Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 12:57 AM EDT

PDB ID	:	9CG6
EMDB ID	:	EMD-45572
Title	:	70S initiation complex (tRNA-fMet M1 + GUG start codon)
Authors	:	Mattingly, J.M.; Nguyen, H.A.; Dunham, C.M.
Deposited on	:	2024-06-28
Resolution	:	2.61 Å(reported)
Based on initial model	:	7K00

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

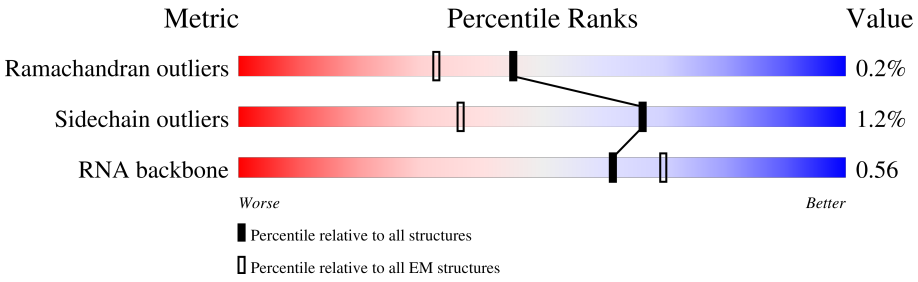
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.61 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	55	5% 93% 7%
2	1	46	98%
3	2	65	98%
4	3	38	100%
5	4	70	30% 81% 14%
6	A	1542	84% 14%
7	B	241	47% 92% 7%
8	C	233	9% 88% 12%

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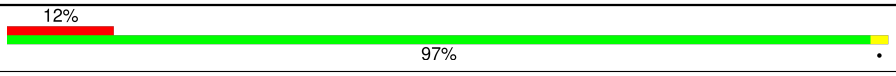
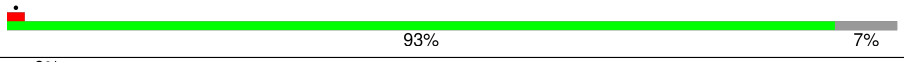
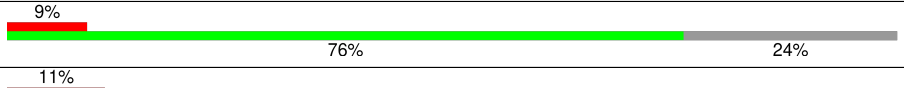
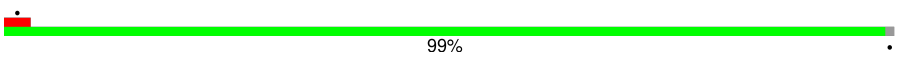
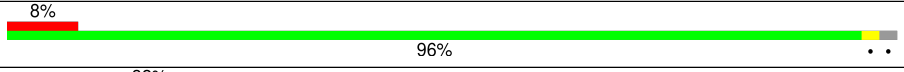
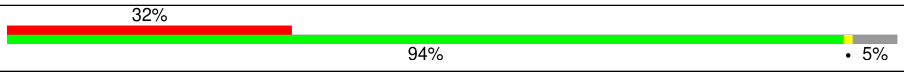
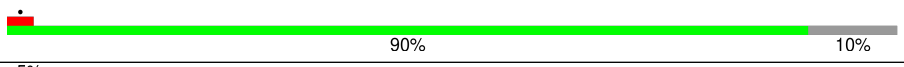
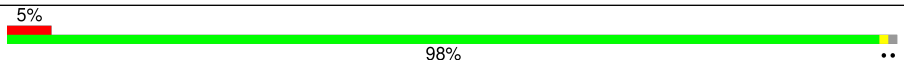
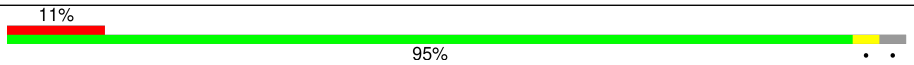
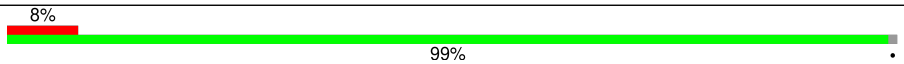
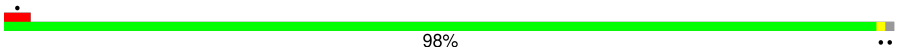
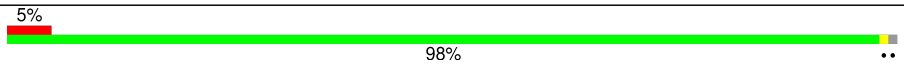
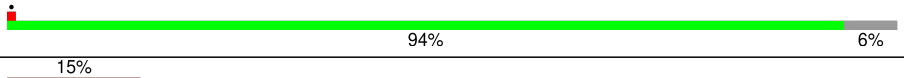
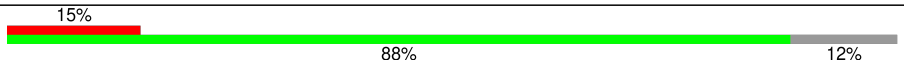
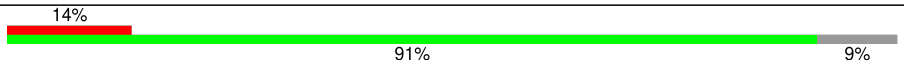
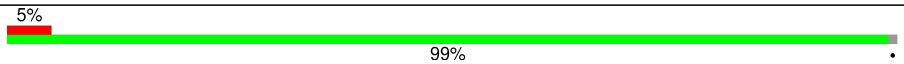
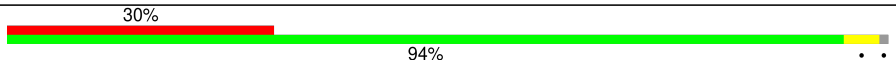
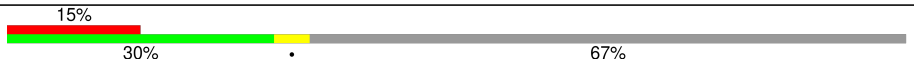
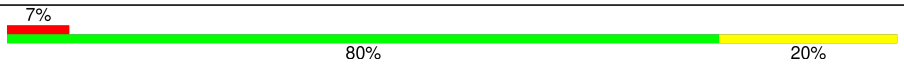
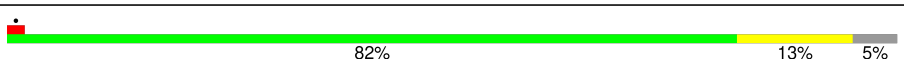
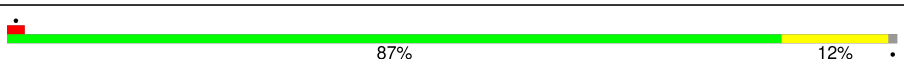
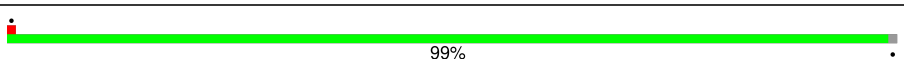
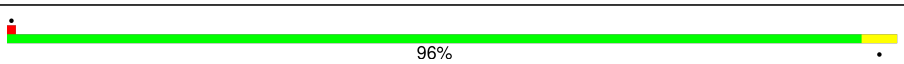
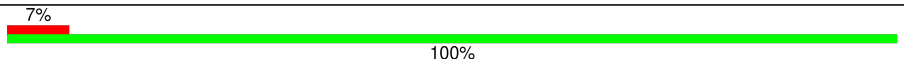
Mol	Chain	Length	Quality of chain
9	D	206	
10	E	167	
11	F	135	
12	G	179	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	X	27	
28	Z	75	
29	a	2904	
30	b	120	
31	c	273	
32	d	209	
33	e	201	

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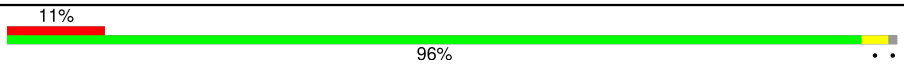
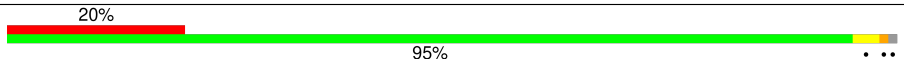
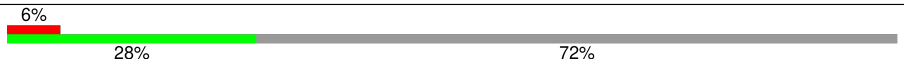
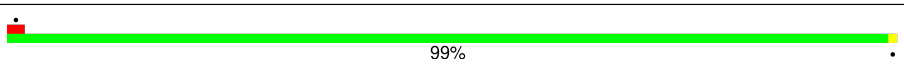
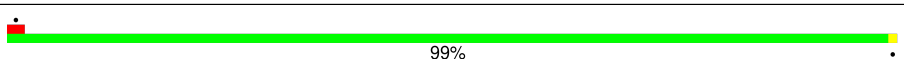
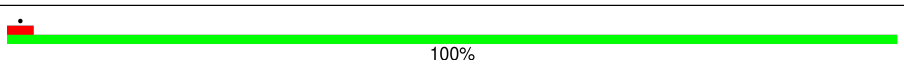
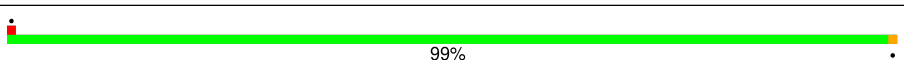
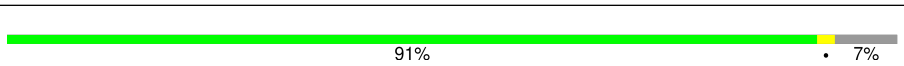
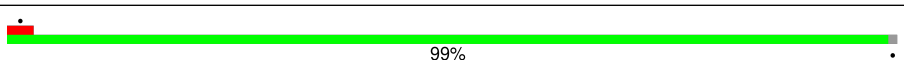
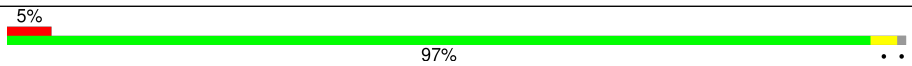
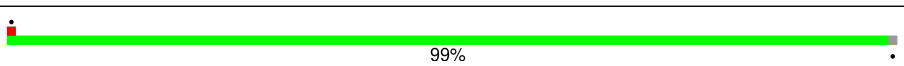
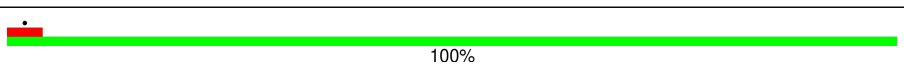
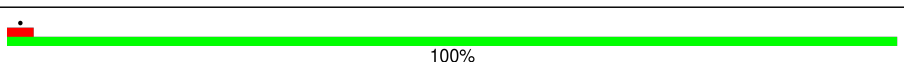
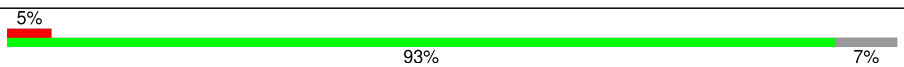
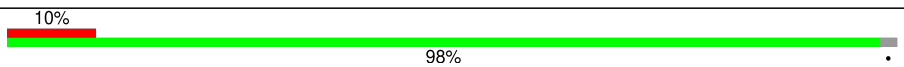
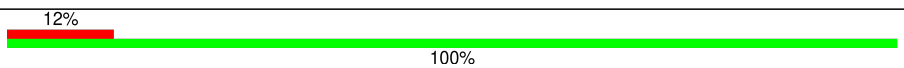
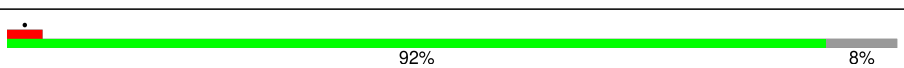
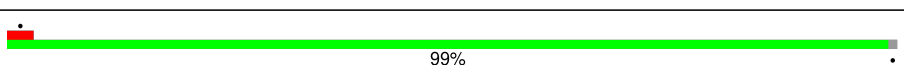
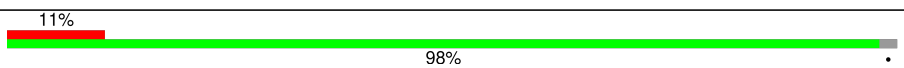
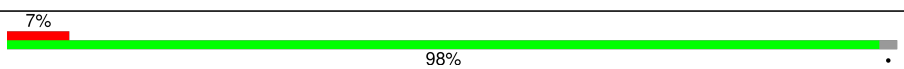
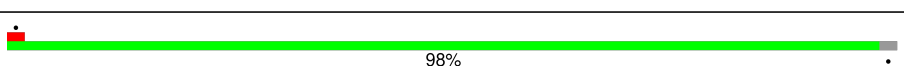
Mol	Chain	Length	Quality of chain
34	f	179	
35	g	177	
36	h	149	
37	i	142	
38	j	123	
39	k	144	
40	l	136	
41	m	127	
42	n	117	
43	o	115	
44	p	118	
45	q	103	
46	r	110	
47	s	100	
48	t	104	
49	u	94	
50	v	85	
51	w	78	
52	x	63	
53	y	59	
54	z	57	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 140170 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 L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 7 is a protein called 30S ribosomal protein S2.

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

- Molecule 8 is a protein called 30S ribosomal protein S3.

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

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

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

- Molecule 11 is a protein called 30S ribosomal protein S6.

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

- Molecule 12 is a protein called 30S ribosomal protein S7.

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

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	116	Total	C	N	O	S	0	0
			869	536	172	158	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	ASP	ASN	conflict	UNP C3SR57

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S13.

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

- Molecule 19 is a protein called 30S ribosomal protein S14.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S16.

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

- Molecule 22 is a protein called 30S ribosomal protein S17.

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

- Molecule 23 is a protein called 30S ribosomal protein S18.

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

- Molecule 24 is a protein called 30S ribosomal protein S19.

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

- Molecule 25 is a protein called 30S ribosomal protein S20.

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

- Molecule 26 is a protein called 30S ribosomal protein S21.

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

- Molecule 27 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	9	Total	C	N	O	P	0	0
			197	88	39	61	9		

- Molecule 28 is a RNA chain called P-site tRNA-fMet M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	75	Total	C	N	O	P	0	0
			1603	714	292	522	75		

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 31 is a protein called 50S ribosomal protein L2.

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

- Molecule 32 is a protein called 50S ribosomal protein L3.

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

- Molecule 33 is a protein called 50S ribosomal protein L4.

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

- Molecule 34 is a protein called 50S ribosomal protein L5.

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

- Molecule 35 is a protein called 50S ribosomal protein L6.

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

- Molecule 36 is a protein called 50S ribosomal protein L9.

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

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP A1AGK1

- Molecule 41 is a protein called 50S ribosomal protein L17.

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

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

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

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

- Molecule 53 is a protein called 50S ribosomal protein L30.

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

- Molecule 54 is a protein called 50S ribosomal protein L32.

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

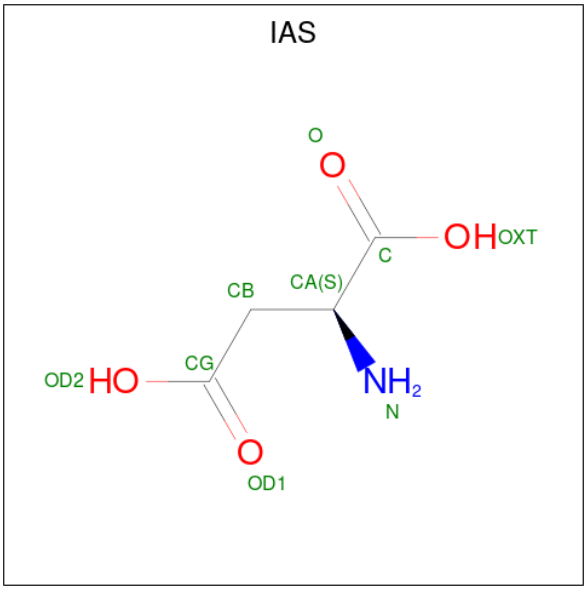
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	93	Total	Mg	0
			93	93	
56	a	210	Total	Mg	0
			210	210	
56	b	5	Total	Mg	0
			5	5	
56	z	1	Total	Mg	0
			1	1	

- Molecule 57 is BETA-L-ASPARTIC ACID (three-letter code: IAS) (formula: $C_4H_7NO_4$).



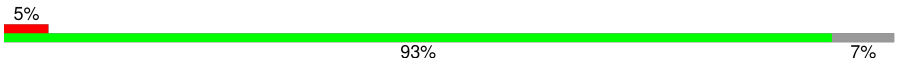
Mol	Chain	Residues	Atoms				AltConf
57	K	1	Total	C	N	O	0
			8	4	1	3	

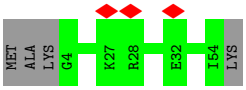
3 Residue-property plots (i)

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 L33

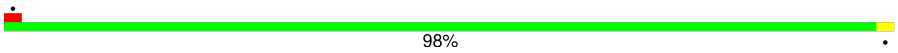
Chain 0:

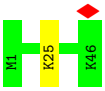




• Molecule 2: 50S ribosomal protein L34

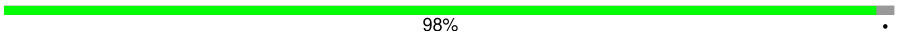
Chain 1:





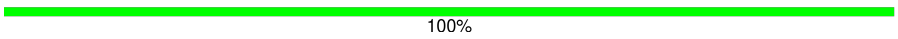
• Molecule 3: 50S ribosomal protein L35

Chain 2:



• Molecule 4: 50S ribosomal protein L36

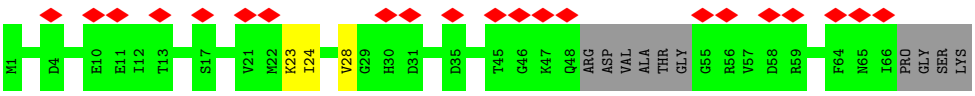
Chain 3:



There are no outlier residues recorded for this chain.

