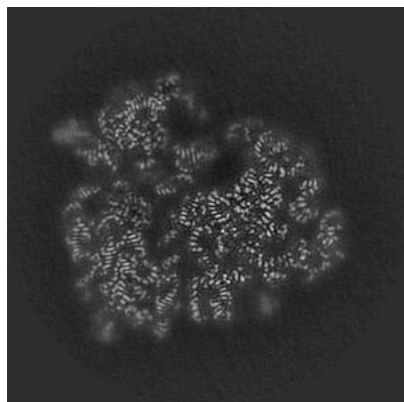


Z

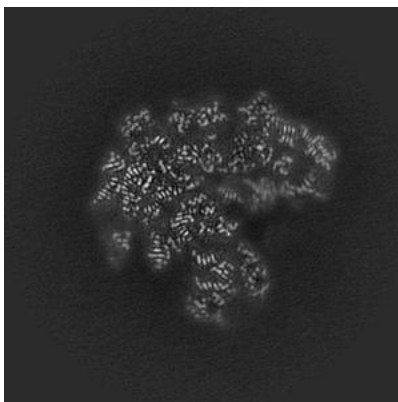
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

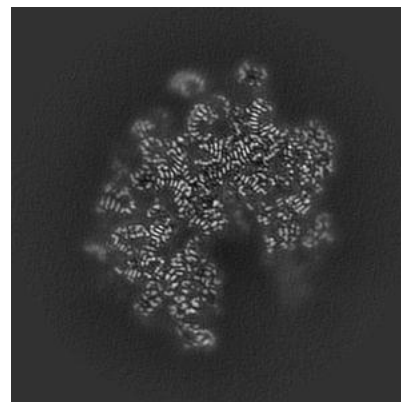
6.2.1 Primary map



X Index: 256

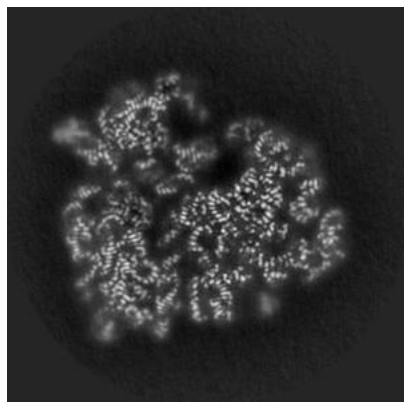


Y Index: 256

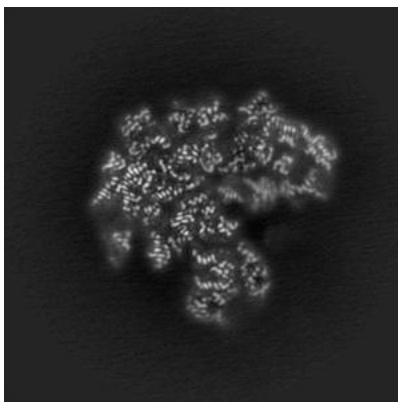


Z Index: 256

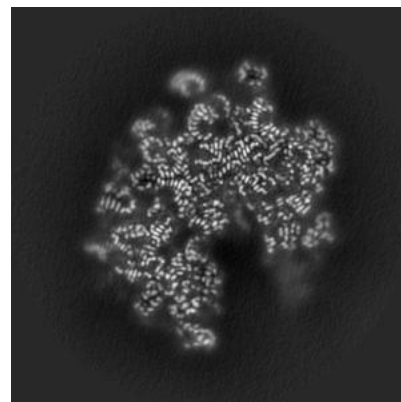
6.2.2 Raw map



X Index: 144



Y Index: 144

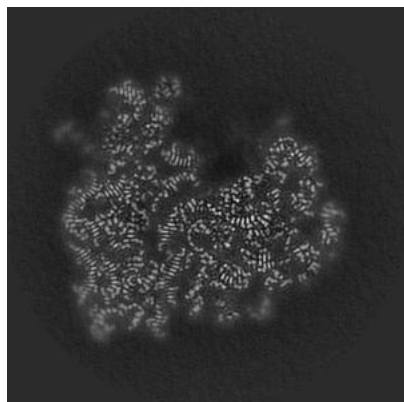


Z Index: 144

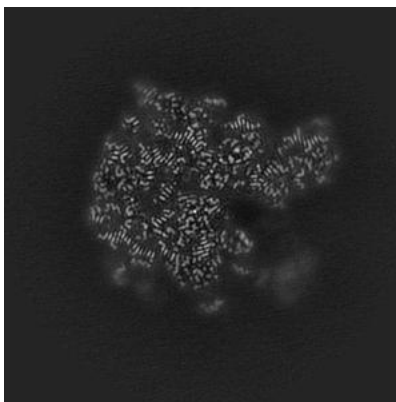
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

