



Full wwPDB EM Validation Report ⓘ

Mar 11, 2025 – 02:14 PM EDT

PDB ID : 6OM6
EMDB ID : EMD-20121
Title : Structure of trans-translation inhibitor bound to E. coli 70S ribosome with P site tRNA
Authors : Hoffer, E.D.; Mehrani, A.; Keiler, K.C.; Stagg, S.M.; Dunham, C.M.
Deposited on : 2019-04-18
Resolution : 3.10 Å(reported)
Based on initial model : 5MDV

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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

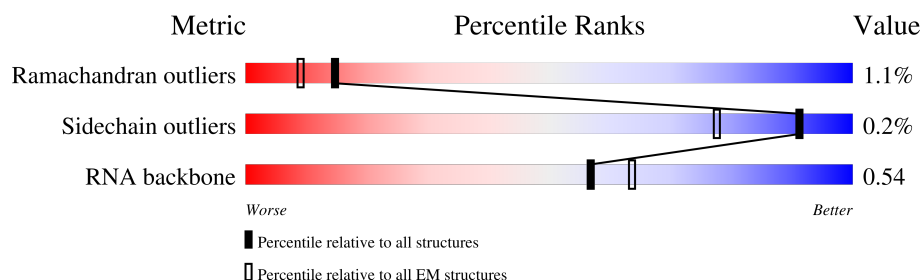
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	2904	
2	2	1534	
3	3	120	
4	4	5	
5	5	76	
6	B	273	
7	C	209	
8	D	201	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	E	179	
10	F	177	
11	G	149	
12	J	142	
13	K	123	
14	L	144	
15	M	136	
16	N	127	
17	O	117	
18	P	115	
19	Q	118	
20	R	103	
21	S	110	
22	T	100	
23	U	104	
24	V	94	
25	X	78	
26	Y	63	
27	Z	59	
28	a	70	
29	b	57	
30	c	55	
31	d	46	
32	e	65	
33	f	38	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	g	241	
35	h	233	
36	i	206	
37	j	167	
38	k	135	
39	l	179	
40	m	130	
41	n	130	
42	o	103	
43	p	129	
44	q	124	
45	r	118	
46	s	101	
47	t	89	
48	u	82	
49	v	84	
50	w	75	
51	x	92	
52	y	87	
53	z	71	
54	W	85	

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 144295 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62334	27814	11470	20147	2903		

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	5	Total	C	N	O	P	0	0
			110	49	23	33	5		

- Molecule 5 is a RNA chain called tRNA(gly).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	76	Total	C	N	O	P	0	0
			1619	722	284	537	76		

- Molecule 6 is a protein called 50S ribosomal protein L2.

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

- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

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

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 11 is a protein called 50S ribosomal protein L9.

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

- Molecule 12 is a protein called 50S ribosomal protein L13.

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

- Molecule 13 is a protein called 50S ribosomal protein L14.

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

- Molecule 14 is a protein called 50S ribosomal protein L15.

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

- Molecule 15 is a protein called 50S ribosomal protein L16.

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

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 17 is a protein called 50S ribosomal protein L18.

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

- Molecule 18 is a protein called 50S ribosomal protein L19.

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

- Molecule 19 is a protein called 50S ribosomal protein L20.

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

- Molecule 20 is a protein called 50S ribosomal protein L21.

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

- Molecule 21 is a protein called 50S ribosomal protein L22.

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

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	103	Total	C	N	O	0	0
			788	498	148	142		

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 28 is a protein called 50S ribosomal protein L31.

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

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

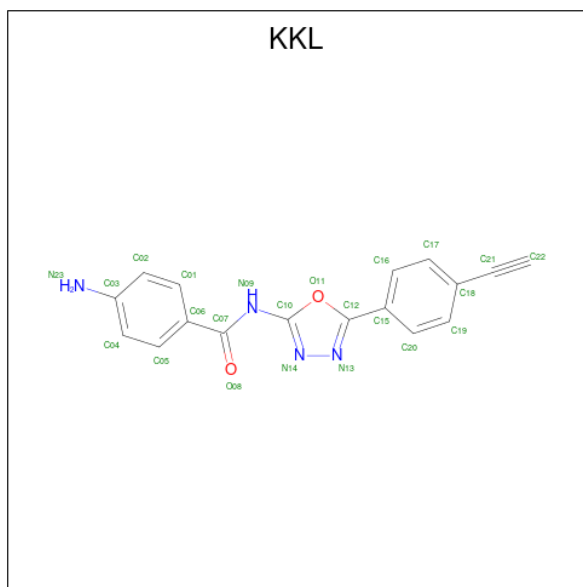
- Molecule 53 is a protein called 30S ribosomal protein S21.

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

- Molecule 54 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 55 is 4-amino-N-[5-(4-ethynylphenyl)-1,3,4-oxadiazol-2-yl]benzamide (three-letter code: KKL) (formula: C₁₇H₁₂N₄O₂) (labeled as "Ligand of Interest" by depositor).