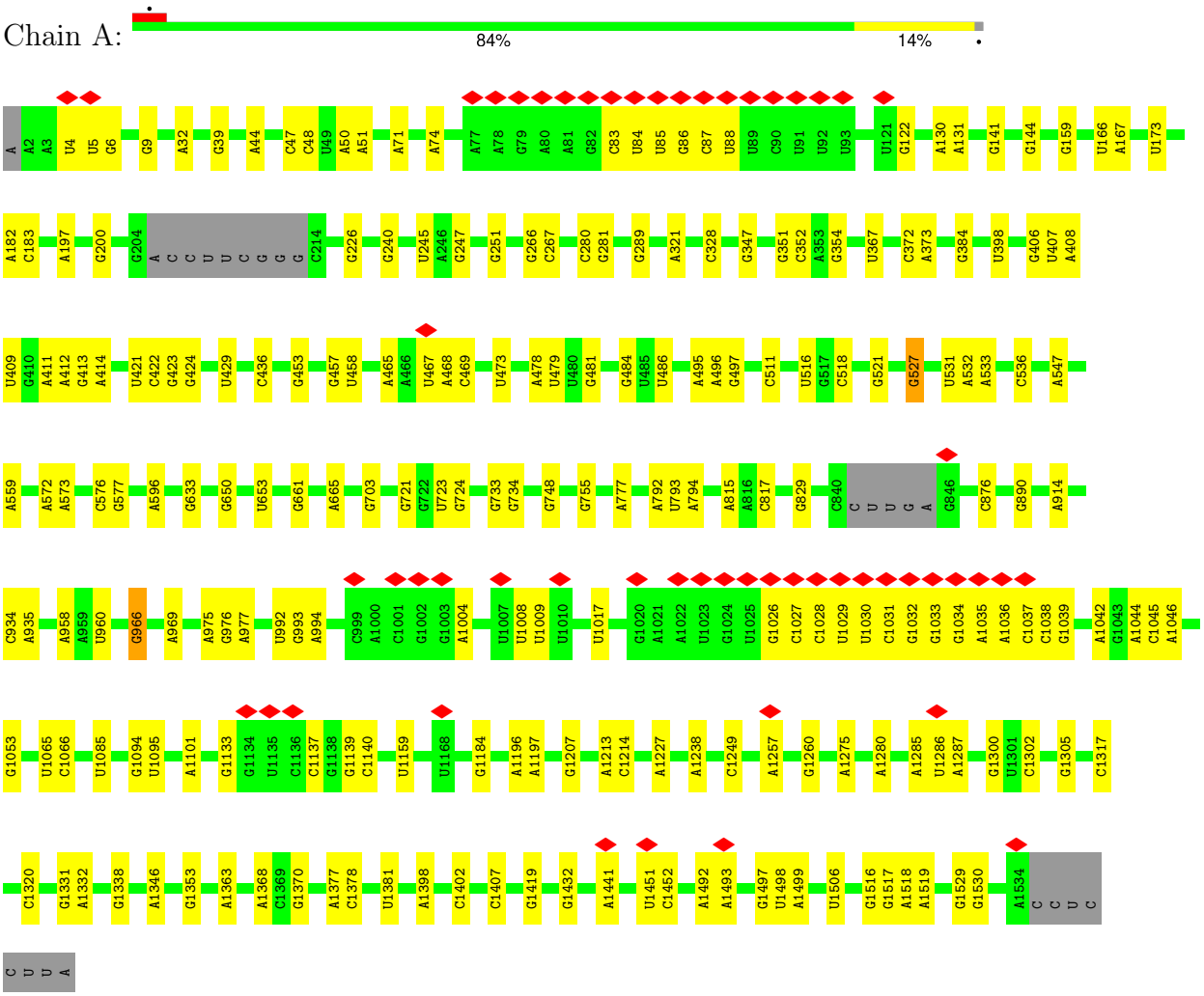
• Molecule 5: 50S ribosomal protein L31

Chain 4:



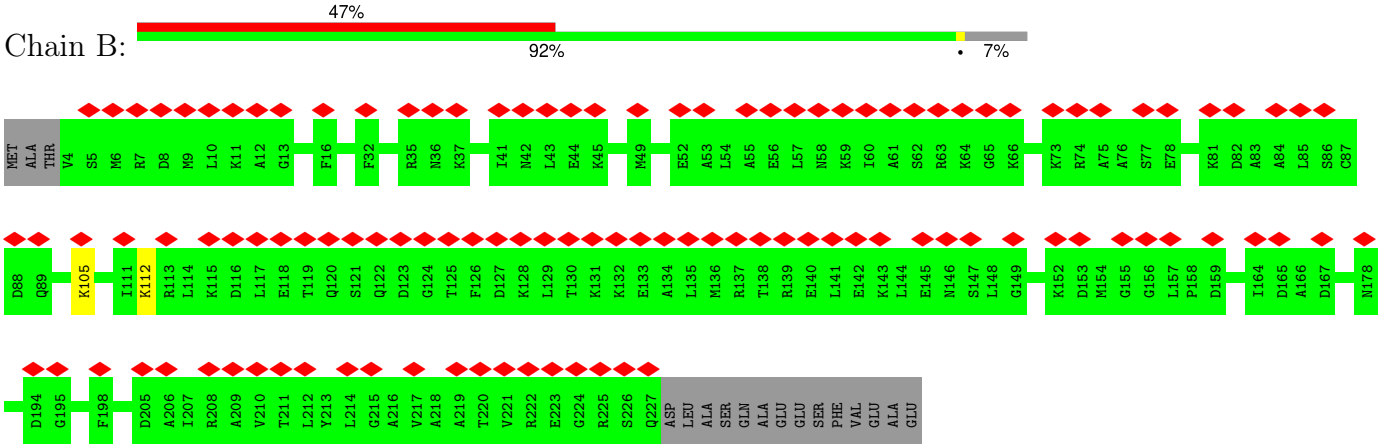
• Molecule 6: 16S ribosomal RNA

Chain A:



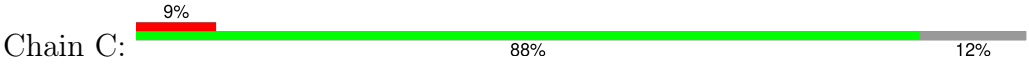
• Molecule 7: 30S ribosomal protein S2

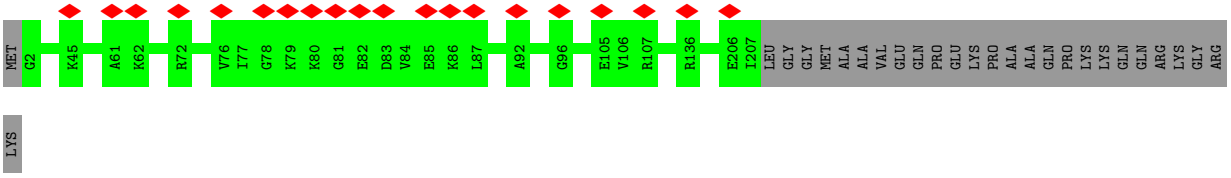
Chain B:



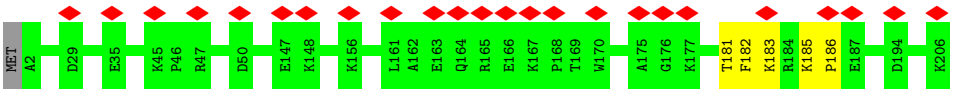
• Molecule 8: 30S ribosomal protein S3

Chain C:

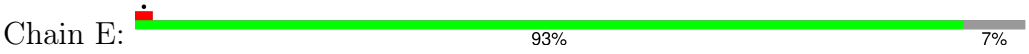


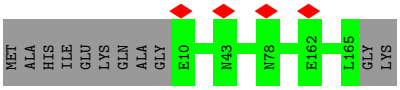


• Molecule 9: 30S ribosomal protein S4

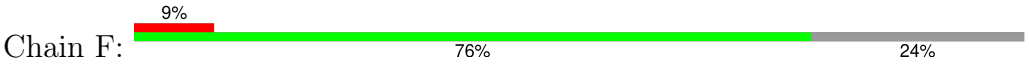


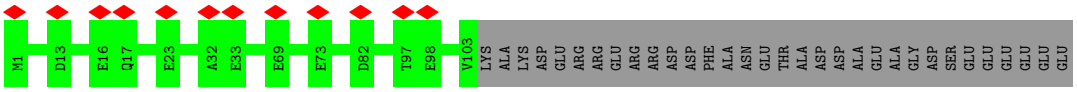
• Molecule 10: 30S ribosomal protein S5



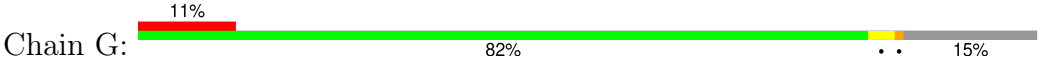


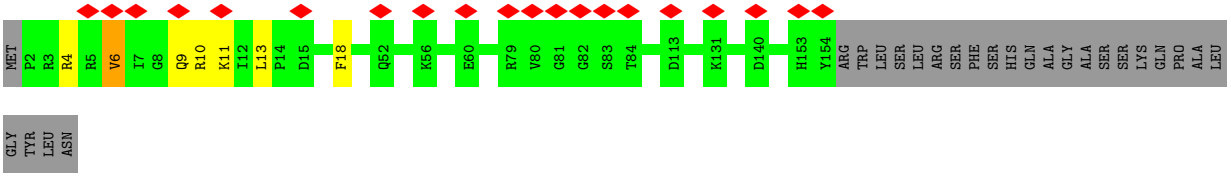
• Molecule 11: 30S ribosomal protein S6



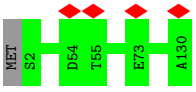


• Molecule 12: 30S ribosomal protein S7

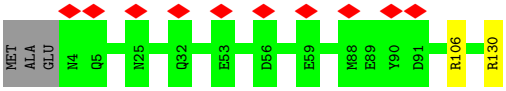




• Molecule 13: 30S ribosomal protein S8

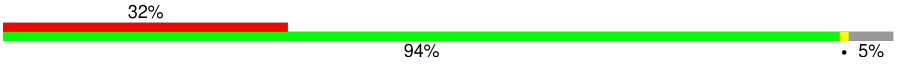


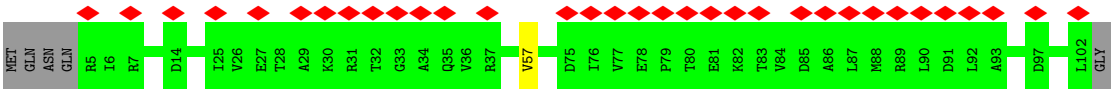
• Molecule 14: 30S ribosomal protein S9



• Molecule 15: 30S ribosomal protein S10

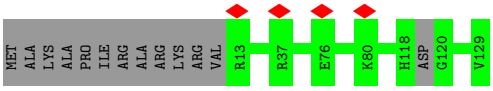
Chain J:





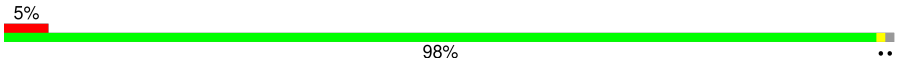
• Molecule 16: 30S ribosomal protein S11

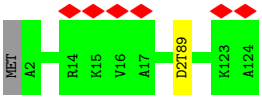
Chain K:



• Molecule 17: 30S ribosomal protein S12

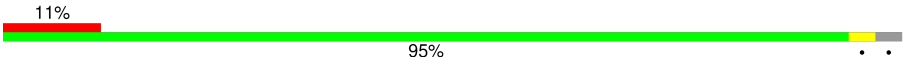
Chain L:

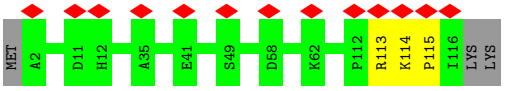




• Molecule 18: 30S ribosomal protein S13

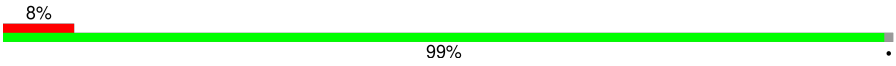
Chain M:

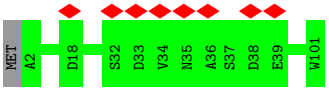




• Molecule 19: 30S ribosomal protein S14

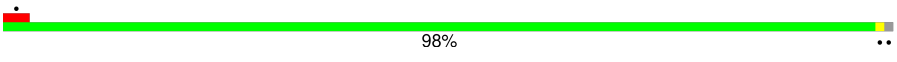
Chain N:

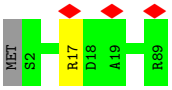




• Molecule 20: 30S ribosomal protein S15

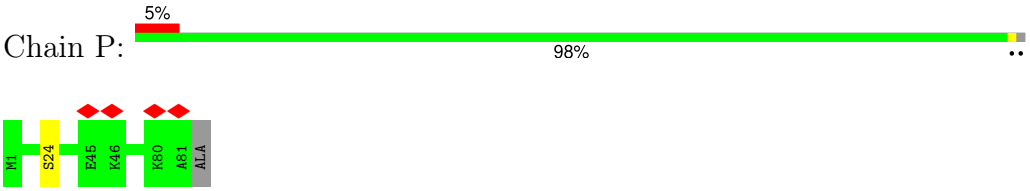
Chain O:





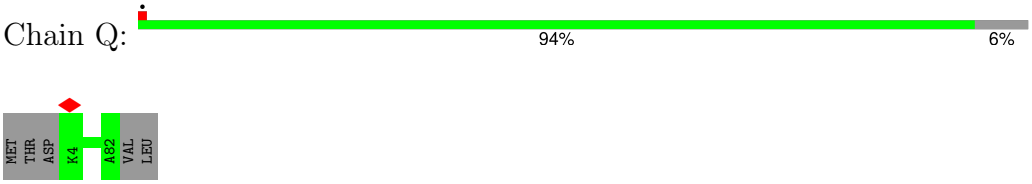
• Molecule 21: 30S ribosomal protein S16

Chain P:



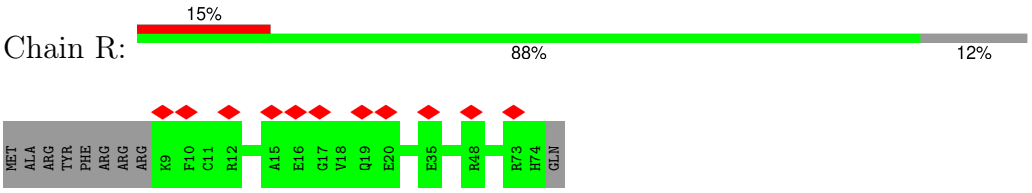
• Molecule 22: 30S ribosomal protein S17

Chain Q:



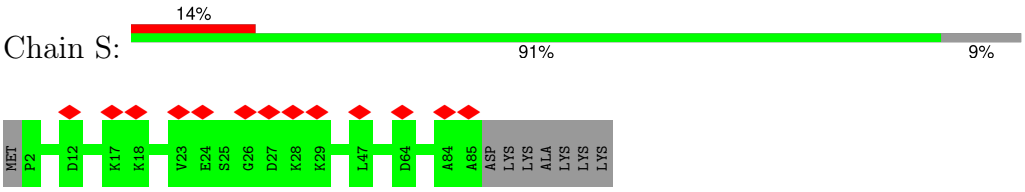
• Molecule 23: 30S ribosomal protein S18

Chain R:



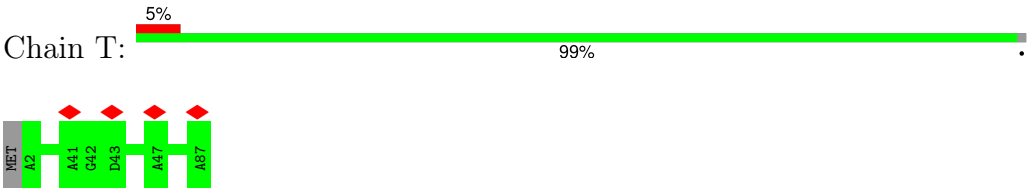
• Molecule 24: 30S ribosomal protein S19

Chain S:



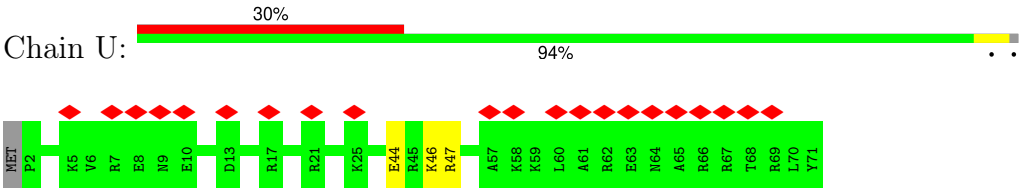
• Molecule 25: 30S ribosomal protein S20

Chain T:



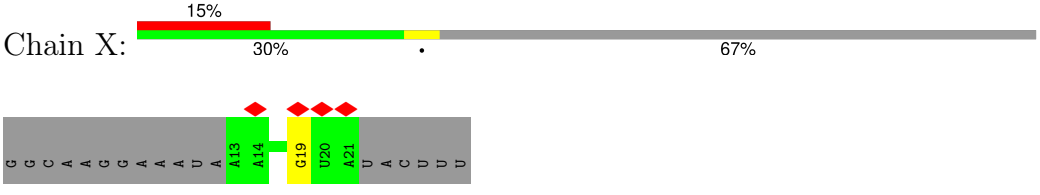
• Molecule 26: 30S ribosomal protein S21

Chain U:



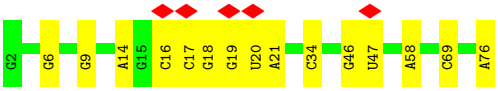
• Molecule 27: mRNA

Chain X:



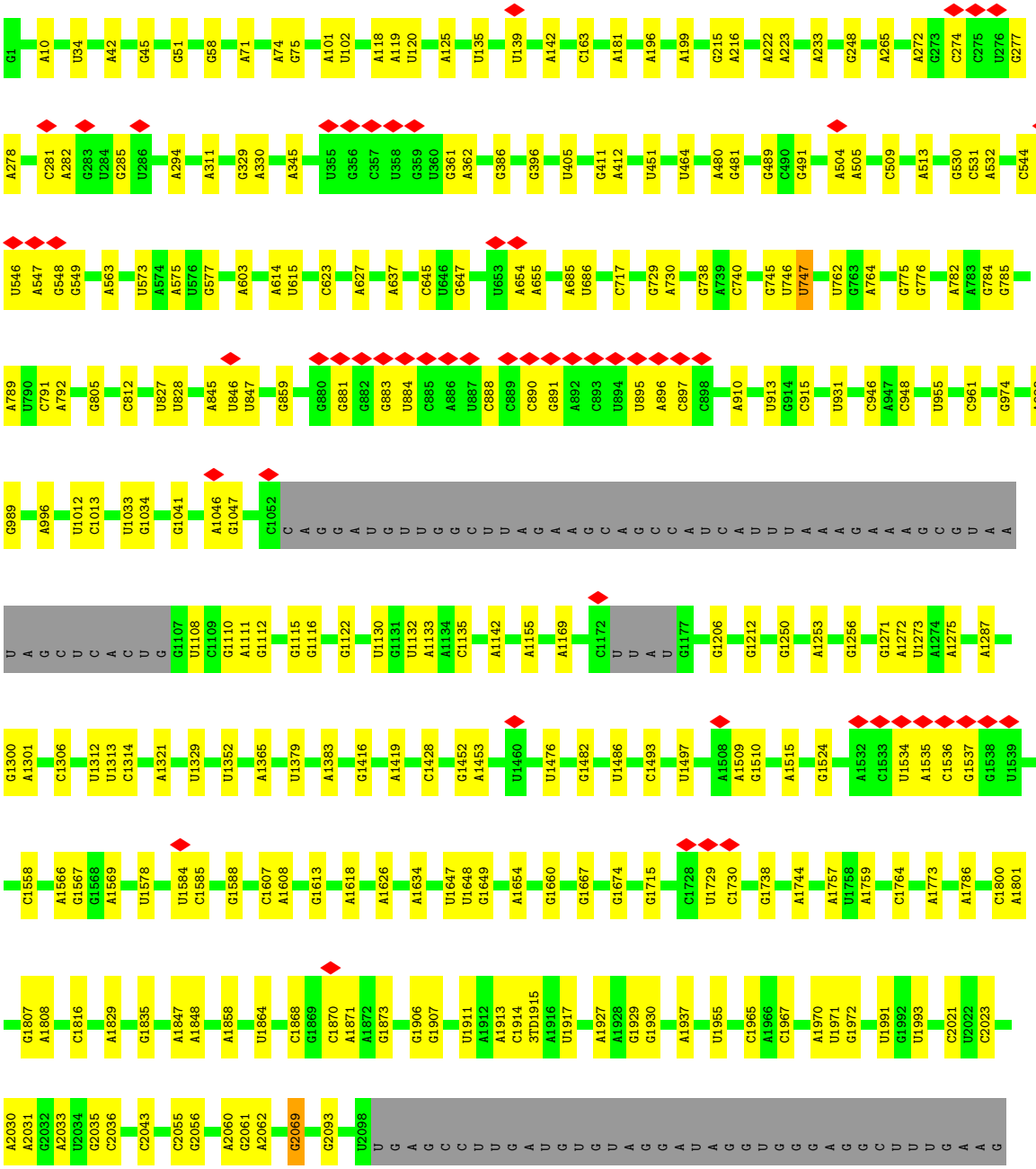
• Molecule 28: P-site tRNA-fMet M1

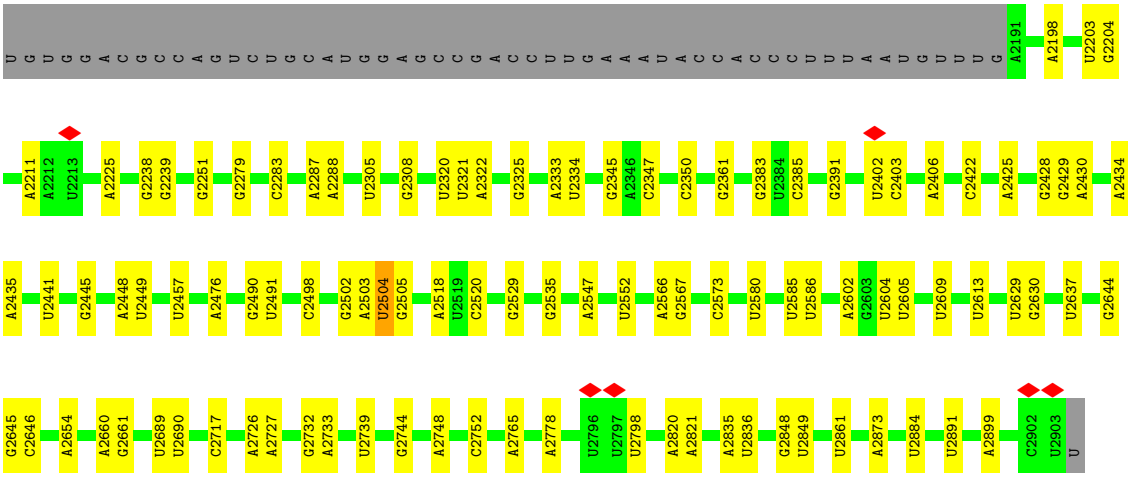
Chain Z:



• Molecule 29: 23S ribosomal RNA

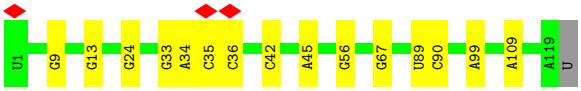
Chain a:





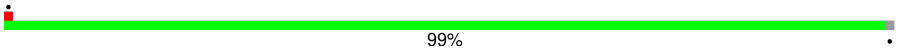
• Molecule 30: 5S ribosomal RNA

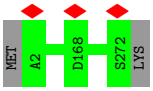
Chain b:



• Molecule 31: 50S ribosomal protein L2

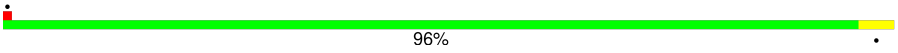
Chain c:

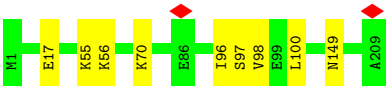




• Molecule 32: 50S ribosomal protein L3

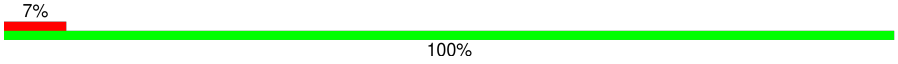
Chain d:

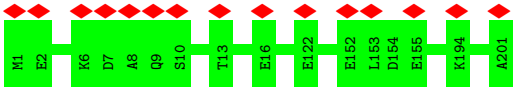




• Molecule 33: 50S ribosomal protein L4

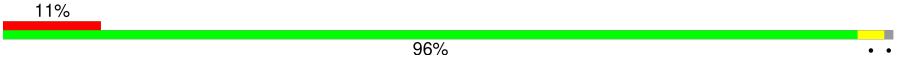
Chain e:

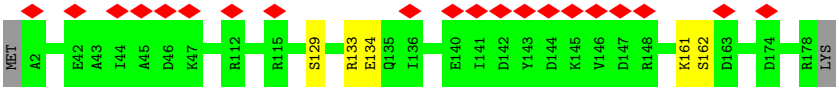




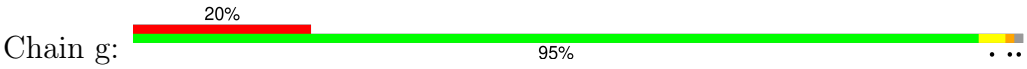
• Molecule 34: 50S ribosomal protein L5

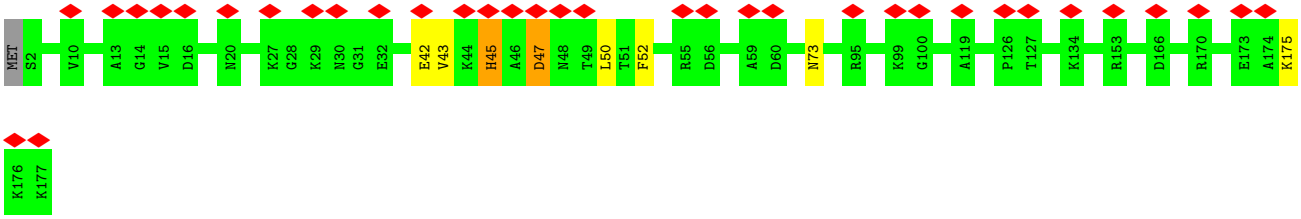
Chain f:



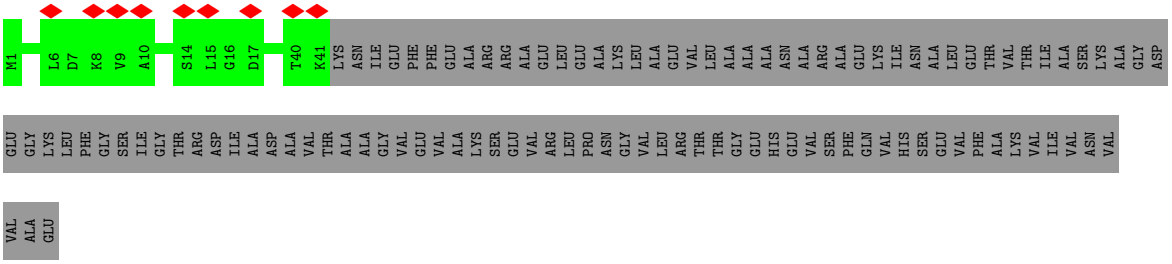


• Molecule 35: 50S ribosomal protein L6

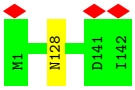




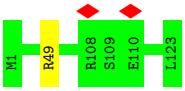
• Molecule 36: 50S ribosomal protein L9



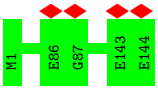
• Molecule 37: 50S ribosomal protein L13



• Molecule 38: 50S ribosomal protein L14

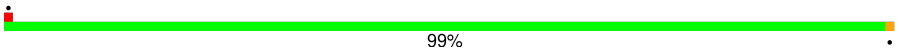


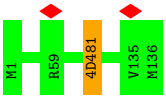
• Molecule 39: 50S ribosomal protein L15



• Molecule 40: 50S ribosomal protein L16

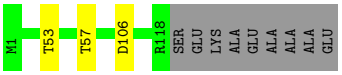
Chain l:





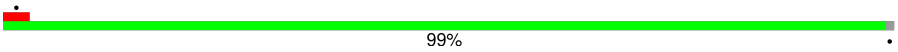
• Molecule 41: 50S ribosomal protein L17

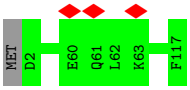
Chain m:



• Molecule 42: 50S ribosomal protein L18

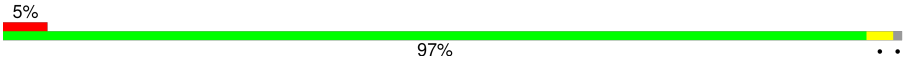
Chain n:

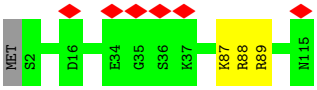




• Molecule 43: 50S ribosomal protein L19

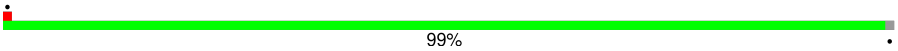
Chain o:





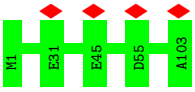
• Molecule 44: 50S ribosomal protein L20

Chain p:



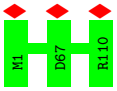
• Molecule 45: 50S ribosomal protein L21

Chain q:



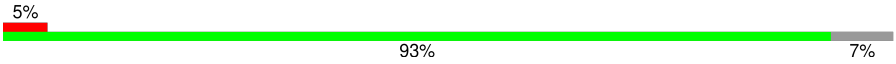
• Molecule 46: 50S ribosomal protein L22

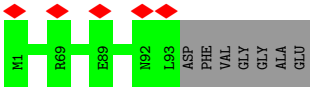
Chain r:



• Molecule 47: 50S ribosomal protein L23

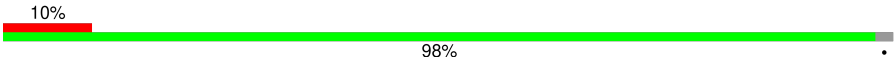
Chain s:

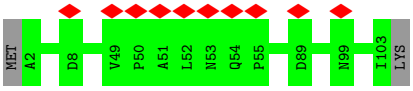




• Molecule 48: 50S ribosomal protein L24

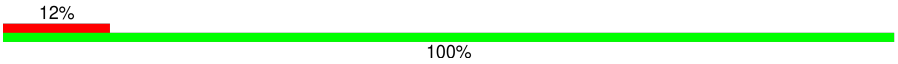
Chain t:

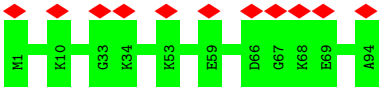




• Molecule 49: 50S ribosomal protein L25

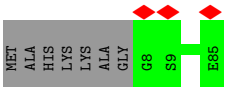
Chain u:





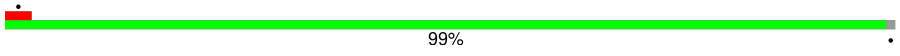
• Molecule 50: 50S ribosomal protein L27

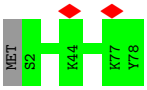
Chain v:



• Molecule 51: 50S ribosomal protein L28

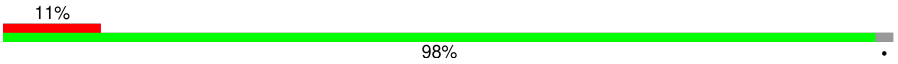
Chain w:

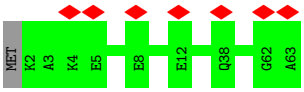




• Molecule 52: 50S ribosomal protein L29

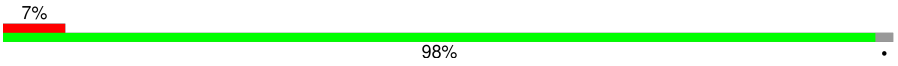
Chain x:

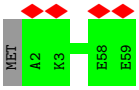




• Molecule 53: 50S ribosomal protein L30

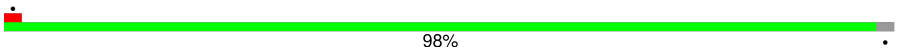
Chain y:





• Molecule 54: 50S ribosomal protein L32

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	149231	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; cryoSPARC patch CTF estimation	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	58.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	79000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.332	Depositor
Minimum map value	-0.745	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	417.99997, 417.99997, 417.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	0	0.39	0/424	0.55	0/565
2	1	0.37	0/380	0.71	0/498
3	2	0.41	0/513	0.56	0/676
4	3	0.40	0/303	0.58	0/397
5	4	0.35	0/488	0.60	0/649
6	A	0.73	0/36236	0.81	0/56520
7	B	0.29	0/1784	0.54	0/2403
8	C	0.33	0/1651	0.55	0/2225
9	D	0.36	0/1665	0.63	0/2227
10	E	0.37	0/1165	0.55	0/1568
11	F	0.34	0/858	0.55	0/1160
12	G	0.31	0/1219	0.53	0/1635
13	H	0.37	0/989	0.55	0/1326
14	I	0.34	0/1034	0.59	0/1375
15	J	0.30	0/796	0.59	0/1077
16	K	0.35	0/884	0.59	0/1191
17	L	0.38	0/960	0.60	0/1286
18	M	0.30	0/900	0.57	0/1204
19	N	0.32	0/817	0.56	0/1088
20	O	0.32	0/722	0.55	0/964
21	P	0.38	0/653	0.60	0/877
22	Q	0.35	0/650	0.55	0/871
23	R	0.36	0/553	0.56	0/742
24	S	0.33	0/685	0.55	0/922
25	T	0.29	0/676	0.46	0/895
26	U	0.35	0/597	0.58	0/792
27	X	0.47	0/221	0.75	0/343
28	Z	0.52	0/1791	0.79	0/2791
29	a	0.93	0/65651	0.85	0/102413
30	b	0.68	0/2850	0.80	0/4444
31	c	0.45	0/2121	0.63	0/2852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
32	d	0.52	0/1576	0.56	0/2119
33	e	0.37	0/1571	0.54	0/2113
34	f	0.35	0/1434	0.54	0/1926
35	g	0.31	0/1343	0.54	0/1816
36	h	0.33	0/306	0.58	0/413
37	i	0.41	0/1152	0.55	0/1551
38	j	0.39	0/955	0.64	0/1279
39	k	0.41	0/1062	0.59	0/1413
40	l	0.41	0/1073	0.59	0/1433
41	m	0.49	0/958	0.63	0/1281
42	n	0.34	0/902	0.57	0/1209
43	o	0.42	0/929	0.56	0/1242
44	p	0.46	0/960	0.56	0/1278
45	q	0.41	0/829	0.59	0/1107
46	r	0.37	0/864	0.55	0/1156
47	s	0.37	0/744	0.54	0/994
48	t	0.34	0/787	0.57	0/1051
49	u	0.36	0/766	0.53	0/1025
50	v	0.39	0/593	0.57	0/785
51	w	0.42	0/635	0.63	0/848
52	x	0.29	0/502	0.52	0/667
53	y	0.35	0/453	0.60	0/605
54	z	0.41	0/450	0.63	0/599
All	All	0.75	0/151080	0.77	0/225886