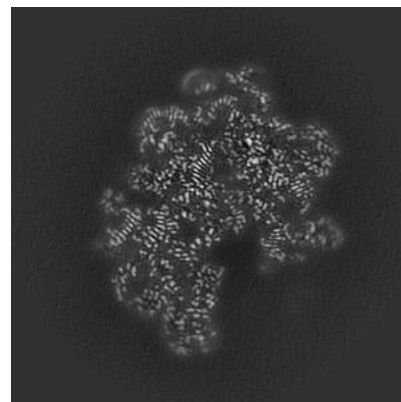
6.3.1 Primary map



X Index: 246

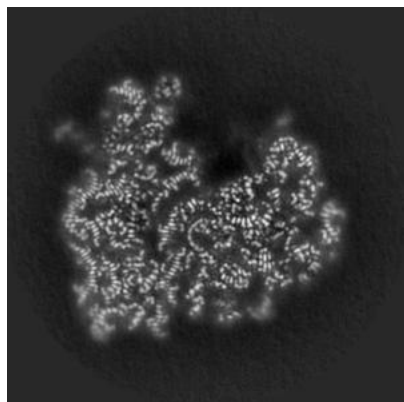


Y Index: 285

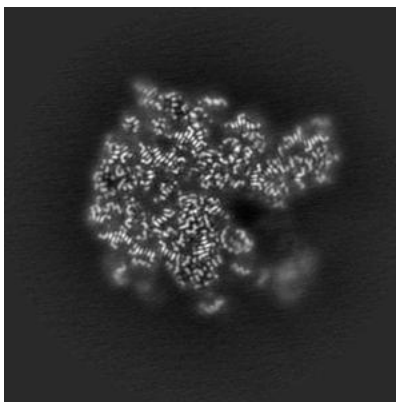


Z Index: 242

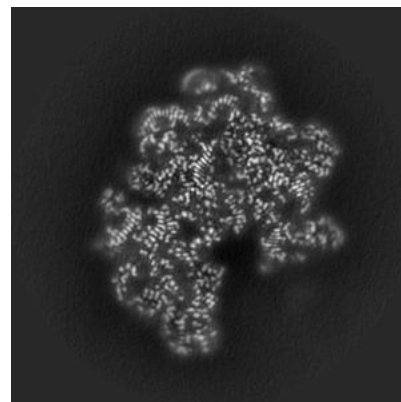
6.3.2 Raw map



X Index: 138



Y Index: 160



Z Index: 136

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y



Z

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

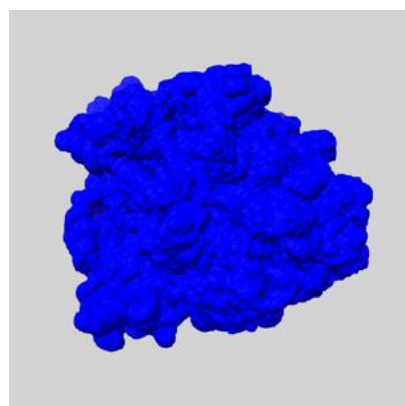
6.5 Mask visualisation [i](#)

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

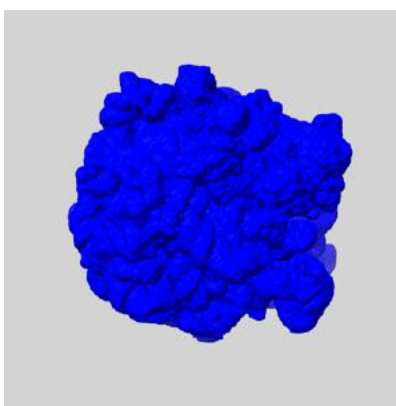
A mask typically either:

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

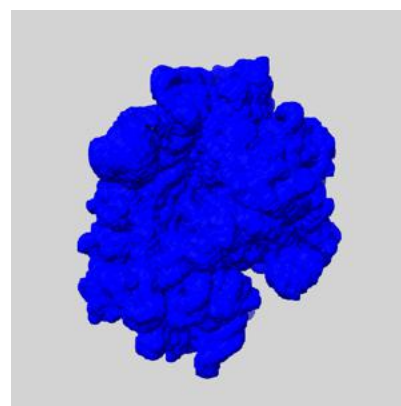
6.5.1 emd_13458_msk_1.map [i](#)