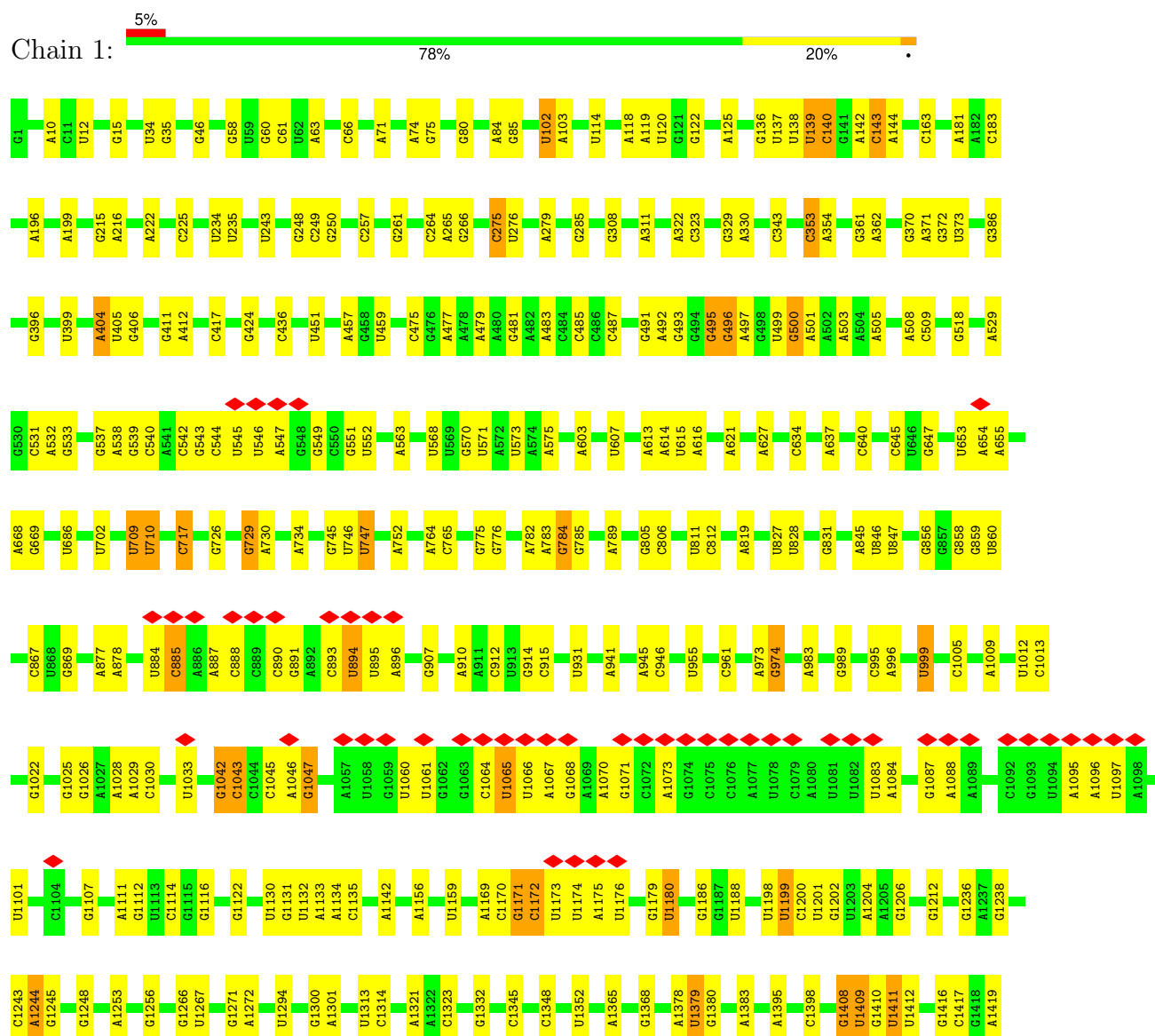


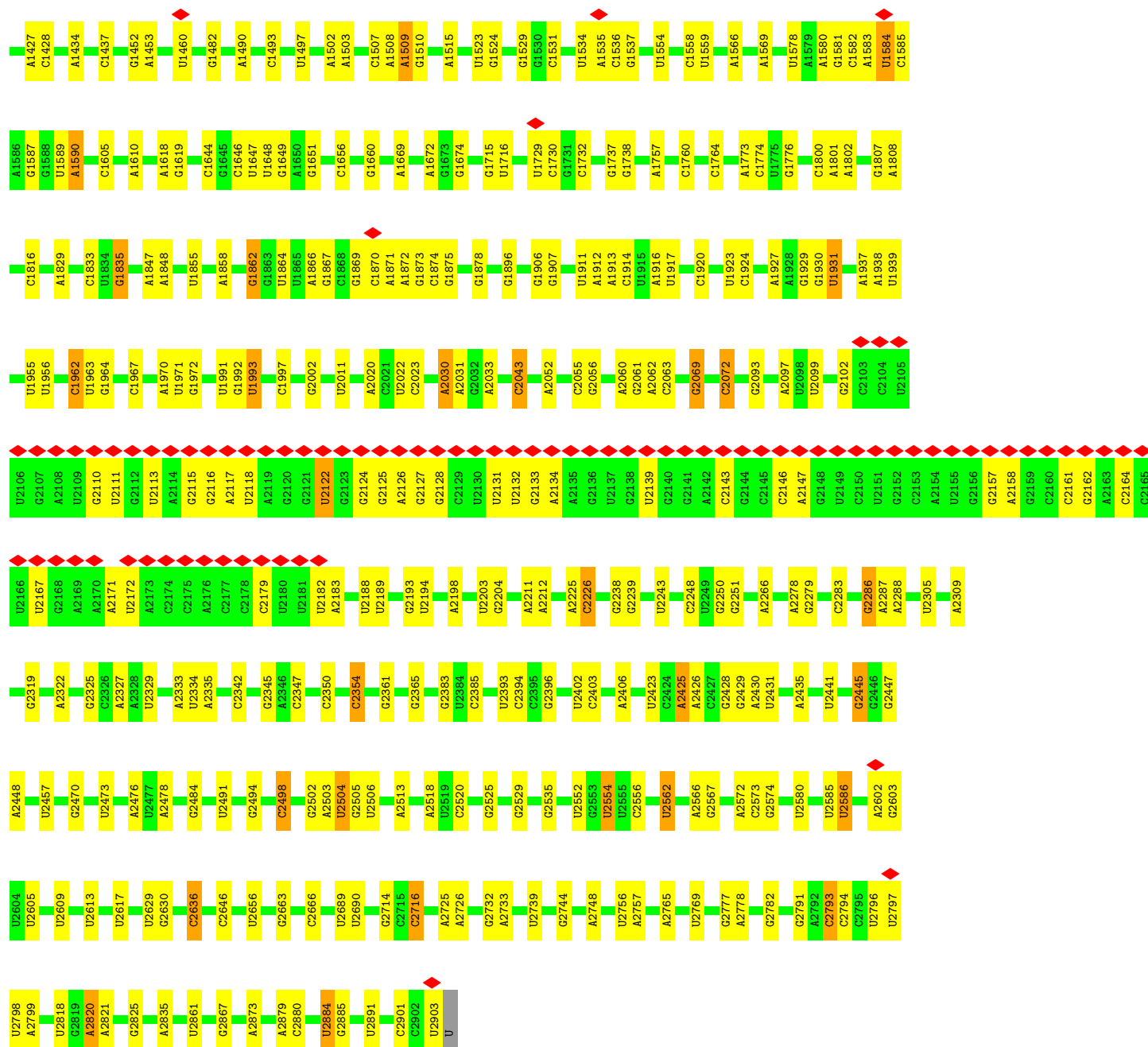
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
55	1	1	23	17	4	2	0