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

Mol	Chain	#Chirality outliers	#Planarity outliers
40	l	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	l	81	4D4	Peptide,Mainchain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
7	B	222/241 (92%)	206 (93%)	16 (7%)	0	100	100
8	C	204/233 (88%)	200 (98%)	4 (2%)	0	100	100
9	D	203/206 (98%)	183 (90%)	19 (9%)	1 (0%)	25	45
10	E	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
11	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
12	G	151/179 (84%)	139 (92%)	10 (7%)	2 (1%)	10	20
13	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
14	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
15	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	13	26
16	K	112/129 (87%)	108 (96%)	4 (4%)	0	100	100
17	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
18	M	113/118 (96%)	108 (96%)	4 (4%)	1 (1%)	14	29
19	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
20	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
21	P	79/82 (96%)	75 (95%)	3 (4%)	1 (1%)	10	20
22	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
24	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
25	T	84/87 (97%)	84 (100%)	0	0	100	100
26	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
31	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
32	d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	25	45
33	e	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
34	f	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
35	g	174/177 (98%)	162 (93%)	10 (6%)	2 (1%)	12	24
36	h	39/149 (26%)	33 (85%)	6 (15%)	0	100	100
37	i	140/142 (99%)	140 (100%)	0	0	100	100
38	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
39	k	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
40	l	132/136 (97%)	131 (99%)	1 (1%)	0	100	100
41	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
42	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
43	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
44	p	115/118 (98%)	115 (100%)	0	0	100	100
45	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
46	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
47	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
48	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
49	u	92/94 (98%)	92 (100%)	0	0	100	100
50	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
51	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
52	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
53	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
54	z	54/57 (95%)	54 (100%)	0	0	100	100
All	All	5480/5913 (93%)	5267 (96%)	204 (4%)	9 (0%)	45	65

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	G	6	VAL
18	M	115	PRO
32	d	149	ASN
12	G	11	LYS
15	J	57	VAL
35	g	45	HIS
35	g	47	ASP
9	D	186	PRO
21	P	24	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	37 (97%)	1 (3%)	41	66
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	52 (94%)	3 (6%)	18	37
7	B	186/199 (94%)	184 (99%)	2 (1%)	70	86
8	C	170/190 (90%)	170 (100%)	0	100	100
9	D	172/173 (99%)	168 (98%)	4 (2%)	45	69
10	E	119/126 (94%)	119 (100%)	0	100	100
11	F	90/116 (78%)	90 (100%)	0	100	100
12	G	126/147 (86%)	120 (95%)	6 (5%)	21	42
13	H	104/105 (99%)	104 (100%)	0	100	100
14	I	105/107 (98%)	103 (98%)	2 (2%)	52	75
15	J	86/90 (96%)	86 (100%)	0	100	100
16	K	89/99 (90%)	89 (100%)	0	100	100
17	L	102/103 (99%)	102 (100%)	0	100	100
18	M	93/96 (97%)	91 (98%)	2 (2%)	47	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	N	83/84 (99%)	83 (100%)	0	100	100
20	O	76/77 (99%)	75 (99%)	1 (1%)	65	83
21	P	65/65 (100%)	65 (100%)	0	100	100
22	Q	73/78 (94%)	73 (100%)	0	100	100
23	R	57/65 (88%)	57 (100%)	0	100	100
24	S	72/79 (91%)	72 (100%)	0	100	100
25	T	65/66 (98%)	65 (100%)	0	100	100
26	U	60/61 (98%)	57 (95%)	3 (5%)	20	41
31	c	216/218 (99%)	216 (100%)	0	100	100
32	d	163/163 (100%)	155 (95%)	8 (5%)	21	41
33	e	165/165 (100%)	165 (100%)	0	100	100
34	f	148/150 (99%)	143 (97%)	5 (3%)	32	56
35	g	137/138 (99%)	129 (94%)	8 (6%)	17	34
36	h	32/114 (28%)	32 (100%)	0	100	100
37	i	116/116 (100%)	115 (99%)	1 (1%)	75	89
38	j	104/104 (100%)	103 (99%)	1 (1%)	73	87
39	k	103/103 (100%)	103 (100%)	0	100	100
40	l	107/107 (100%)	107 (100%)	0	100	100
41	m	98/103 (95%)	95 (97%)	3 (3%)	35	60
42	n	86/87 (99%)	86 (100%)	0	100	100
43	o	99/100 (99%)	96 (97%)	3 (3%)	36	61
44	p	89/90 (99%)	89 (100%)	0	100	100
45	q	84/84 (100%)	84 (100%)	0	100	100
46	r	93/93 (100%)	93 (100%)	0	100	100
47	s	80/84 (95%)	80 (100%)	0	100	100
48	t	83/85 (98%)	83 (100%)	0	100	100
49	u	78/78 (100%)	78 (100%)	0	100	100
50	v	58/63 (92%)	58 (100%)	0	100	100
51	w	67/68 (98%)	67 (100%)	0	100	100
52	x	54/55 (98%)	54 (100%)	0	100	100
53	y	48/49 (98%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	z	47/48 (98%)	47 (100%)	0	100 100
All	All	4572/4826 (95%)	4519 (99%)	53 (1%)	66 84

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	25	LYS
5	4	23	LYS
5	4	24	ILE
5	4	28	VAL
7	B	105	LYS
7	B	112	LYS
9	D	181	THR
9	D	182	PHE
9	D	183	LYS
9	D	185	LYS
12	G	4	ARG
12	G	6	VAL
12	G	9	GLN
12	G	10	ARG
12	G	13	LEU
12	G	18	PHE
14	I	106	ARG
14	I	130	ARG
18	M	113	ARG
18	M	114	LYS
20	O	17	ARG
26	U	44	GLU
26	U	46	LYS
26	U	47	ARG
32	d	17	GLU
32	d	55	LYS
32	d	56	LYS
32	d	70	LYS
32	d	96	ILE
32	d	97	SER
32	d	98	VAL
32	d	100	LEU
34	f	129	SER
34	f	133	ARG
34	f	134	GLU
34	f	161	LYS

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Mol	Chain	Res	Type
34	f	162	SER
35	g	42	GLU
35	g	43	VAL
35	g	45	HIS
35	g	47	ASP
35	g	50	LEU
35	g	52	PHE
35	g	73	ASN
35	g	175	LYS
37	i	128	ASN
38	j	49	ARG
41	m	53	THR
41	m	57	THR
41	m	106	ASP
43	o	87	LYS
43	o	88	ARG
43	o	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
9	D	100	ASN
11	F	11	HIS
11	F	14	GLN
13	H	18	GLN
13	H	118	GLN
35	g	45	HIS
42	n	116	GLN
47	s	48	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	8/27 (29%)	1 (12%)	0
28	Z	74/75 (98%)	14 (18%)	3 (4%)
29	a	2745/2904 (94%)	355 (12%)	0
30	b	118/120 (98%)	15 (12%)	0
6	A	1513/1542 (98%)	209 (13%)	4 (0%)
All	All	4458/4668 (95%)	594 (13%)	7 (0%)

All (594) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	5	U
6	A	6	G
6	A	9	G
6	A	32	A
6	A	39	G
6	A	44	A
6	A	47	C
6	A	48	C
6	A	50	A
6	A	51	A
6	A	71	A
6	A	74	A
6	A	83	C
6	A	84	U
6	A	85	U
6	A	86	G
6	A	87	C
6	A	88	U
6	A	122	G
6	A	130	A
6	A	131	A
6	A	141	G
6	A	144	G
6	A	159	G
6	A	166	U
6	A	167	A
6	A	173	U
6	A	182	A
6	A	183	C
6	A	197	A
6	A	200	G
6	A	226	G
6	A	240	G
6	A	245	U
6	A	247	G
6	A	251	G
6	A	266	G
6	A	267	C
6	A	280	C
6	A	281	G
6	A	289	G

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Mol	Chain	Res	Type
6	A	321	A
6	A	328	C
6	A	347	G
6	A	351	G
6	A	352	C
6	A	354	G
6	A	367	U
6	A	372	C
6	A	373	A
6	A	384	G
6	A	398	U
6	A	406	G
6	A	407	U
6	A	408	A
6	A	409	U
6	A	411	A
6	A	412	A
6	A	413	G
6	A	414	A
6	A	421	U
6	A	422	C
6	A	423	G
6	A	424	G
6	A	429	U
6	A	436	C
6	A	453	G
6	A	457	G
6	A	458	U
6	A	465	A
6	A	467	U
6	A	468	A
6	A	469	C
6	A	473	U
6	A	478	A
6	A	479	U
6	A	481	G
6	A	484	G
6	A	486	U
6	A	495	A
6	A	496	A
6	A	497	G
6	A	511	C

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Mol	Chain	Res	Type
6	A	518	C
6	A	521	G
6	A	527	G7M
6	A	531	U
6	A	532	A
6	A	533	A
6	A	536	C
6	A	547	A
6	A	559	A
6	A	572	A
6	A	573	A
6	A	576	C
6	A	577	G
6	A	596	A
6	A	633	G
6	A	650	G
6	A	653	U
6	A	661	G
6	A	665	A
6	A	703	G
6	A	721	G
6	A	723	U
6	A	724	G
6	A	733	G
6	A	734	G
6	A	748	G
6	A	755	G
6	A	777	A
6	A	793	U
6	A	794	A
6	A	815	A
6	A	817	C
6	A	829	G
6	A	876	C
6	A	890	G
6	A	914	A
6	A	934	C
6	A	935	A
6	A	958	A
6	A	960	U
6	A	966	2MG
6	A	969	A

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Mol	Chain	Res	Type
6	A	975	A
6	A	976	G
6	A	977	A
6	A	992	U
6	A	993	G
6	A	994	A
6	A	1004	A
6	A	1008	U
6	A	1009	U
6	A	1017	U
6	A	1027	C
6	A	1028	C
6	A	1029	U
6	A	1030	U
6	A	1031	C
6	A	1032	G
6	A	1033	G
6	A	1034	G
6	A	1036	A
6	A	1037	C
6	A	1038	C
6	A	1039	G
6	A	1042	A
6	A	1044	A
6	A	1045	C
6	A	1046	A
6	A	1053	G
6	A	1065	U
6	A	1066	C
6	A	1085	U
6	A	1094	G
6	A	1095	U
6	A	1101	A
6	A	1133	G
6	A	1137	C
6	A	1139	G
6	A	1140	C
6	A	1159	U
6	A	1184	G
6	A	1196	A
6	A	1197	A
6	A	1213	A

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Mol	Chain	Res	Type
6	A	1214	C
6	A	1227	A
6	A	1238	A
6	A	1249	C
6	A	1257	A
6	A	1260	G
6	A	1275	A
6	A	1280	A
6	A	1285	A
6	A	1286	U
6	A	1287	A
6	A	1300	G
6	A	1302	C
6	A	1305	G
6	A	1317	C
6	A	1320	C
6	A	1331	G
6	A	1332	A
6	A	1338	G
6	A	1346	A
6	A	1353	G
6	A	1363	A
6	A	1368	A
6	A	1370	G
6	A	1377	A
6	A	1378	C
6	A	1381	U
6	A	1398	A
6	A	1419	G
6	A	1432	G
6	A	1441	A
6	A	1451	U
6	A	1452	C
6	A	1492	A
6	A	1493	A
6	A	1497	G
6	A	1499	A
6	A	1506	U
6	A	1517	G
6	A	1529	G
6	A	1530	G
27	X	19	G

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Mol	Chain	Res	Type
28	Z	6	G
28	Z	9	G
28	Z	14	A
28	Z	17	C
28	Z	18	G
28	Z	19	G
28	Z	20	U
28	Z	21	A
28	Z	34	C
28	Z	46	G
28	Z	47	U
28	Z	58	A
28	Z	69	C
28	Z	76	A
29	a	10	A
29	a	34	U
29	a	42	A
29	a	45	G
29	a	51	G
29	a	58	G
29	a	71	A
29	a	74	A
29	a	75	G
29	a	101	A
29	a	102	U
29	a	118	A
29	a	119	A
29	a	120	U
29	a	125	A
29	a	135	U
29	a	139	U
29	a	142	A
29	a	163	C
29	a	181	A
29	a	196	A
29	a	199	A
29	a	215	G
29	a	216	A
29	a	222	A
29	a	223	A
29	a	233	A
29	a	248	G

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Mol	Chain	Res	Type
29	a	265	A
29	a	272	A
29	a	274	C
29	a	277	G
29	a	278	A
29	a	281	C
29	a	282	A
29	a	285	G
29	a	294	A
29	a	311	A
29	a	329	G
29	a	330	A
29	a	345	A
29	a	361	G
29	a	362	A
29	a	386	G
29	a	396	G
29	a	405	U
29	a	411	G
29	a	412	A
29	a	451	U
29	a	464	U
29	a	480	A
29	a	481	G
29	a	489	G
29	a	491	G
29	a	504	A
29	a	505	A
29	a	509	C
29	a	513	A
29	a	530	G
29	a	531	C
29	a	532	A
29	a	544	C
29	a	545	U
29	a	546	U
29	a	547	A
29	a	548	G
29	a	549	G
29	a	563	A
29	a	573	U
29	a	575	A

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Mol	Chain	Res	Type
29	a	577	G
29	a	603	A
29	a	614	A
29	a	615	U
29	a	623	C
29	a	627	A
29	a	637	A
29	a	645	C
29	a	647	G
29	a	654	A
29	a	655	A
29	a	685	A
29	a	686	U
29	a	717	C
29	a	729	G
29	a	730	A
29	a	738	G
29	a	740	C
29	a	747	5MU
29	a	762	U
29	a	764	A
29	a	775	G
29	a	776	G
29	a	782	A
29	a	784	G
29	a	785	G
29	a	789	A
29	a	791	C
29	a	792	A
29	a	805	G
29	a	812	C
29	a	827	U
29	a	828	U
29	a	845	A
29	a	846	U
29	a	847	U
29	a	859	G
29	a	881	G
29	a	883	G
29	a	884	U
29	a	888	C
29	a	890	C

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Mol	Chain	Res	Type
29	a	891	G
29	a	895	U
29	a	896	A
29	a	897	C
29	a	910	A
29	a	913	U
29	a	915	C
29	a	931	U
29	a	946	C
29	a	948	C
29	a	961	C
29	a	974	G
29	a	983	A
29	a	985	C
29	a	989	G
29	a	996	A
29	a	1012	U
29	a	1013	C
29	a	1033	U
29	a	1034	G
29	a	1041	G
29	a	1046	A
29	a	1047	G
29	a	1108	U
29	a	1110	G
29	a	1111	A
29	a	1112	G
29	a	1115	G
29	a	1116	G
29	a	1122	G
29	a	1130	U
29	a	1132	U
29	a	1133	A
29	a	1135	C
29	a	1142	A
29	a	1155	A
29	a	1169	A
29	a	1206	G
29	a	1212	G
29	a	1250	G
29	a	1253	A
29	a	1256	G

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Mol	Chain	Res	Type
29	a	1271	G
29	a	1272	A
29	a	1273	U
29	a	1275	A
29	a	1287	A
29	a	1300	G
29	a	1301	A
29	a	1306	C
29	a	1312	U
29	a	1313	U
29	a	1314	C
29	a	1321	A
29	a	1329	U
29	a	1352	U
29	a	1365	A
29	a	1379	U
29	a	1383	A
29	a	1416	G
29	a	1419	A
29	a	1428	C
29	a	1452	G
29	a	1453	A
29	a	1476	U
29	a	1482	G
29	a	1486	U
29	a	1493	C
29	a	1497	U
29	a	1509	A
29	a	1510	G
29	a	1515	A
29	a	1524	G
29	a	1534	U
29	a	1535	A
29	a	1536	C
29	a	1537	G
29	a	1554	U
29	a	1558	C
29	a	1566	A
29	a	1567	G
29	a	1569	A
29	a	1578	U
29	a	1584	U