X



Y

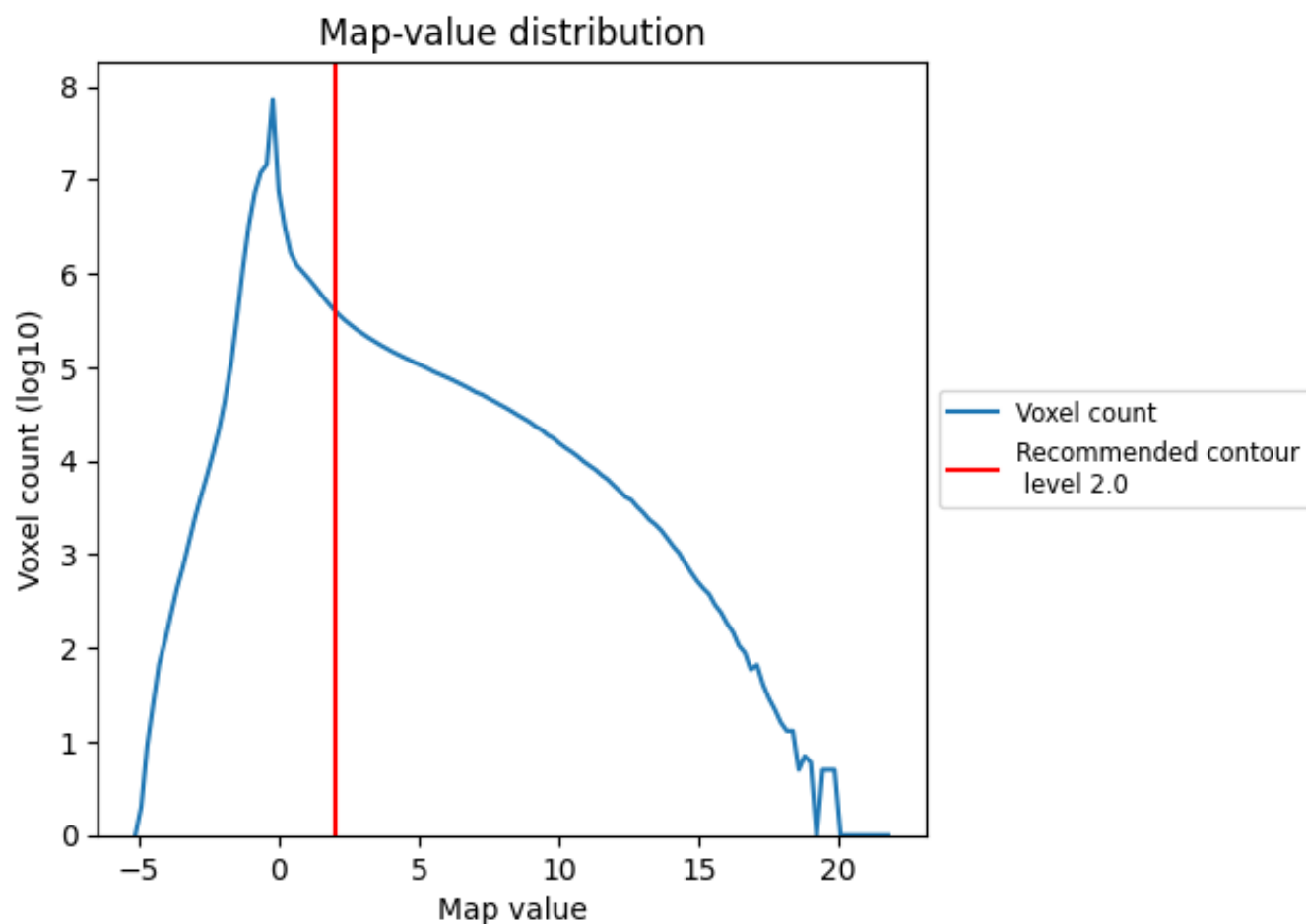


Z

7 Map analysis [i](#)

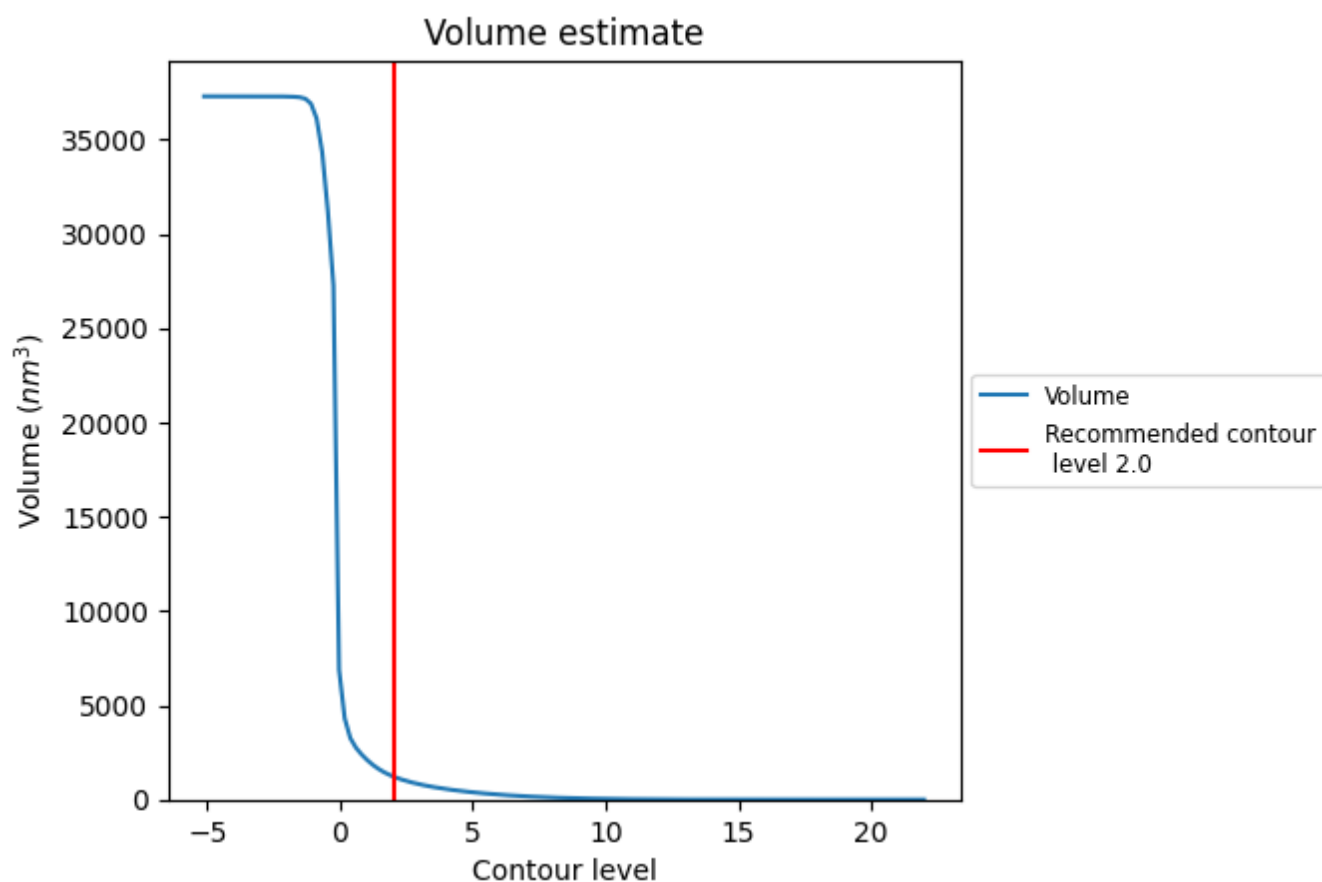
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1226 nm³; this corresponds to an approximate mass of 1108 kDa.