3 Residue-property plots

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

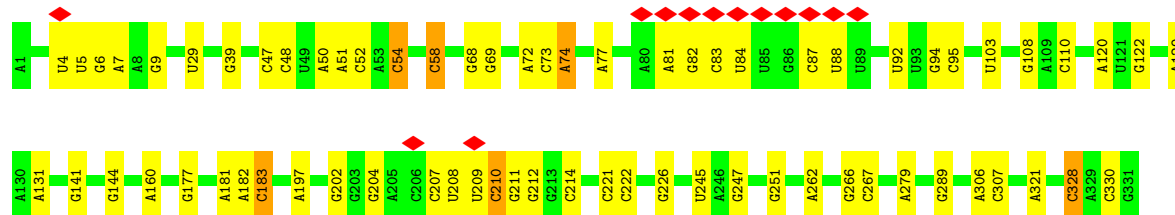
• Molecule 1: 23S ribosomal RNA

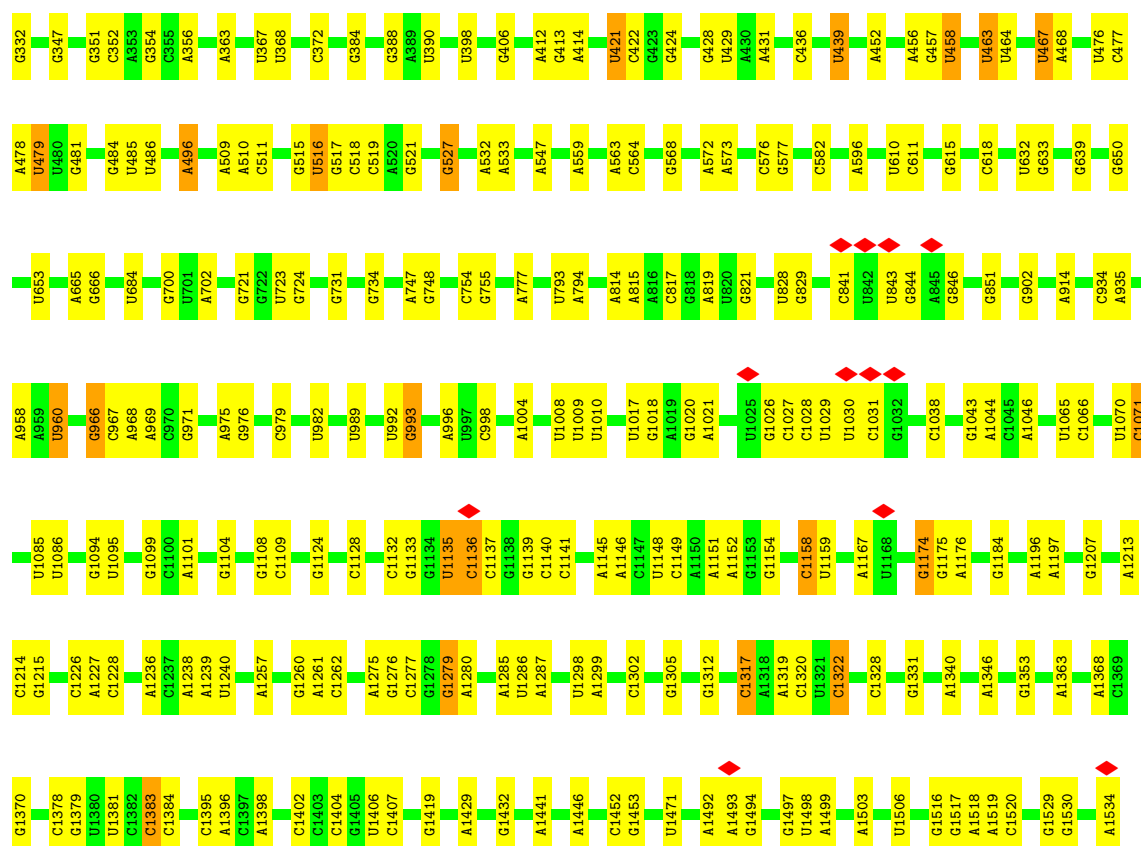




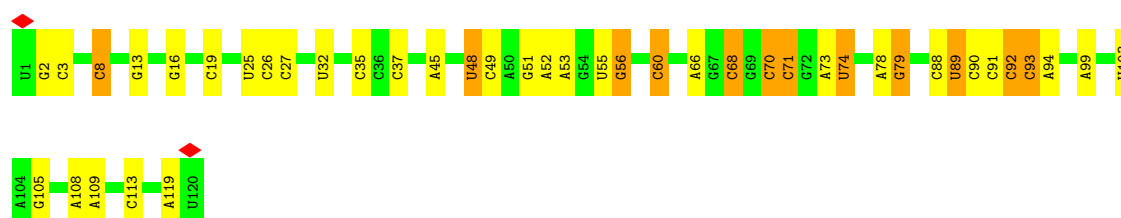
• Molecule 2: 16S ribosomal RNA

Chain 2: 79% 19%





• Molecule 3: 5S ribosomal RNA

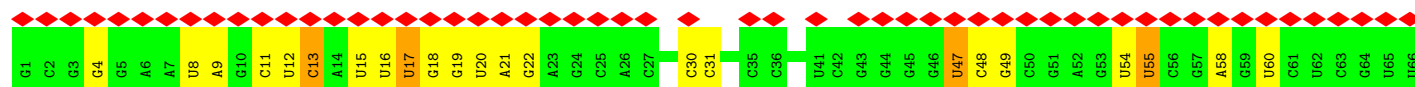
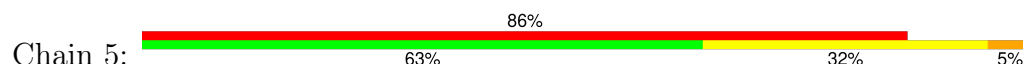


• Molecule 4: mRNA



There are no outlier residues recorded for this chain.

• Molecule 5: tRNA(gly)





- Molecule 6: 50S ribosomal protein L2

Chain B: 92% 7% .



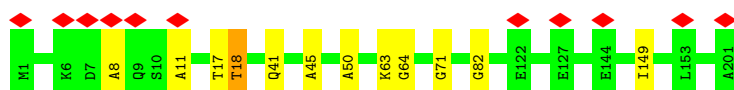
- Molecule 7: 50S ribosomal protein L3

Chain C: 95% 5%



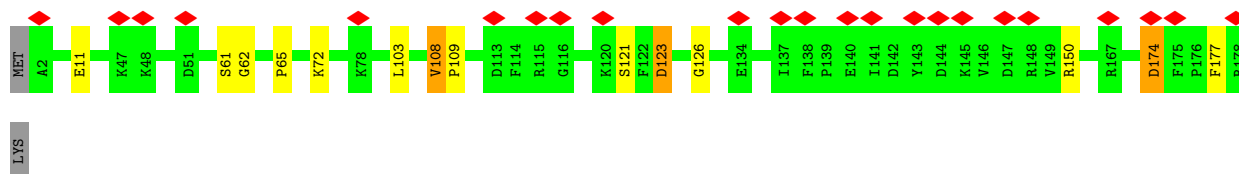
- Molecule 8: 50S ribosomal protein L4

Chain D: 5% 94% 5%



- Molecule 9: 50S ribosomal protein L5

Chain E: 13% 91% 6% ..