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Mol	Chain	Res	Type
29	a	1585	C
29	a	1588	G
29	a	1607	C
29	a	1608	A
29	a	1613	G
29	a	1626	A
29	a	1634	A
29	a	1647	U
29	a	1648	U
29	a	1649	G
29	a	1654	A
29	a	1660	G
29	a	1667	G
29	a	1674	G
29	a	1715	G
29	a	1729	U
29	a	1730	C
29	a	1738	G
29	a	1744	A
29	a	1757	A
29	a	1759	A
29	a	1764	C
29	a	1773	A
29	a	1786	A
29	a	1800	C
29	a	1801	A
29	a	1807	G
29	a	1808	A
29	a	1816	C
29	a	1829	A
29	a	1847	A
29	a	1848	A
29	a	1858	A
29	a	1864	U
29	a	1868	C
29	a	1870	C
29	a	1871	A
29	a	1873	G
29	a	1906	G
29	a	1907	G
29	a	1913	A
29	a	1914	C

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Mol	Chain	Res	Type
29	a	1927	A
29	a	1929	G
29	a	1930	G
29	a	1937	A
29	a	1955	U
29	a	1965	C
29	a	1967	C
29	a	1970	A
29	a	1971	U
29	a	1972	G
29	a	1991	U
29	a	1993	U
29	a	2021	C
29	a	2023	C
29	a	2031	A
29	a	2033	A
29	a	2035	G
29	a	2036	C
29	a	2043	C
29	a	2055	C
29	a	2056	G
29	a	2060	A
29	a	2061	G
29	a	2062	A
29	a	2069	G7M
29	a	2093	G
29	a	2198	A
29	a	2203	U
29	a	2204	G
29	a	2211	A
29	a	2225	A
29	a	2238	G
29	a	2239	G
29	a	2279	G
29	a	2283	C
29	a	2287	A
29	a	2288	A
29	a	2305	U
29	a	2308	G
29	a	2320	U
29	a	2321	U
29	a	2322	A

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Mol	Chain	Res	Type
29	a	2325	G
29	a	2333	A
29	a	2334	U
29	a	2345	G
29	a	2347	C
29	a	2350	C
29	a	2361	G
29	a	2383	G
29	a	2385	C
29	a	2391	G
29	a	2402	U
29	a	2403	C
29	a	2406	A
29	a	2422	C
29	a	2425	A
29	a	2428	G
29	a	2429	G
29	a	2430	A
29	a	2434	A
29	a	2435	A
29	a	2441	U
29	a	2448	A
29	a	2476	A
29	a	2490	G
29	a	2491	U
29	a	2502	G
29	a	2504	PSU
29	a	2505	G
29	a	2518	A
29	a	2520	C
29	a	2529	G
29	a	2535	G
29	a	2547	A
29	a	2566	A
29	a	2567	G
29	a	2573	C
29	a	2585	U
29	a	2586	U
29	a	2602	A
29	a	2609	U
29	a	2613	U
29	a	2629	U

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Mol	Chain	Res	Type
29	a	2630	G
29	a	2637	U
29	a	2644	G
29	a	2645	G
29	a	2646	C
29	a	2654	A
29	a	2660	A
29	a	2661	G
29	a	2689	U
29	a	2690	U
29	a	2717	C
29	a	2726	A
29	a	2727	A
29	a	2732	G
29	a	2733	A
29	a	2739	U
29	a	2744	G
29	a	2748	A
29	a	2752	C
29	a	2765	A
29	a	2778	A
29	a	2798	U
29	a	2820	A
29	a	2821	A
29	a	2835	A
29	a	2836	U
29	a	2848	G
29	a	2849	U
29	a	2861	U
29	a	2873	A
29	a	2884	U
29	a	2891	U
29	a	2899	A
30	b	9	G
30	b	13	G
30	b	24	G
30	b	33	G
30	b	34	A
30	b	35	C
30	b	36	C
30	b	42	C
30	b	45	A

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Mol	Chain	Res	Type
30	b	56	G
30	b	67	G
30	b	89	U
30	b	90	C
30	b	99	A
30	b	109	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	5	U
6	A	792	A
6	A	1026	G
6	A	1035	A
28	Z	16	C
28	Z	17	C
28	Z	18	G

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

38 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	$\#\|Z\| > 2$
29	1MG	a	745	29	19,26,27	2.93	6 (31%)	18,39,42	1.60	3 (16%)
6	PSU	A	516	56,6	18,21,22	1.01	1 (5%)	21,30,33	1.98	6 (28%)
40	4D4	l	81	40	9,11,12	1.96	2 (22%)	7,13,15	2.12	3 (42%)
29	PSU	a	746	56,29	18,21,22	1.11	2 (11%)	21,30,33	1.98	4 (19%)
6	4OC	A	1402	6	20,23,24	2.91	8 (40%)	25,32,35	0.96	2 (8%)
6	5MC	A	1407	6	19,22,23	0.89	1 (5%)	26,32,35	0.73	0
29	5MC	a	1962	29	19,22,23	0.81	0	26,32,35	0.70	0
29	2MG	a	2445	29	18,26,27	1.45	3 (16%)	16,38,41	0.86	1 (6%)
29	PSU	a	1917	29	18,21,22	1.04	1 (5%)	21,30,33	1.86	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	6MZ	a	1618	29	17,25,26	1.47	1 (5%)	15,36,39	3.85	3 (20%)
29	2MA	a	2503	56,29	17,25,26	2.25	5 (29%)	16,37,40	1.99	5 (31%)
17	D2T	L	89	17	8,9,10	1.71	2 (25%)	6,11,13	1.73	3 (50%)
29	2MG	a	1835	29	18,26,27	1.37	3 (16%)	16,38,41	0.95	1 (6%)
29	PSU	a	2604	29	18,21,22	1.07	1 (5%)	21,30,33	2.24	5 (23%)
6	2MG	A	1516	6	18,26,27	1.28	3 (16%)	16,38,41	0.97	1 (6%)
29	3TD	a	1915	29	19,22,23	4.07	7 (36%)	23,32,35	1.92	4 (17%)
29	PSU	a	2504	29	18,21,22	1.08	2 (11%)	21,30,33	1.85	4 (19%)
29	G7M	a	2069	29	20,26,27	2.41	7 (35%)	16,39,42	1.22	2 (12%)
6	MA6	A	1519	6	19,26,27	1.76	2 (10%)	18,38,41	3.54	4 (22%)
6	UR3	A	1498	6	19,22,23	2.63	7 (36%)	26,32,35	1.73	4 (15%)
29	PSU	a	1911	29	18,21,22	1.07	2 (11%)	21,30,33	2.08	5 (23%)
29	OMG	a	2251	28,29	19,26,27	1.39	3 (15%)	21,38,41	0.84	1 (4%)
29	PSU	a	2580	29	18,21,22	1.09	3 (16%)	21,30,33	2.03	5 (23%)
6	2MG	A	1207	6	18,26,27	1.22	3 (16%)	16,38,41	0.89	1 (6%)
32	MEQ	d	150	32	8,9,10	0.98	0	5,10,12	0.52	0
6	2MG	A	966	6	18,26,27	1.30	3 (16%)	16,38,41	0.87	1 (6%)
29	6MZ	a	2030	29	17,25,26	1.39	1 (5%)	15,36,39	4.06	5 (33%)
29	5MU	a	747	29	19,22,23	0.60	0	27,32,35	0.77	2 (7%)
6	G7M	A	527	6	20,26,27	2.54	7 (35%)	16,39,42	1.24	2 (12%)
29	PSU	a	2605	29	18,21,22	1.10	2 (11%)	21,30,33	1.95	3 (14%)
29	PSU	a	2457	29	18,21,22	1.11	2 (11%)	21,30,33	2.16	5 (23%)
29	PSU	a	955	29	18,21,22	1.07	1 (5%)	21,30,33	1.97	4 (19%)
29	OMU	a	2552	29	19,22,23	2.84	7 (36%)	25,31,34	1.83	4 (16%)
29	5MU	a	1939	29	19,22,23	0.77	0	27,32,35	0.56	0
6	5MC	A	967	6	19,22,23	0.67	0	26,32,35	0.58	0
29	OMC	a	2498	56,29	19,22,23	0.79	1 (5%)	25,31,34	0.86	1 (4%)
29	H2U	a	2449	29	18,21,22	0.65	0	19,30,33	1.07	1 (5%)
6	MA6	A	1518	6	19,26,27	1.79	3 (15%)	18,38,41	3.35	3 (16%)

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
29	1MG	a	745	29	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	A	516	56,6	-	0/7/25/26	0/2/2/2
40	4D4	l	81	40	-	4/11/12/14	-
29	PSU	a	746	56,29	-	2/7/25/26	0/2/2/2
6	4OC	A	1402	6	-	1/9/29/30	0/2/2/2
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
29	5MC	a	1962	29	-	0/7/25/26	0/2/2/2
29	2MG	a	2445	29	-	1/5/27/28	0/3/3/3
29	PSU	a	1917	29	-	0/7/25/26	0/2/2/2
29	6MZ	a	1618	29	-	2/5/27/28	0/3/3/3
29	2MA	a	2503	56,29	-	1/3/25/26	0/3/3/3
17	D2T	L	89	17	-	4/7/12/14	-
29	2MG	a	1835	29	-	2/5/27/28	0/3/3/3
29	PSU	a	2604	29	-	0/7/25/26	0/2/2/2
6	2MG	A	1516	6	-	0/5/27/28	0/3/3/3
29	3TD	a	1915	29	-	0/7/25/26	0/2/2/2
29	PSU	a	2504	29	-	2/7/25/26	0/2/2/2
29	G7M	a	2069	29	-	1/3/25/26	0/3/3/3
6	MA6	A	1519	6	-	3/7/29/30	0/3/3/3
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
29	PSU	a	1911	29	-	0/7/25/26	0/2/2/2
29	OMG	a	2251	28,29	-	0/5/27/28	0/3/3/3
29	PSU	a	2580	29	-	0/7/25/26	0/2/2/2
6	2MG	A	1207	6	-	0/5/27/28	0/3/3/3
32	MEQ	d	150	32	-	2/8/9/11	-
6	2MG	A	966	6	-	2/5/27/28	0/3/3/3
29	6MZ	a	2030	29	-	2/5/27/28	0/3/3/3
29	5MU	a	747	29	-	1/7/25/26	0/2/2/2
6	G7M	A	527	6	-	3/3/25/26	0/3/3/3
29	PSU	a	2605	29	-	0/7/25/26	0/2/2/2
29	PSU	a	2457	29	-	0/7/25/26	0/2/2/2
29	PSU	a	955	29	-	0/7/25/26	0/2/2/2
29	OMU	a	2552	29	-	1/9/27/28	0/2/2/2
29	5MU	a	1939	29	-	0/7/25/26	0/2/2/2
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
29	OMC	a	2498	56,29	-	0/9/27/28	0/2/2/2
29	H2U	a	2449	29	-	0/7/38/39	0/2/2/2
6	MA6	A	1518	6	-	0/7/29/30	0/3/3/3

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	1915	3TD	C6-C5	12.31	1.48	1.35
29	a	1915	3TD	C2-N1	9.14	1.48	1.37
29	a	745	1MG	C2-N3	8.28	1.46	1.33
6	A	1498	UR3	C2-N1	6.91	1.48	1.38
29	a	2552	OMU	C2-N1	6.60	1.48	1.38
6	A	1402	4OC	C4-N3	6.52	1.43	1.32
29	a	2552	OMU	C2-N3	6.11	1.48	1.38
6	A	1402	4OC	C6-C5	6.06	1.49	1.35
29	a	745	1MG	C2-N2	5.85	1.44	1.34
29	a	2503	2MA	C2-N3	5.78	1.44	1.31
29	a	1915	3TD	C6-N1	5.71	1.45	1.36
6	A	1498	UR3	C6-C5	5.66	1.48	1.35
6	A	527	G7M	C2-N2	5.62	1.47	1.34
29	a	2069	G7M	C2-N2	5.48	1.47	1.34
6	A	1402	4OC	C2-N3	5.39	1.47	1.36
6	A	1518	MA6	C6-N6	5.38	1.49	1.37
29	a	2552	OMU	C6-C5	5.29	1.47	1.35
6	A	1519	MA6	C6-N6	5.25	1.49	1.37
6	A	527	G7M	C4-N3	4.89	1.49	1.37
6	A	527	G7M	C2-N3	4.84	1.45	1.33
29	a	745	1MG	C4-N3	4.84	1.48	1.37
29	a	1618	6MZ	C6-C5	-4.81	1.37	1.44
29	a	1915	3TD	C2-N3	4.76	1.48	1.38
40	l	81	4D4	CZ-NE	4.74	1.42	1.33
29	a	2503	2MA	C4-N3	4.67	1.48	1.37
29	a	2069	G7M	C4-N3	4.66	1.48	1.37
29	a	2069	G7M	C2-N3	4.44	1.44	1.33
6	A	1518	MA6	C6-C5	-4.42	1.38	1.44
6	A	1498	UR3	C2-N3	4.42	1.47	1.39
29	a	2030	6MZ	C6-C5	-4.42	1.38	1.44
6	A	1519	MA6	C6-C5	-4.39	1.38	1.44
29	a	745	1MG	C5-C4	-3.94	1.33	1.43
6	A	1402	4OC	C4-N4	3.93	1.44	1.36
29	a	2445	2MG	C8-N7	-3.81	1.28	1.34
29	a	1835	2MG	C8-N7	-3.79	1.28	1.34
29	a	2251	OMG	C8-N7	-3.66	1.29	1.34
6	A	1402	4OC	C2-N1	3.56	1.47	1.40
6	A	966	2MG	C8-N7	-3.55	1.29	1.34
29	a	2552	OMU	C4-N3	3.54	1.44	1.38
29	a	2552	OMU	O4-C4	-3.50	1.17	1.24
6	A	527	G7M	C6-N1	3.47	1.43	1.37
6	A	1402	4OC	C5-C4	3.43	1.48	1.41
6	A	527	G7M	C2-N1	3.41	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	2503	2MA	C5-C4	-3.41	1.34	1.43
6	A	1402	4OC	O2-C2	-3.37	1.17	1.23
6	A	1516	2MG	C8-N7	-3.31	1.29	1.34
6	A	527	G7M	C5-C6	3.28	1.53	1.45
17	L	89	D2T	CB-CA	-3.21	1.53	1.54
29	a	1917	PSU	C6-C5	3.20	1.38	1.35
29	a	1911	PSU	C6-C5	3.14	1.38	1.35
29	a	2251	OMG	C5-C6	-3.12	1.41	1.47
6	A	1207	2MG	C8-N7	-3.08	1.30	1.34
29	a	2069	G7M	C6-N1	3.02	1.42	1.37
29	a	1915	3TD	O2-C2	-3.00	1.17	1.23
29	a	2069	G7M	C2-N1	2.99	1.44	1.37
29	a	2504	PSU	C6-C5	2.99	1.38	1.35
29	a	2552	OMU	O2-C2	-2.98	1.17	1.23
29	a	746	PSU	C6-C5	2.98	1.38	1.35
29	a	2069	G7M	C5-C6	2.98	1.53	1.45
29	a	2605	PSU	C6-C5	2.92	1.38	1.35
29	a	955	PSU	C6-C5	2.90	1.38	1.35
6	A	1402	4OC	C6-N1	2.90	1.45	1.38
29	a	745	1MG	C2-N1	2.87	1.42	1.37
29	a	2069	G7M	O6-C6	-2.82	1.16	1.23
29	a	2445	2MG	C5-C6	-2.82	1.41	1.47
29	a	2604	PSU	C6-C5	2.78	1.38	1.35
6	A	966	2MG	C5-C6	-2.77	1.42	1.47
29	a	1835	2MG	C5-C6	-2.77	1.42	1.47
6	A	1498	UR3	C6-N1	2.76	1.44	1.38
6	A	516	PSU	C6-C5	2.76	1.38	1.35
6	A	527	G7M	O6-C6	-2.74	1.17	1.23
29	a	2503	2MA	C6-N1	2.70	1.43	1.37
29	a	2457	PSU	C6-C5	2.68	1.38	1.35
6	A	1498	UR3	O2-C2	-2.65	1.17	1.22
6	A	1498	UR3	O4-C4	-2.59	1.18	1.23
40	l	81	4D4	CZ-NH1	2.59	1.43	1.34
6	A	1516	2MG	C5-C6	-2.59	1.42	1.47
6	A	1207	2MG	C5-C6	-2.57	1.42	1.47
29	a	2445	2MG	C5-C4	-2.55	1.36	1.43
29	a	745	1MG	C5-C6	2.49	1.54	1.47
29	a	2552	OMU	C6-N1	2.49	1.44	1.38
29	a	2503	2MA	C2-N1	2.48	1.43	1.36
29	a	1915	3TD	C4-N3	2.41	1.45	1.40
29	a	2580	PSU	C6-C5	2.40	1.37	1.35
29	a	2251	OMG	C5-C4	-2.37	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	2580	PSU	O4'-C1'	-2.25	1.40	1.43
6	A	966	2MG	C5-C4	-2.24	1.37	1.43
6	A	1516	2MG	C5-C4	-2.24	1.37	1.43
29	a	1835	2MG	C5-C4	-2.23	1.37	1.43
29	a	746	PSU	C4-C5	-2.22	1.38	1.44
29	a	2605	PSU	C4-C5	-2.15	1.38	1.44
29	a	1915	3TD	O4-C4	-2.14	1.18	1.23
6	A	1207	2MG	C5-C4	-2.11	1.37	1.43
29	a	2580	PSU	C4-C5	-2.11	1.38	1.44
6	A	1518	MA6	C2-N3	2.10	1.35	1.32
6	A	1407	5MC	C4-N3	-2.09	1.30	1.34
17	L	89	D2T	CB1-SB	-2.08	1.75	1.79
6	A	1498	UR3	C4-N3	2.06	1.44	1.40
29	a	2498	OMC	C4-N3	-2.05	1.30	1.34
29	a	2457	PSU	C4-C5	-2.04	1.38	1.44
29	a	2504	PSU	C4-C5	-2.01	1.38	1.44
29	a	1911	PSU	C4-C5	-2.00	1.38	1.44