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

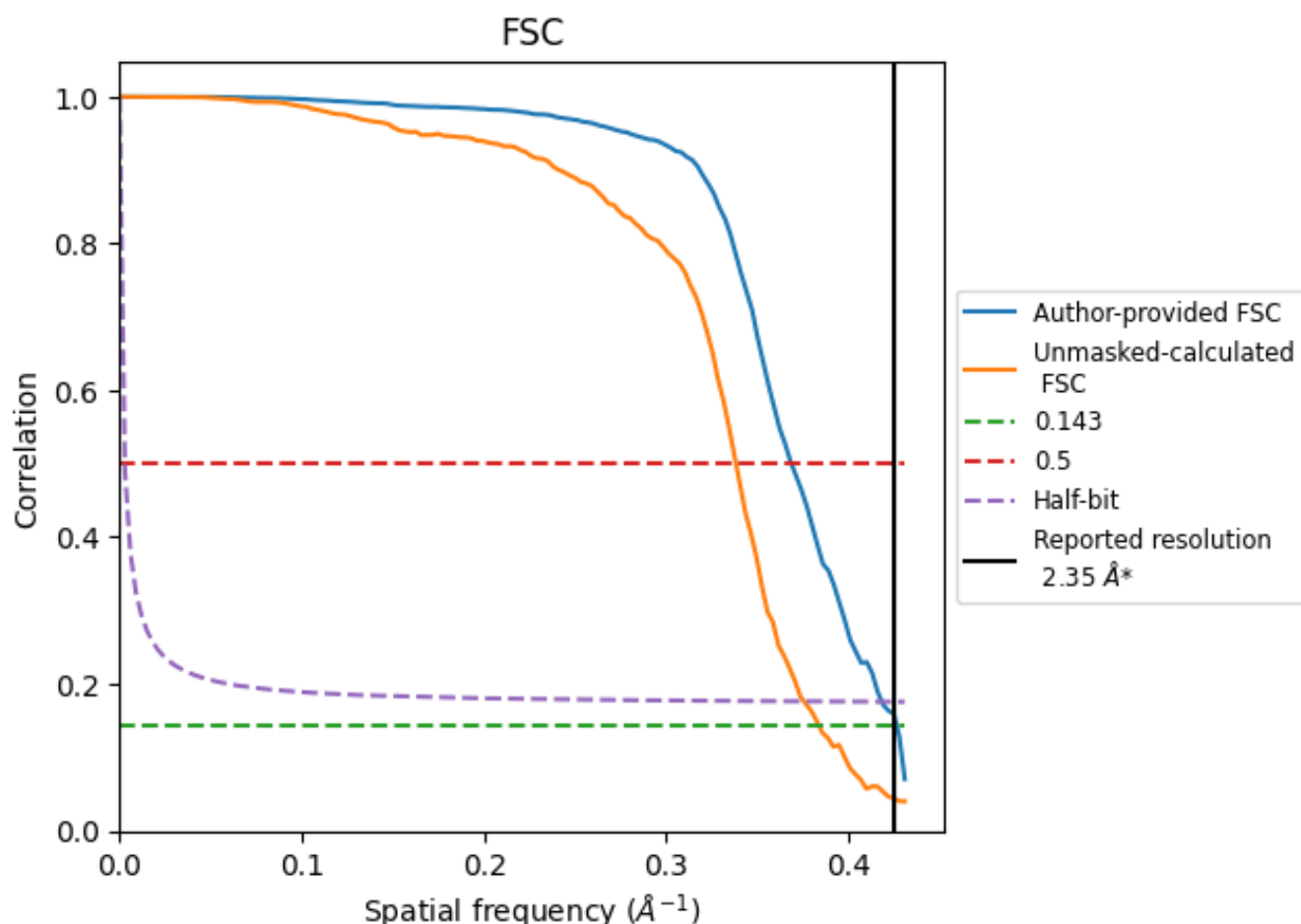
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

8.2 Resolution estimates [i](#)

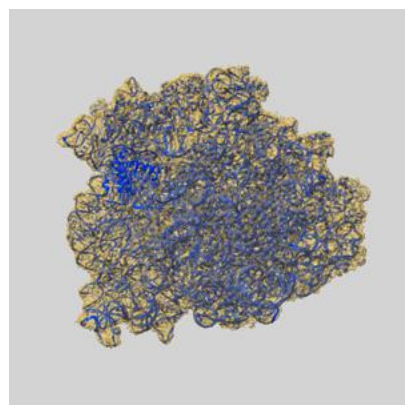
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.34	2.71	2.39
Unmasked-calculated*	2.60	2.96	2.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.60 differs from the reported value 2.35 by more than 10 %

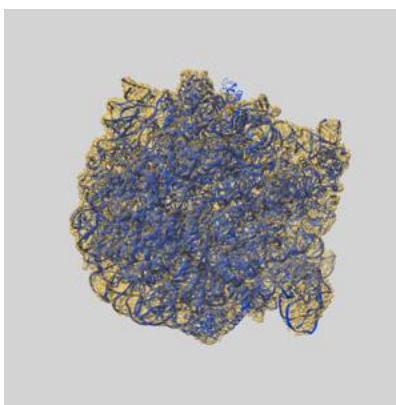
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13458 and PDB model 7PJS. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