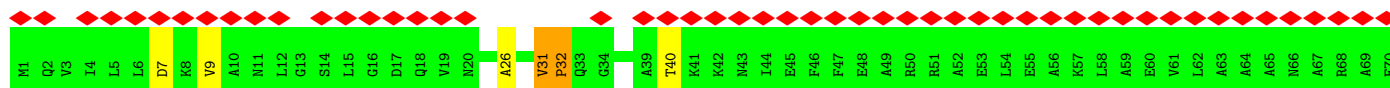
- Molecule 10: 50S ribosomal protein L6

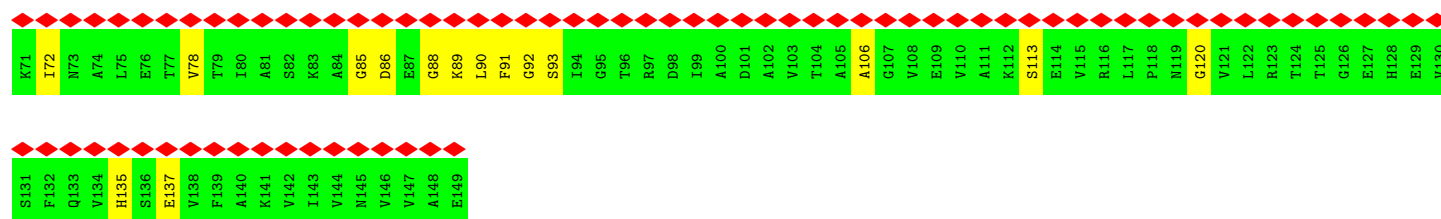
Chain F: 7% 93% 6% ..



- Molecule 11: 50S ribosomal protein L9

Chain G: 87% 86% 13% .





- Molecule 12: 50S ribosomal protein L13

Chain J:  96%

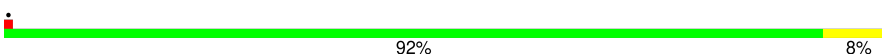


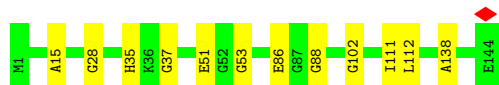
- Molecule 13: 50S ribosomal protein L14

Chain K:  96%



- Molecule 14: 50S ribosomal protein L15

Chain L:  92% 8%



- Molecule 15: 50S ribosomal protein L16

Chain M:  99%



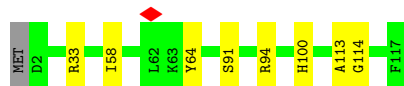
- Molecule 16: 50S ribosomal protein L17

Chain N:  90% 6%



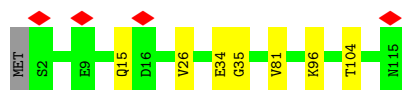
- Molecule 17: 50S ribosomal protein L18

Chain O:  92% 7%



- Molecule 18: 50S ribosomal protein L19

Chain P:  93% 6%




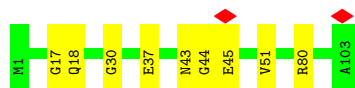
- Molecule 19: 50S ribosomal protein L20

Chain Q:  95%



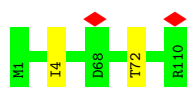
- Molecule 20: 50S ribosomal protein L21

Chain R:  91% 9%




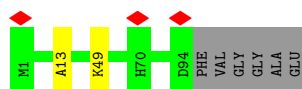
- Molecule 21: 50S ribosomal protein L22

Chain S:  98%




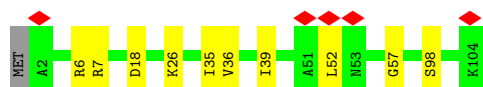
- Molecule 22: 50S ribosomal protein L23

Chain T:  92% 6%



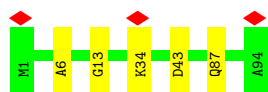
- Molecule 23: 50S ribosomal protein L24

Chain U:  5% 89% 10%



- Molecule 24: 50S ribosomal protein L25

Chain V:  95% 5%



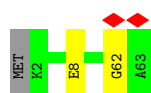
- Molecule 25: 50S ribosomal protein L28

Chain X: 90% 9%



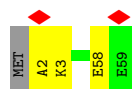
- Molecule 26: 50S ribosomal protein L29

Chain Y: 95%



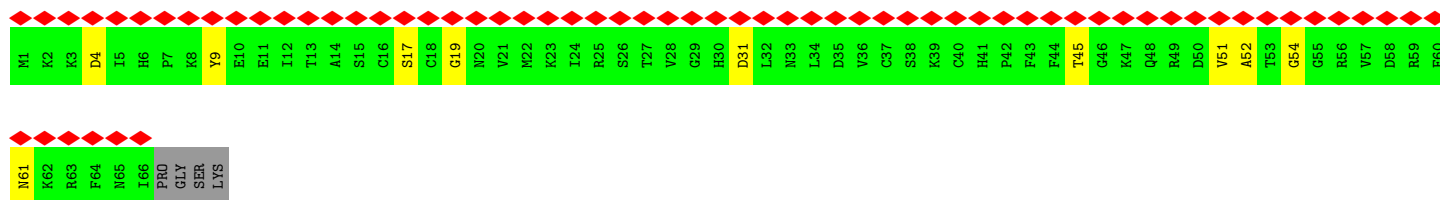
- Molecule 27: 50S ribosomal protein L30

Chain Z: 93% 5%



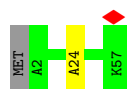
- Molecule 28: 50S ribosomal protein L31

Chain a: 80% 94% 14% 6%



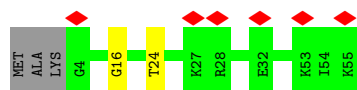
- Molecule 29: 50S ribosomal protein L32