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1519	MA6	N1-C6-N6	-12.62	102.26	116.83
6	A	1518	MA6	N1-C6-N6	-11.97	103.00	116.83
29	a	2030	6MZ	C1'-N9-C4	11.96	147.66	126.64
29	a	1618	6MZ	C1'-N9-C4	11.72	147.24	126.64
29	a	1618	6MZ	N3-C2-N1	-6.89	119.32	128.67
6	A	1519	MA6	N3-C2-N1	-6.80	119.44	128.67
29	a	2030	6MZ	N3-C2-N1	-6.79	119.46	128.67
29	a	2030	6MZ	C2-N1-C6	6.48	121.63	116.60
6	A	1518	MA6	N3-C2-N1	-6.43	119.95	128.67
29	a	1915	3TD	N1-C2-N3	6.17	120.62	116.13
6	A	1498	UR3	C4-N3-C2	-6.00	119.75	124.58
29	a	2552	OMU	C4-N3-C2	-5.59	119.67	126.61
29	a	2457	PSU	N1-C2-N3	5.58	121.05	115.17
29	a	2604	PSU	N1-C2-N3	5.54	121.01	115.17
29	a	2604	PSU	C4-N3-C2	-5.49	118.81	126.37
29	a	2457	PSU	C4-N3-C2	-5.44	118.87	126.37
29	a	1911	PSU	N1-C2-N3	5.26	120.71	115.17
29	a	1618	6MZ	C2-N1-C6	5.25	120.67	116.60
29	a	2580	PSU	N1-C2-N3	5.21	120.67	115.17
29	a	955	PSU	N1-C2-N3	5.17	120.62	115.17
29	a	746	PSU	C4-N3-C2	-5.12	119.32	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	746	PSU	N1-C2-N3	5.05	120.49	115.17
29	a	2580	PSU	C4-N3-C2	-4.96	119.54	126.37
29	a	2605	PSU	C4-N3-C2	-4.96	119.54	126.37
29	a	2605	PSU	N1-C2-N3	4.94	120.38	115.17
29	a	955	PSU	C4-N3-C2	-4.93	119.57	126.37
29	a	1911	PSU	C4-N3-C2	-4.92	119.59	126.37
6	A	516	PSU	N1-C2-N3	4.91	120.34	115.17
29	a	2504	PSU	C4-N3-C2	-4.87	119.66	126.37
6	A	516	PSU	C4-N3-C2	-4.83	119.72	126.37
29	a	1917	PSU	C4-N3-C2	-4.81	119.74	126.37
29	a	2504	PSU	N1-C2-N3	4.74	120.17	115.17
29	a	1917	PSU	N1-C2-N3	4.72	120.15	115.17
29	a	2503	2MA	C4-N3-C2	-4.54	119.81	123.30
29	a	1915	3TD	C4-N3-C2	-4.35	120.00	124.61
29	a	745	1MG	C5-C6-N1	4.26	120.12	113.96
29	a	2552	OMU	C5-C4-N3	4.03	120.44	114.80
6	A	1498	UR3	C5-C4-N3	3.89	120.16	115.04
40	l	81	4D4	NE-CZ-NH2	3.85	127.29	120.67
29	a	2503	2MA	C8-N7-C5	3.76	108.96	102.55
29	a	2552	OMU	N3-C2-N1	3.76	119.79	114.89
29	a	2604	PSU	O2-C2-N1	-3.67	119.00	122.79
29	a	745	1MG	C8-N7-C5	3.45	108.42	102.55
6	A	1518	MA6	C2-N1-C6	3.44	120.21	116.84
29	a	2457	PSU	O2-C2-N1	-3.39	119.29	122.79
29	a	2449	H2U	C5-C4-N3	-3.34	113.13	116.69
6	A	527	G7M	C2-N1-C6	-3.29	119.08	125.11
29	a	2503	2MA	C5-C6-N1	3.28	120.24	114.12
6	A	516	PSU	O2-C2-N1	-3.28	119.41	122.79
6	A	1519	MA6	C2-N1-C6	3.16	119.94	116.84
29	a	1911	PSU	O2-C2-N1	-3.09	119.60	122.79
29	a	2604	PSU	C6-C5-C4	3.04	120.22	118.17
29	a	746	PSU	O2-C2-N1	-2.98	119.71	122.79
40	l	81	4D4	O-C-CA	-2.94	117.20	124.77
29	a	2069	G7M	C2-N1-C6	-2.90	119.81	125.11
29	a	2552	OMU	O4-C4-C5	-2.83	120.27	125.16
29	a	1911	PSU	C6-C5-C4	2.81	120.07	118.17
29	a	2503	2MA	CM2-C2-N1	2.74	121.96	116.27
29	a	1915	3TD	C6-C5-C4	2.72	120.02	118.19
29	a	955	PSU	O2-C2-N1	-2.69	120.01	122.79
29	a	2580	PSU	C6-N1-C2	-2.69	120.20	122.69
29	a	1835	2MG	O6-C6-C5	2.68	129.63	124.32
6	A	1516	2MG	O6-C6-C5	2.66	129.60	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	1911	PSU	C6-N1-C2	-2.65	120.23	122.69
6	A	1498	UR3	C6-N1-C2	-2.65	119.64	121.80
29	a	955	PSU	C6-N1-C2	-2.54	120.33	122.69
29	a	1917	PSU	O2-C2-N1	-2.53	120.17	122.79
29	a	2580	PSU	O4'-C1'-C2'	2.48	108.58	105.15
29	a	2503	2MA	N1-C2-N3	-2.46	119.26	123.15
29	a	2580	PSU	O2-C2-N1	-2.46	120.25	122.79
6	A	516	PSU	C6-N1-C2	-2.45	120.41	122.69
29	a	746	PSU	C6-N1-C2	-2.44	120.43	122.69
29	a	2457	PSU	C6-N1-C2	-2.40	120.46	122.69
29	a	745	1MG	O6-C6-C5	-2.39	120.25	124.18
29	a	2504	PSU	O2-C2-N1	-2.36	120.36	122.79
40	l	81	4D4	NH1-CZ-NE	-2.34	113.95	119.27
17	L	89	D2T	OD2-CG-CB	2.33	118.19	113.15
6	A	1402	4OC	CM4-N4-C4	-2.33	117.90	122.45
29	a	2251	OMG	O6-C6-C5	2.32	128.92	124.32
29	a	2605	PSU	C6-N1-C2	-2.30	120.56	122.69
29	a	2445	2MG	O6-C6-C5	2.27	128.83	124.32
6	A	1519	MA6	C1'-N9-C4	-2.27	122.66	126.64
29	a	2504	PSU	C6-N1-C2	-2.24	120.61	122.69
6	A	966	2MG	O6-C6-C5	2.23	128.74	124.32
6	A	516	PSU	O4'-C1'-C2'	2.21	108.20	105.15
29	a	747	5MU	C1'-N1-C6	-2.20	117.53	121.15
29	a	2069	G7M	N2-C2-N1	2.20	121.40	116.76
6	A	1207	2MG	O6-C6-C5	2.20	128.67	124.32
29	a	2604	PSU	C6-N1-C2	-2.18	120.67	122.69
29	a	2030	6MZ	C9-N6-C6	2.15	124.84	122.85
6	A	1498	UR3	C1'-N1-C2	2.13	120.53	117.04
29	a	747	5MU	C1'-N1-C2	2.12	121.39	117.59
29	a	1917	PSU	C6-N1-C2	-2.11	120.73	122.69
17	L	89	D2T	CB-CA-N	2.11	113.38	109.10
6	A	1402	4OC	C6-C5-C4	2.11	119.54	117.00
6	A	527	G7M	N2-C2-N1	2.07	121.12	116.76
29	a	2498	OMC	C1'-N1-C2	2.06	122.98	118.44
6	A	516	PSU	C6-C5-C4	2.05	119.56	118.17
29	a	2457	PSU	C6-C5-C4	2.04	119.55	118.17
29	a	1915	3TD	C1'-C5-C4	2.03	120.69	117.61
17	L	89	D2T	O-C-CA	-2.01	119.61	124.77
29	a	2030	6MZ	C4-C5-N7	-2.00	107.22	109.34

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CG-CB-SB-CB1
17	L	89	D2T	CA-CB-CG-OD1
17	L	89	D2T	CA-CB-CG-OD2
17	L	89	D2T	SB-CB-CG-OD2
40	l	81	4D4	O-C-CA-CB
40	l	81	4D4	CA-CB-CG-CD
29	a	1618	6MZ	C5-C6-N6-C9
29	a	1618	6MZ	N1-C6-N6-C9
6	A	527	G7M	C3'-C4'-C5'-O5'
6	A	966	2MG	O4'-C4'-C5'-O5'
6	A	966	2MG	C3'-C4'-C5'-O5'
29	a	2030	6MZ	O4'-C4'-C5'-O5'
29	a	2030	6MZ	C3'-C4'-C5'-O5'
29	a	2504	PSU	O4'-C4'-C5'-O5'
6	A	1519	MA6	O4'-C4'-C5'-O5'
40	l	81	4D4	OB-CB-CG-CD
32	d	150	MEQ	OE1-CD-CG-CB
32	d	150	MEQ	NE2-CD-CG-CB
29	a	1835	2MG	O4'-C4'-C5'-O5'
6	A	527	G7M	O4'-C4'-C5'-O5'
29	a	1835	2MG	C3'-C4'-C5'-O5'
6	A	1402	4OC	O4'-C4'-C5'-O5'
29	a	2504	PSU	C3'-C4'-C5'-O5'
29	a	2445	2MG	C3'-C4'-C5'-O5'
40	l	81	4D4	NE-CD-CG-CB
6	A	1519	MA6	C5-C6-N6-C9
6	A	527	G7M	C4'-C5'-O5'-P
6	A	1519	MA6	C3'-C4'-C5'-O5'
29	a	2552	OMU	C3'-C2'-O2'-CM2
29	a	2503	2MA	C4'-C5'-O5'-P
29	a	2069	G7M	C4'-C5'-O5'-P
29	a	746	PSU	O4'-C1'-C5-C6
29	a	746	PSU	C2'-C1'-C5-C6
29	a	747	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 312 ligands modelled in this entry, 311 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
57	IAS	K	201	-	6,7,8	1.02	0	3,8,10	1.98	2 (66%)

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
57	IAS	K	201	-	-	3/7/7/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	K	201	IAS	OXT-C-O	-2.21	119.06	124.08
57	K	201	IAS	OD1-CG-CB	-2.09	119.28	125.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	K	201	IAS	N-CA-CB-CG
57	K	201	IAS	C-CA-CB-CG
57	K	201	IAS	CA-CB-CG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

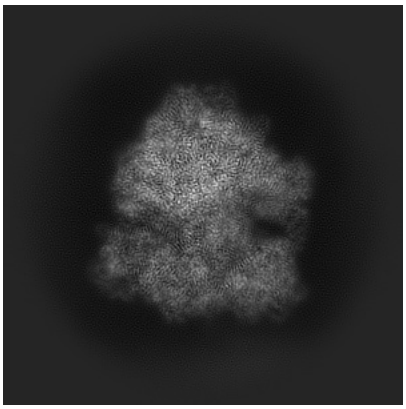
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45572. These allow visual inspection of the internal detail of the map and identification of artifacts.

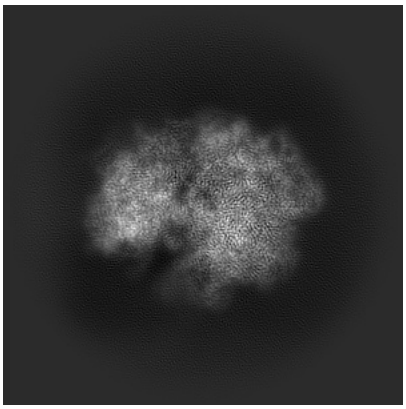
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

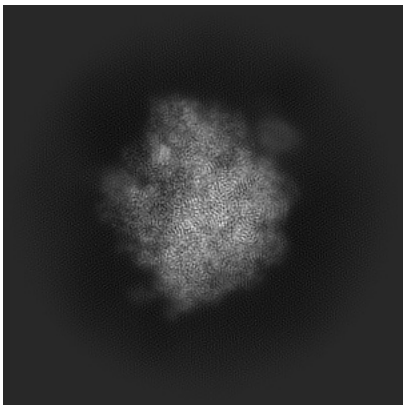
6.1.1 Primary map



X

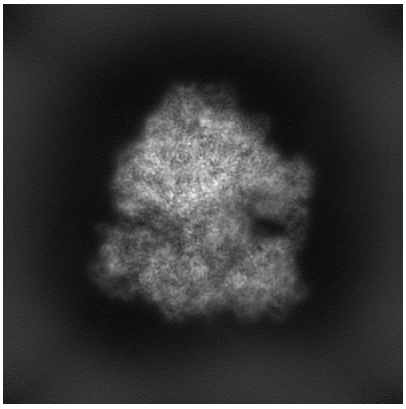


Y

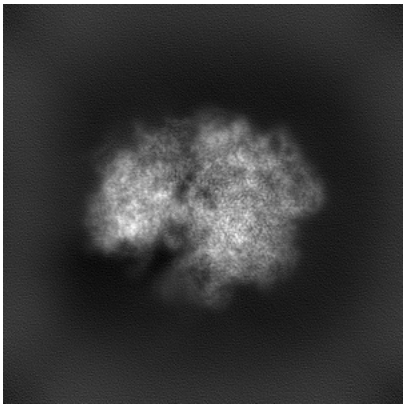


Z

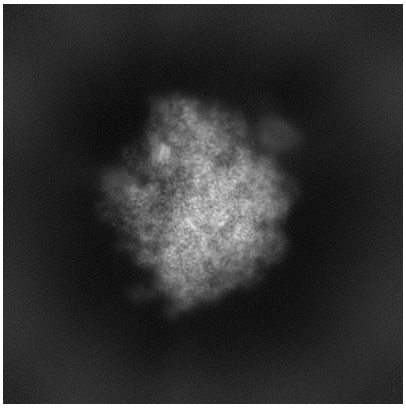
6.1.2 Raw map



X



Y

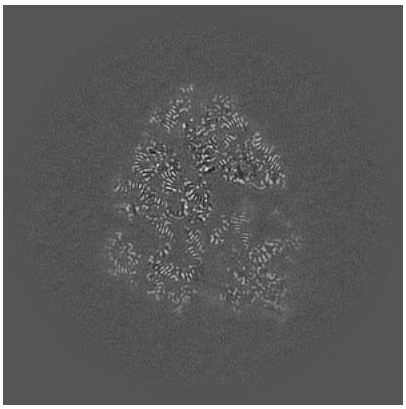


Z

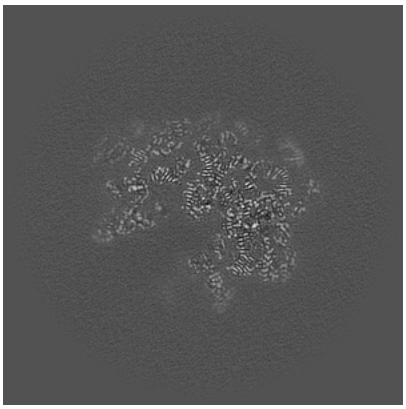
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

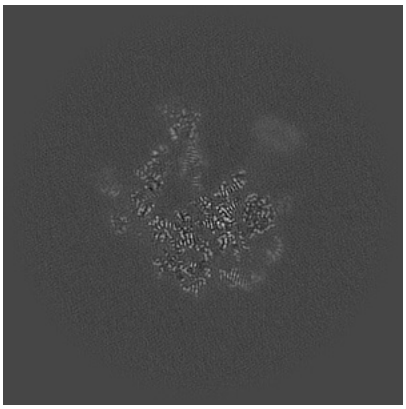
6.2.1 Primary map



X Index: 200

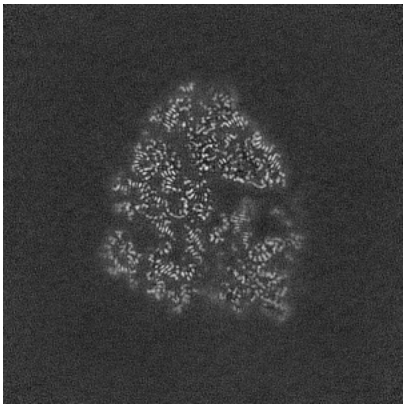


Y Index: 200

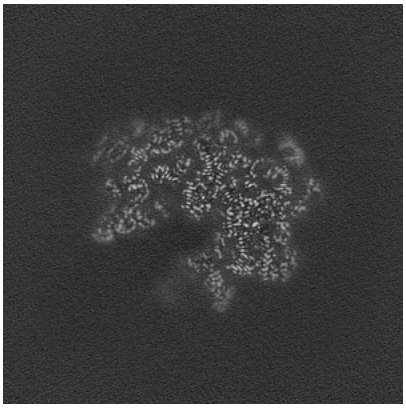


Z Index: 200

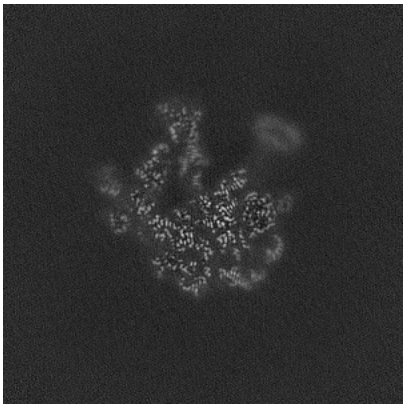
6.2.2 Raw map



X Index: 200



Y Index: 200

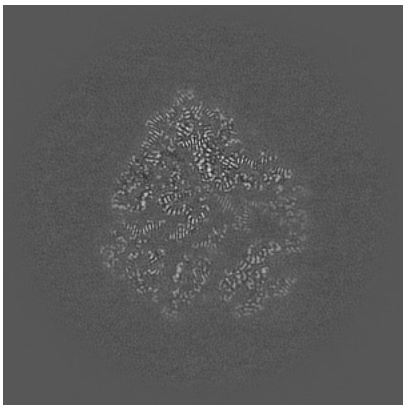


Z Index: 200

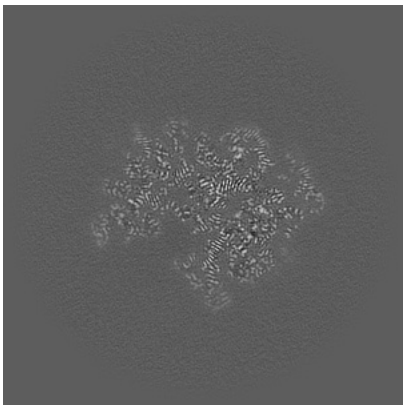
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