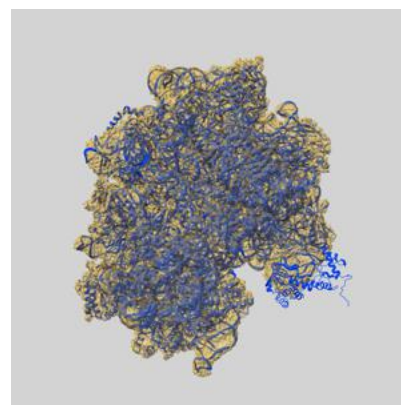
9.1 Map-model overlay [i](#)



X



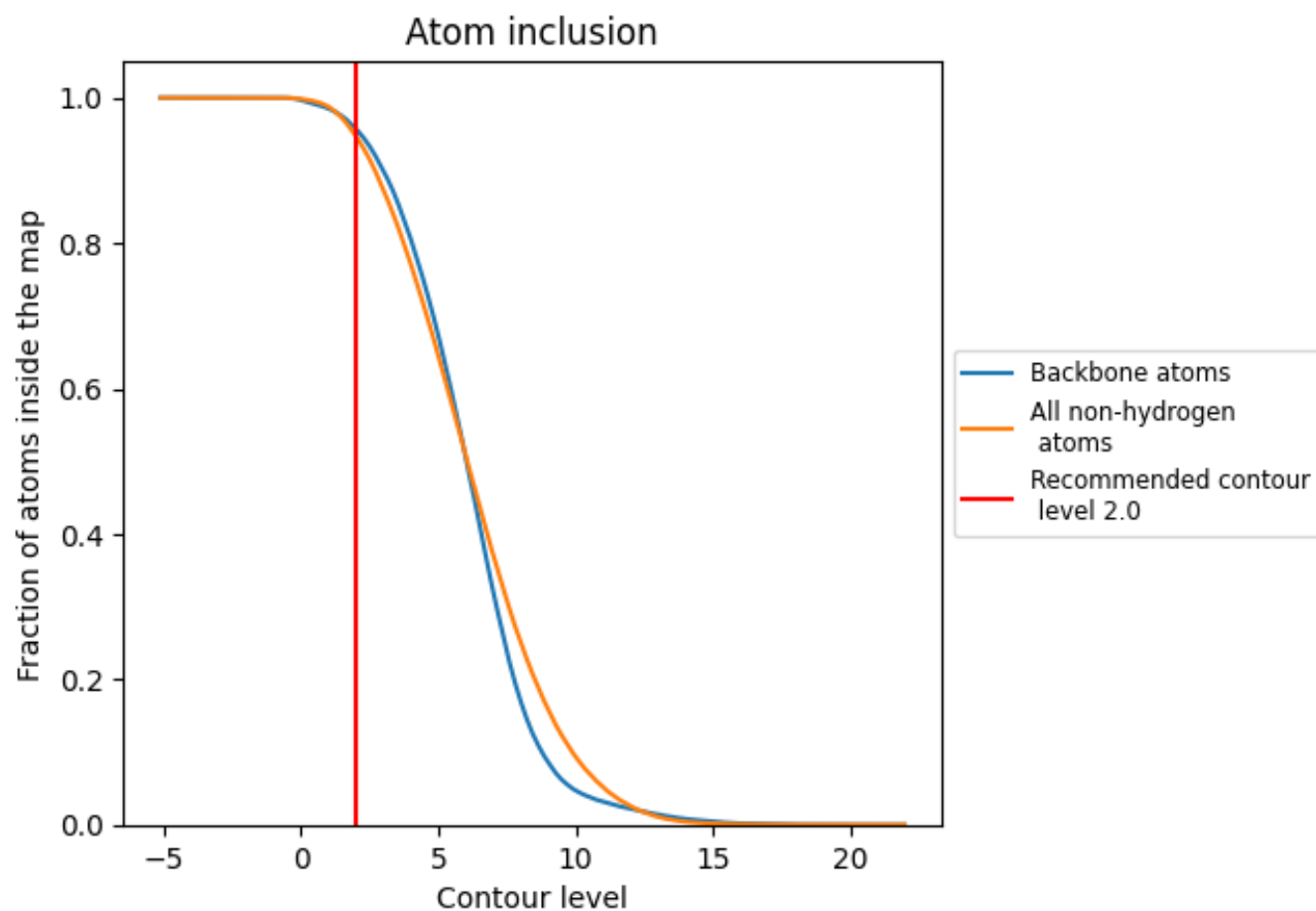
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.