Chain b: 96%



- Molecule 30: 50S ribosomal protein L33

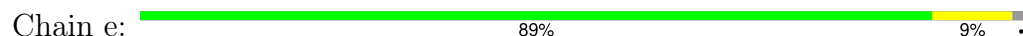
Chain c: 11% 91% 5%



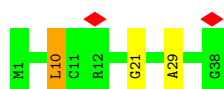
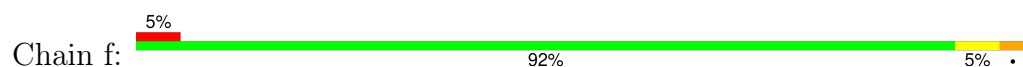
- Molecule 31: 50S ribosomal protein L34



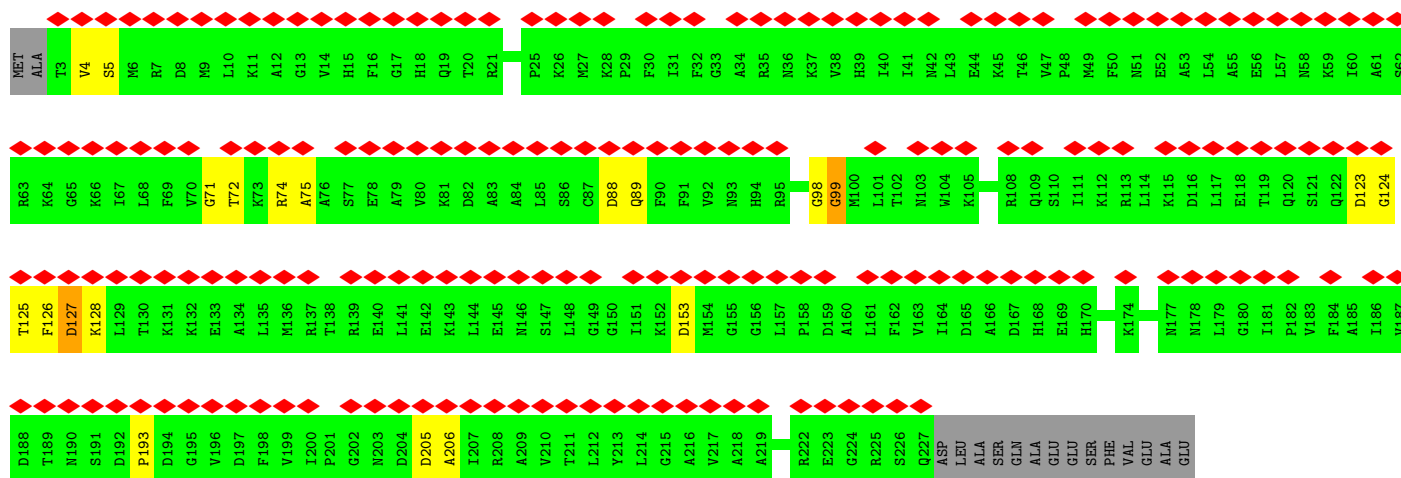
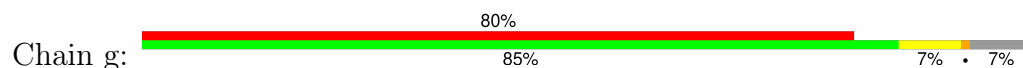
- Molecule 32: 50S ribosomal protein L35



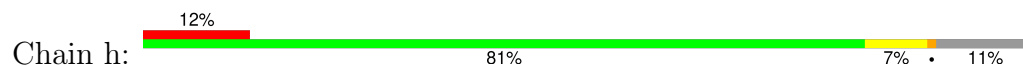
- Molecule 33: 50S ribosomal protein L36

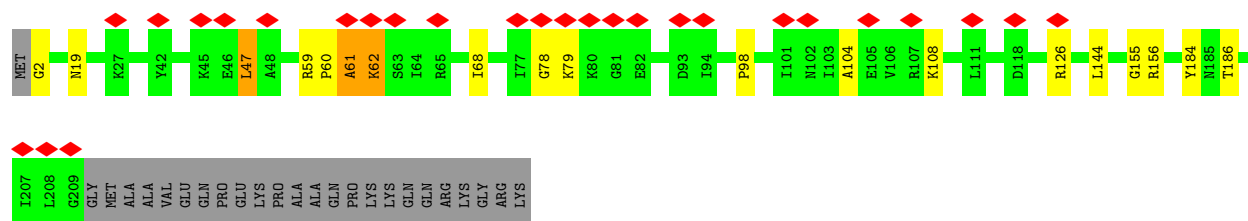


- Molecule 34: 30S ribosomal protein S2

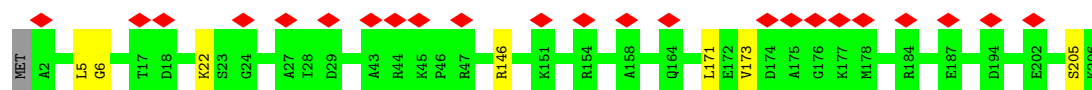


- Molecule 35: 30S ribosomal protein S3

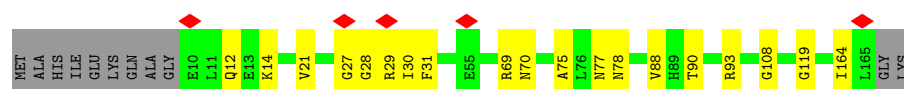
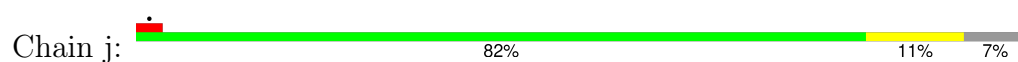