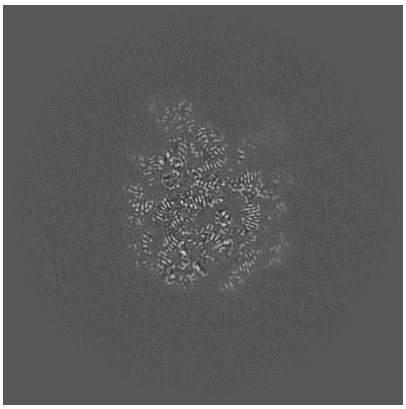
6.3.1 Primary map



X Index: 192

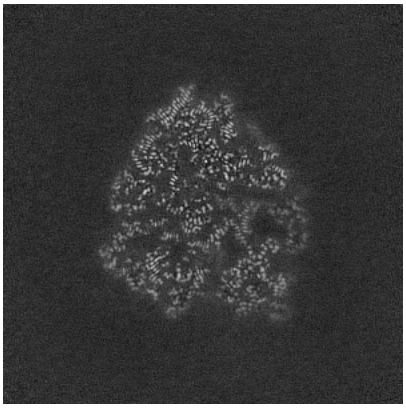


Y Index: 190

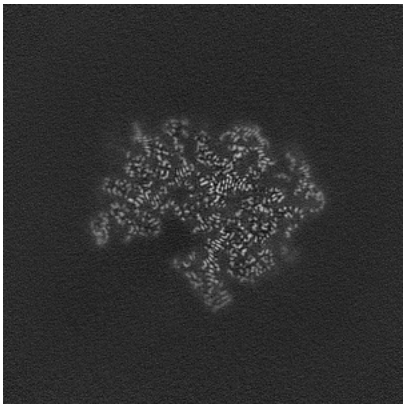


Z Index: 237

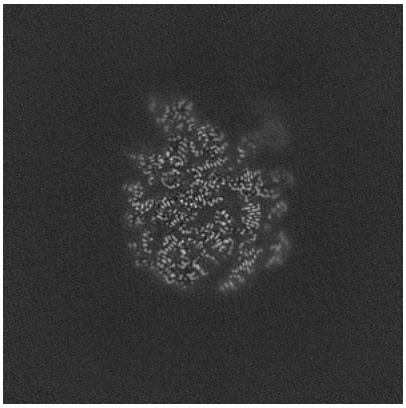
6.3.2 Raw map



X Index: 195



Y Index: 190

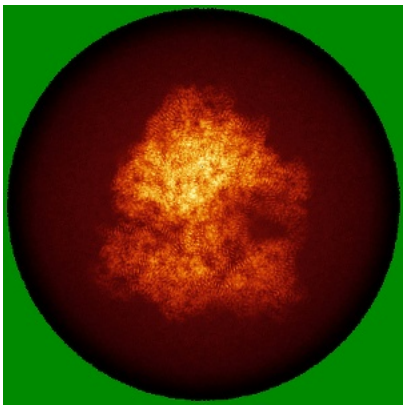


Z Index: 237

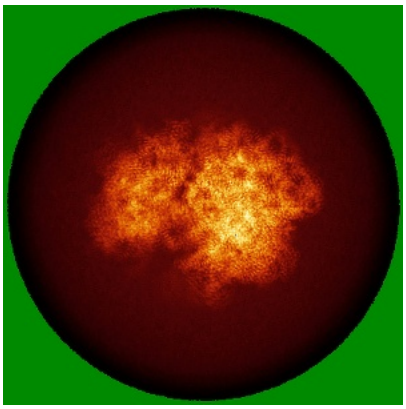
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

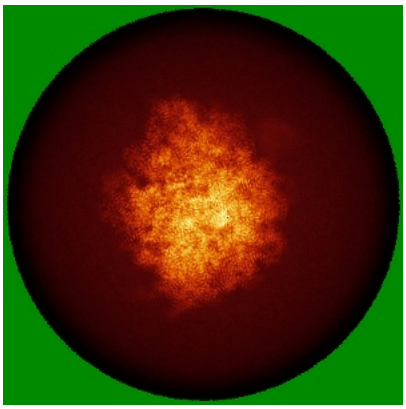
6.4.1 Primary map



X

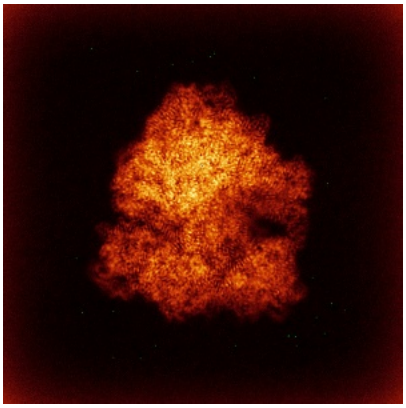


Y

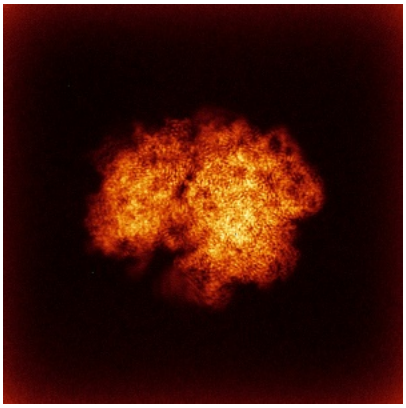


Z

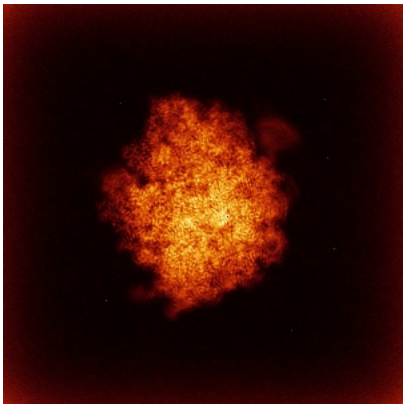
6.4.2 Raw map



X



Y

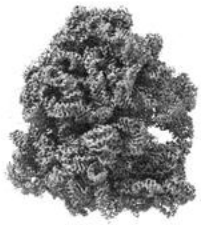


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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.

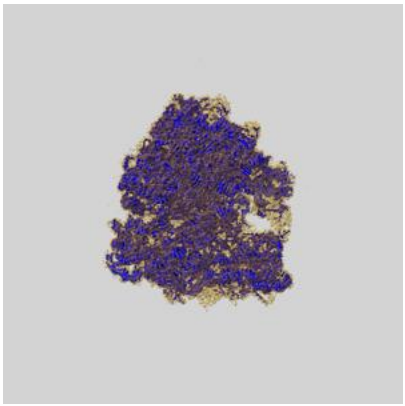
6.6 Mask visualisation

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

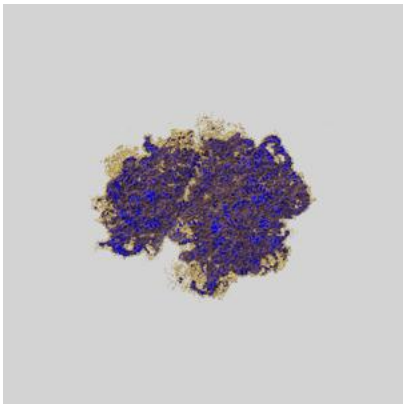
A mask typically either:

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

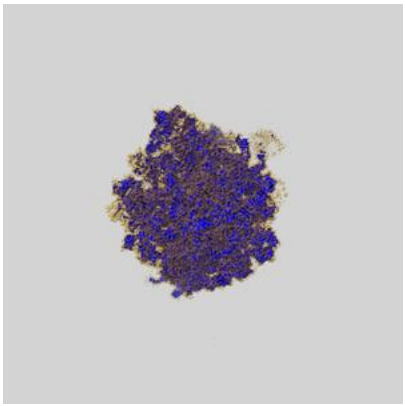
6.6.1 emd_45572_msk_1.map



X



Y

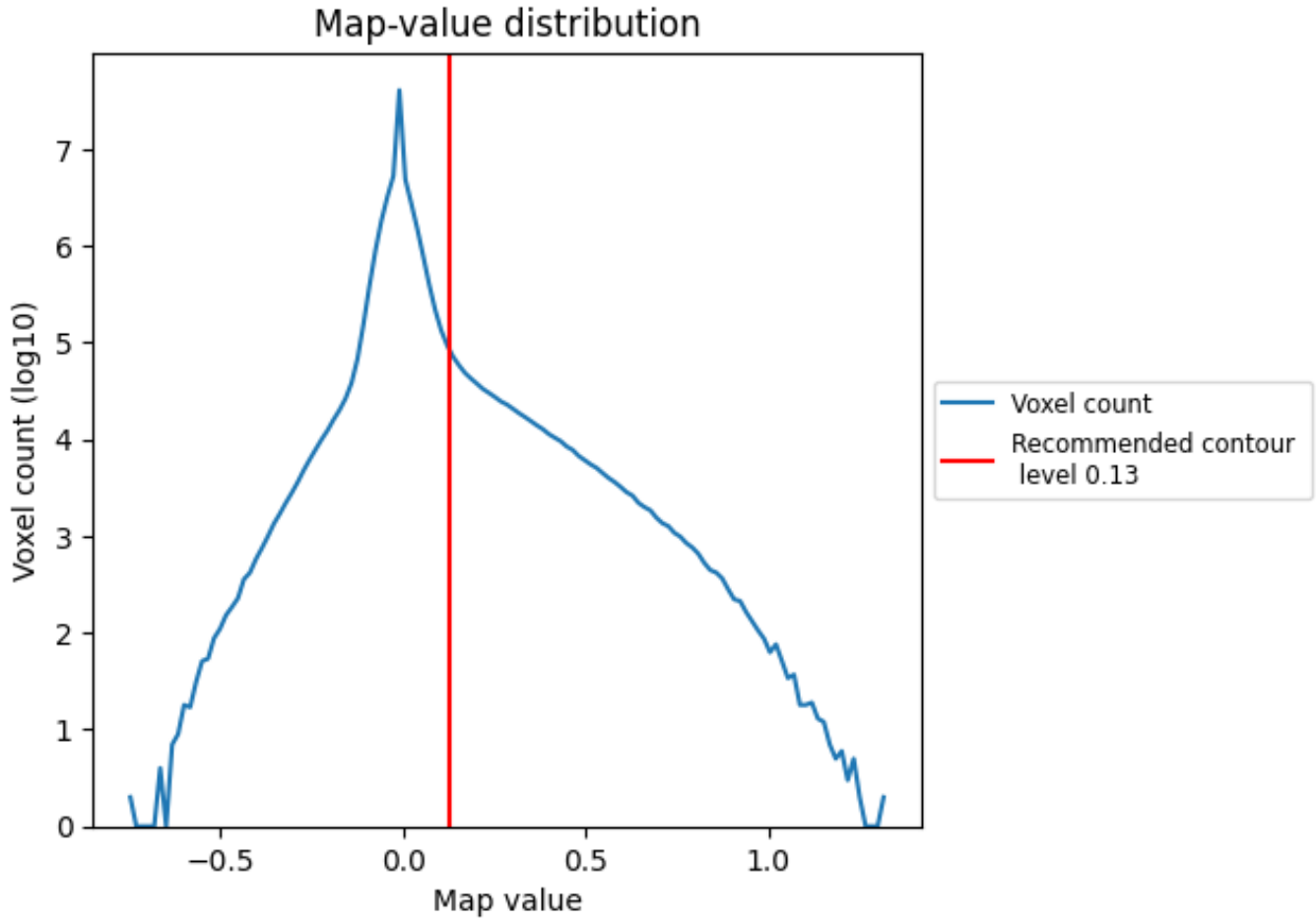


Z

7 Map analysis

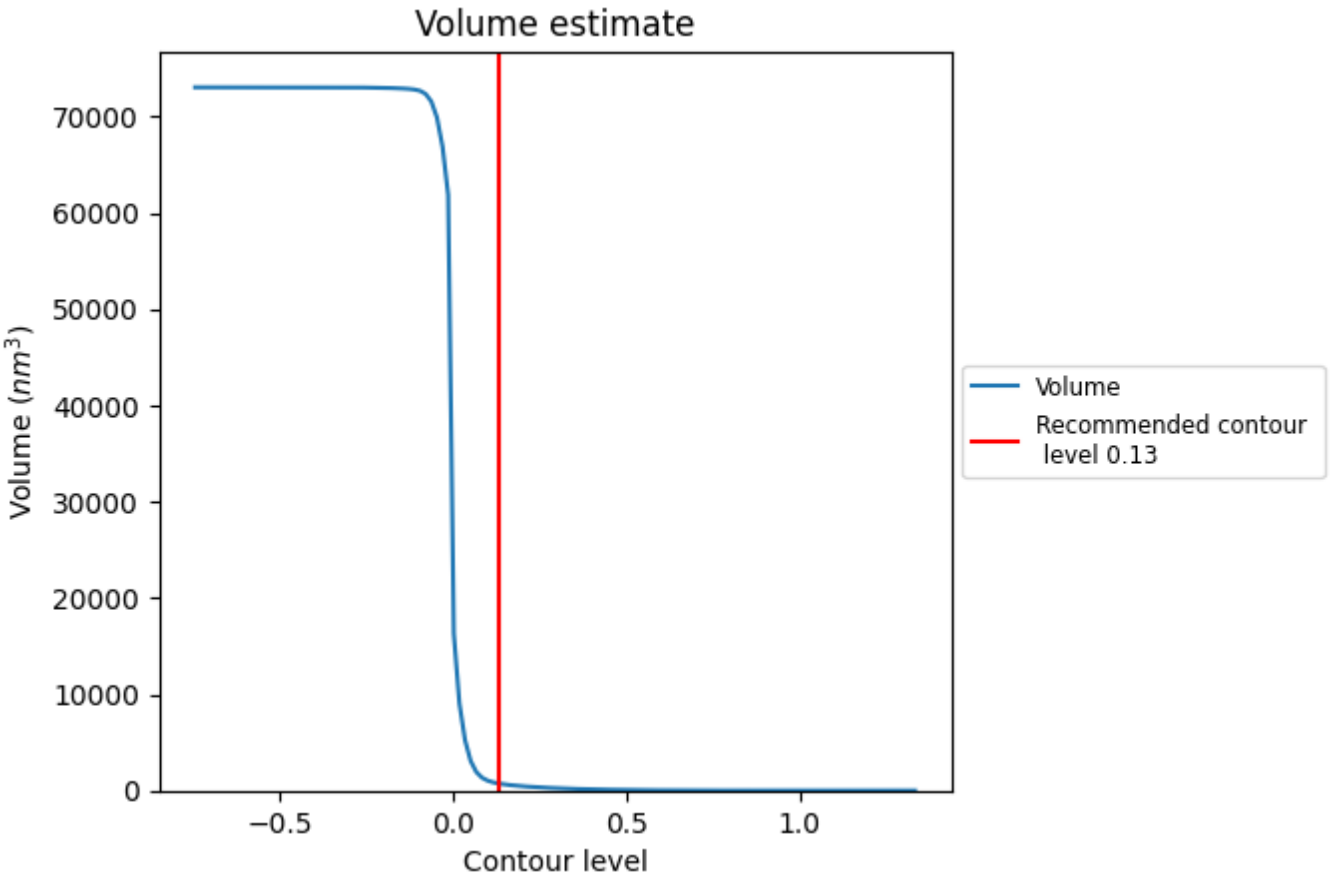
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

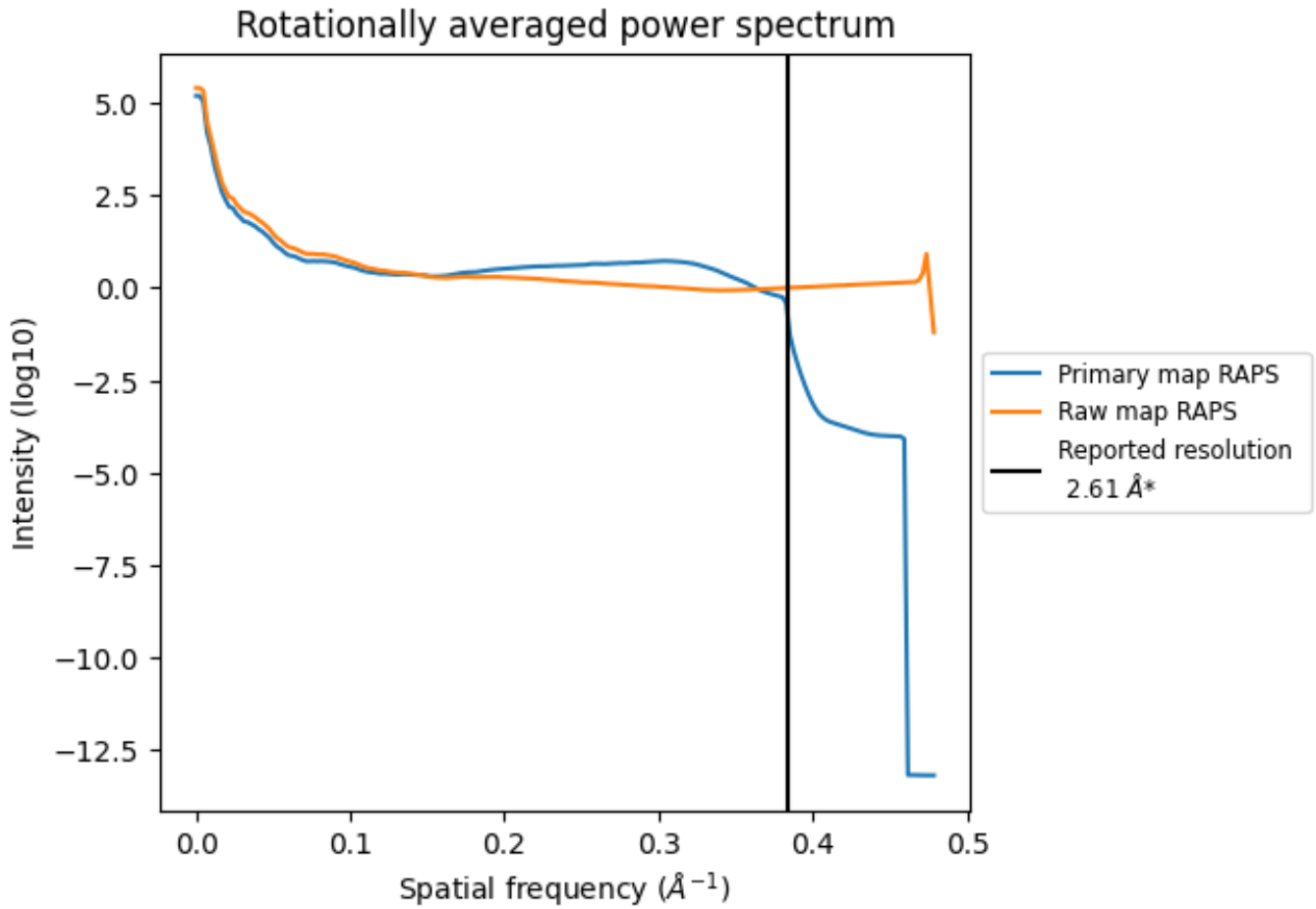
7.2 Volume estimate



The volume at the recommended contour level is 740 nm^3; this corresponds to an approximate mass of 669 kDa.

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

7.3 Rotationally averaged power spectrum (i)

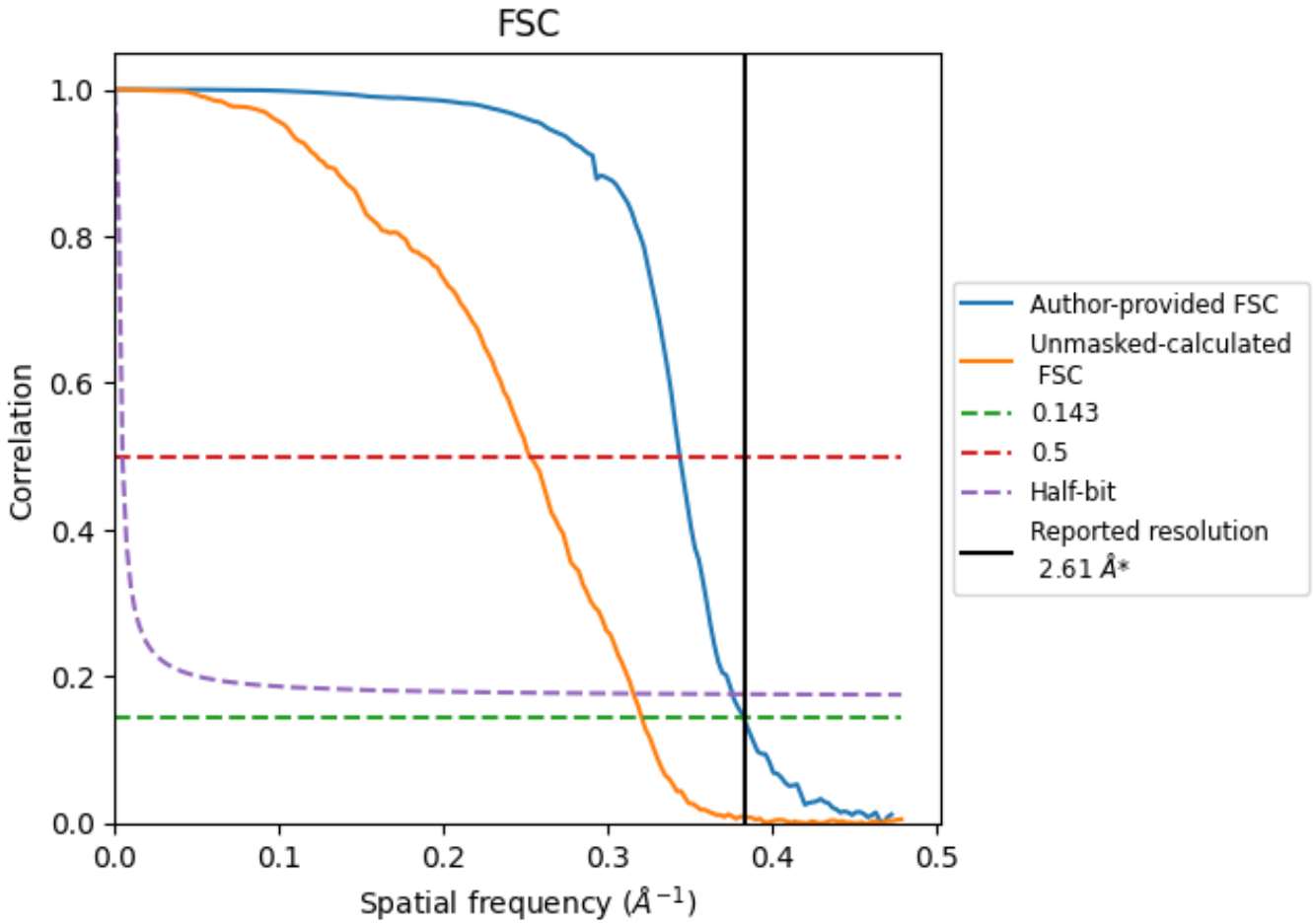


*Reported resolution corresponds to spatial frequency of 0.383 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.383 $Å^{-1}$

8.2 Resolution estimates (i)

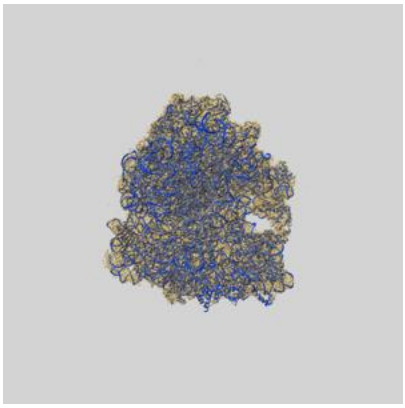
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	2.61	2.91	2.66
Unmasked-calculated*	3.12	3.96	3.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.61 by more than 10 %

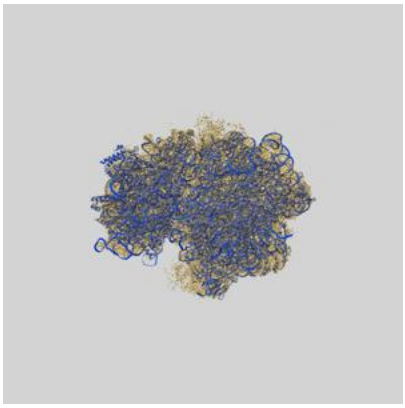
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45572 and PDB model 9CG6. Per-residue inclusion information can be found in section 3 on page 15.

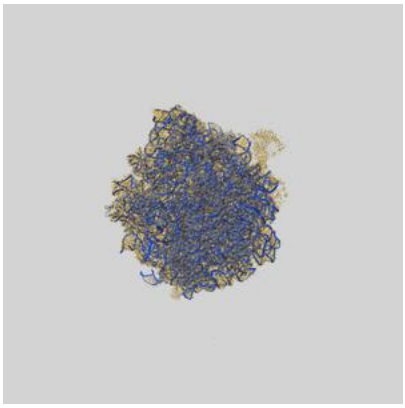
9.1 Map-model overlay



X



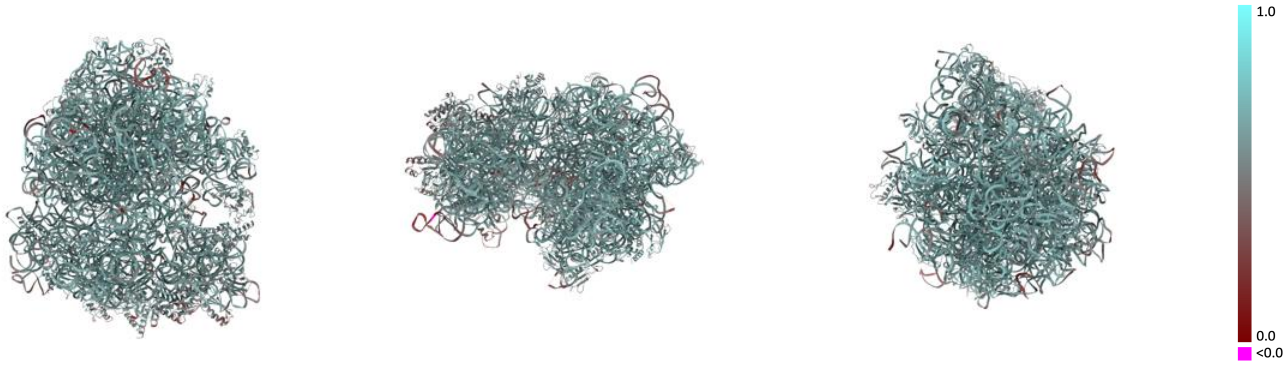
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

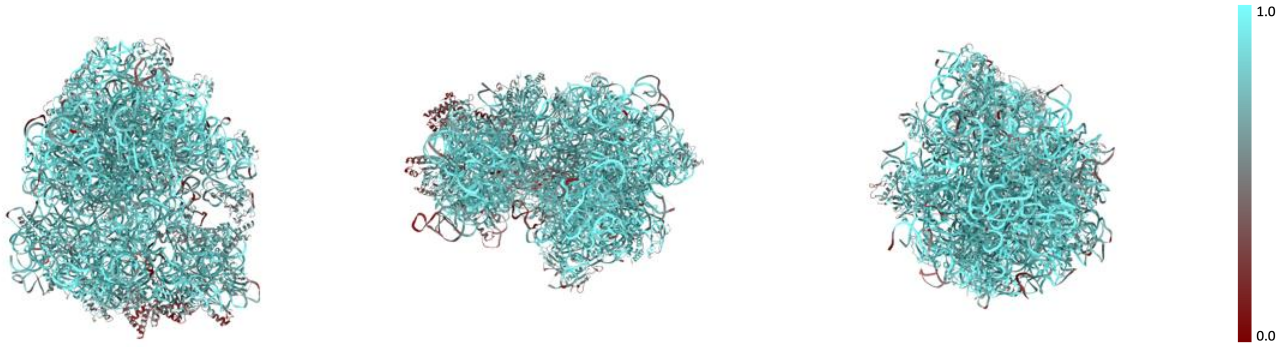
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

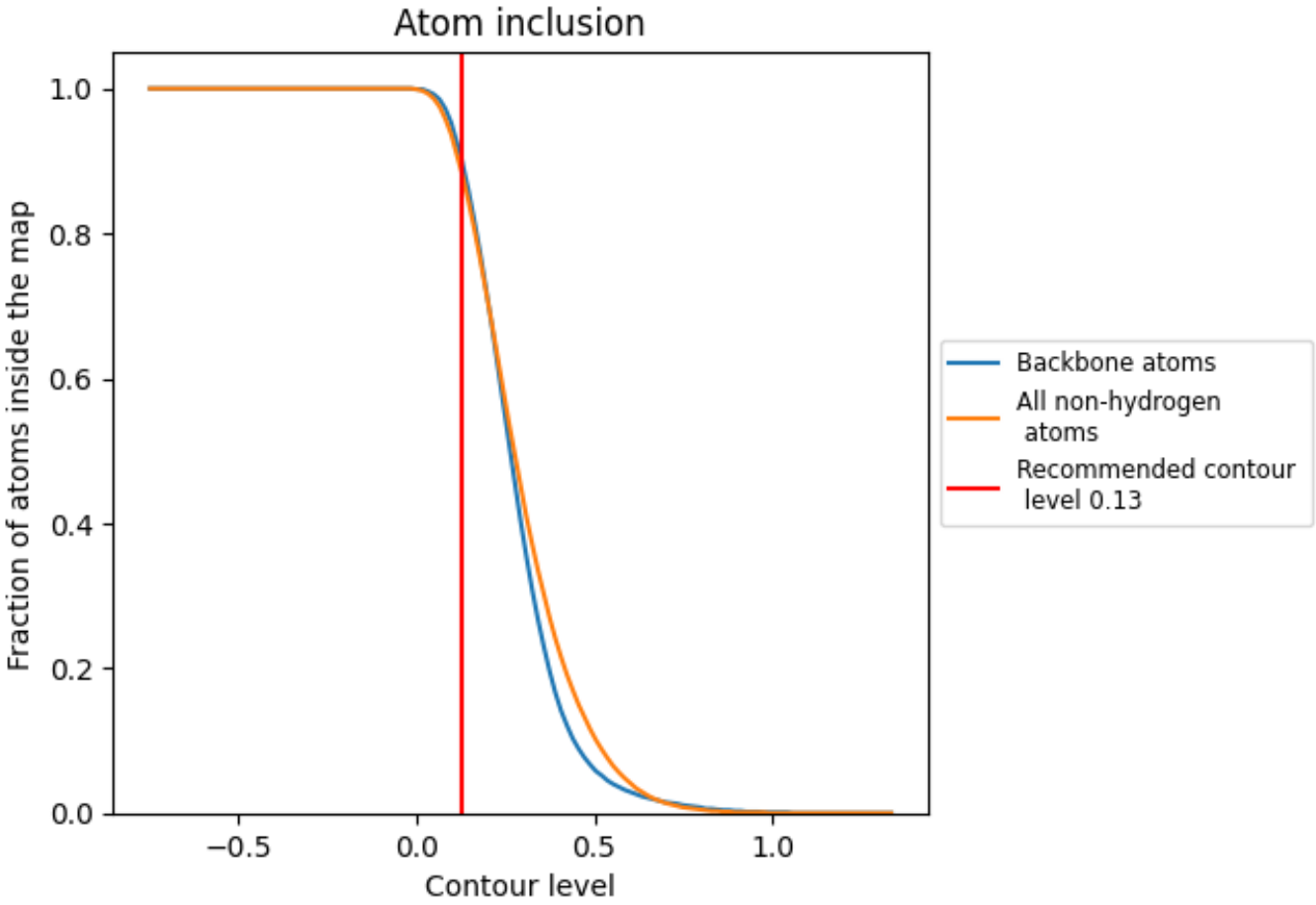
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8820	0.6150
0	0.8190	0.6070
1	0.9520	0.6620
2	0.9490	0.6600
3	0.9080	0.6370
4	0.5020	0.5000
A	0.9080	0.6090
B	0.4220	0.5120
C	0.7520	0.5800
D	0.7420	0.5590
E	0.8540	0.6200
F	0.6930	0.5560
G	0.6560	0.5570
H	0.8420	0.6170
I	0.7470	0.5660
J	0.5970	0.5300
K	0.7970	0.6030
L	0.8300	0.6170
M	0.7140	0.5690
N	0.7750	0.5910
O	0.8040	0.6070
P	0.8310	0.5970
Q	0.7790	0.5950
R	0.7480	0.5870
S	0.6750	0.5480
T	0.8170	0.6080
U	0.5370	0.5270
X	0.5330	0.4720
Z	0.7290	0.5530
a	0.9400	0.6330
b	0.9140	0.6090
c	0.9230	0.6520
d	0.8990	0.6460
e	0.8230	0.6140
f	0.6990	0.5760

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	0.6340	0.5410
h	0.6270	0.5400
i	0.9040	0.6350
j	0.8630	0.6300
k	0.8700	0.6330
l	0.8720	0.6300
m	0.9540	0.6530
n	0.8080	0.6000
o	0.8400	0.6280
p	0.9420	0.6580
q	0.8480	0.6200
r	0.8850	0.6250
s	0.8210	0.6070
t	0.7640	0.5780
u	0.7780	0.5960
v	0.8900	0.6450
w	0.8880	0.6350
x	0.7610	0.5860
y	0.8580	0.6180
z	0.8740	0.6320