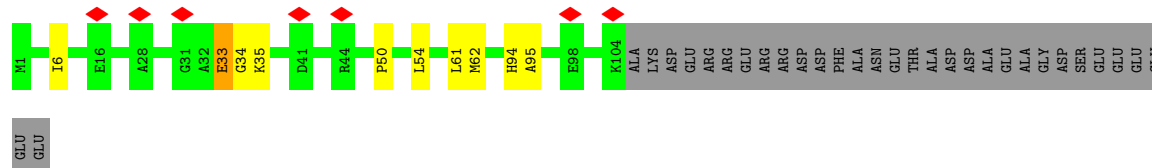
- Molecule 36: 30S ribosomal protein S4



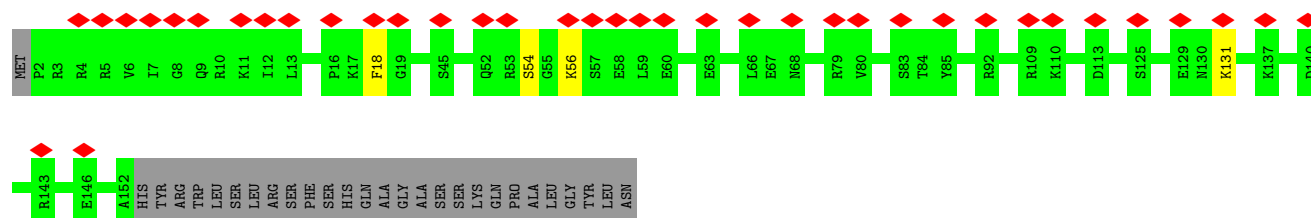
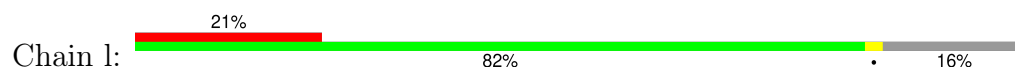
- Molecule 37: 30S ribosomal protein S5



- Molecule 38: 30S ribosomal protein S6

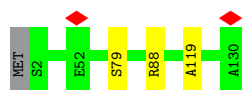


- Molecule 39: 30S ribosomal protein S7

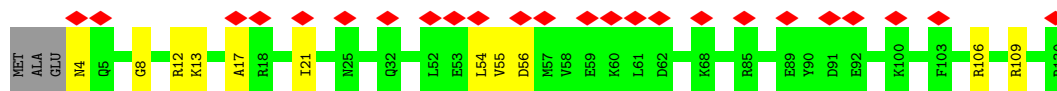
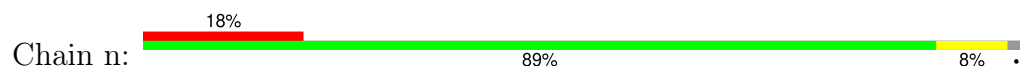


- Molecule 40: 30S ribosomal protein S8

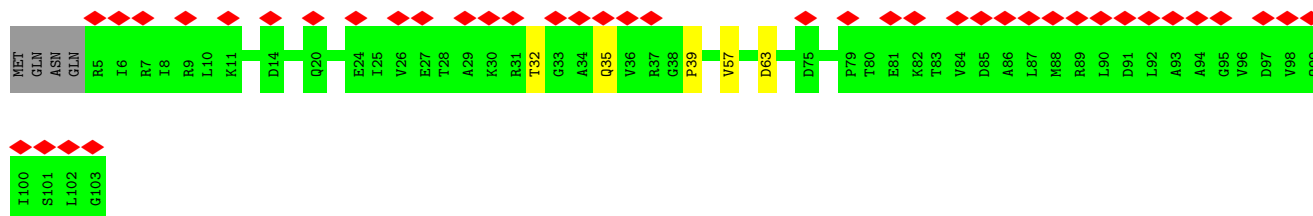




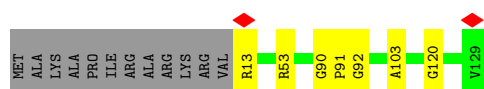
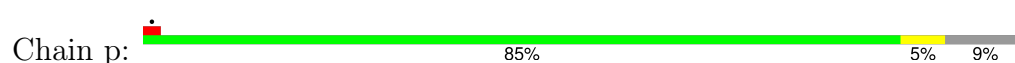
- Molecule 41: 30S ribosomal protein S9



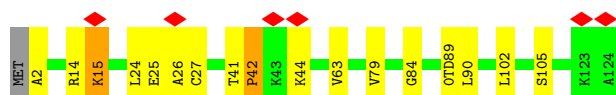
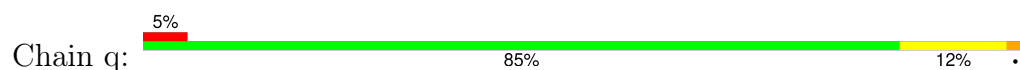
- Molecule 42: 30S ribosomal protein S10



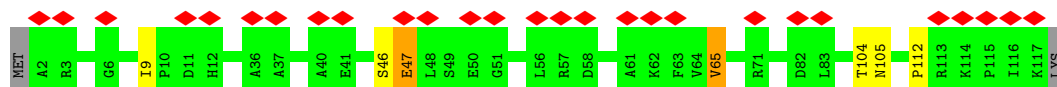
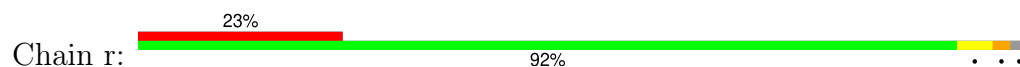
- Molecule 43: 30S ribosomal protein S11



- Molecule 44: 30S ribosomal protein S12

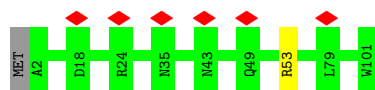


- Molecule 45: 30S ribosomal protein S13



- Molecule 46: 30S ribosomal protein S14

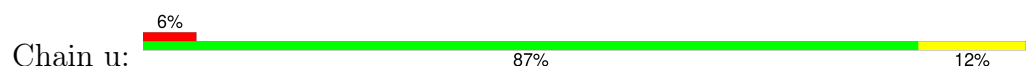




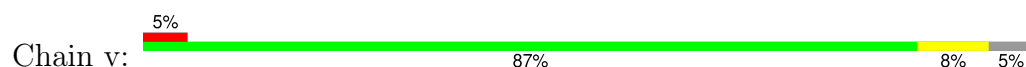
- Molecule 47: 30S ribosomal protein S15



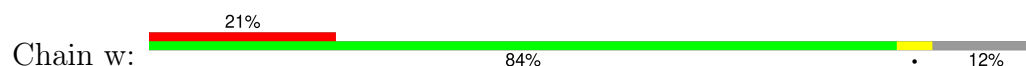
- Molecule 48: 30S ribosomal protein S16



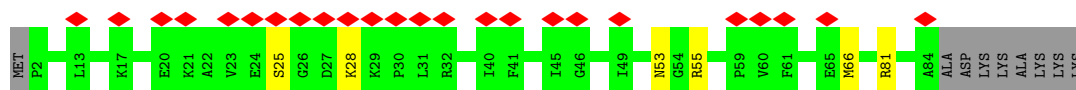
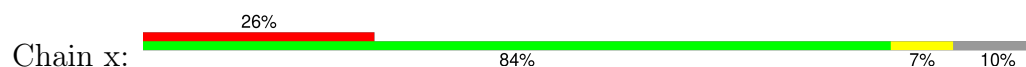
- Molecule 49: 30S ribosomal protein S17



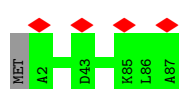
- Molecule 50: 30S ribosomal protein S18



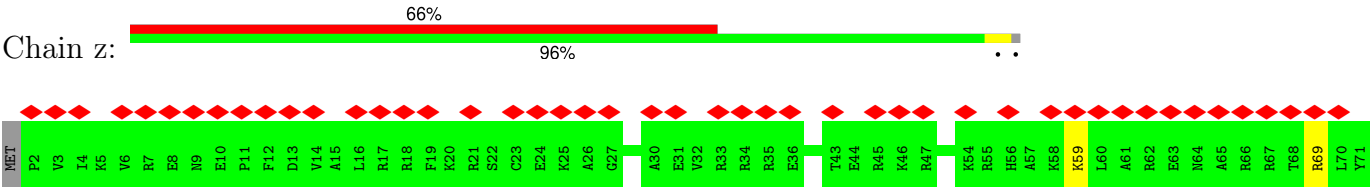
- Molecule 51: 30S ribosomal protein S19



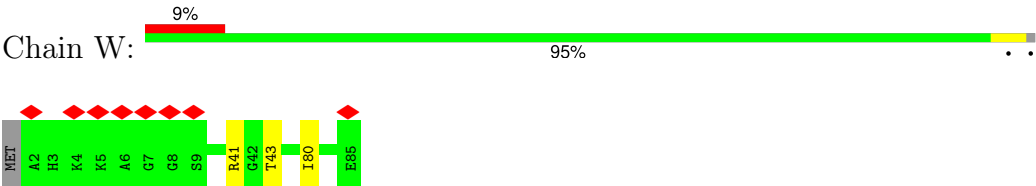
- Molecule 52: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S21



• Molecule 54: 50S ribosomal protein L27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	28121	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.00	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	DIRECT ELECTRON DE-64 (8k x 8k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	457.344, 457.344, 457.344	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.191, 1.191, 1.191	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: KKL, 2MA, 0TD, OMG, 4OC, G7M, 5MC, MA6, 5MU, 2MG, OMC, PSU, OMU, 7MG, 6MZ, UR3, 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	1	0.84	2/69335 (0.0%)	1.06	246/108168 (0.2%)
2	2	0.69	2/36590 (0.0%)	1.04	104/57074 (0.2%)
3	3	0.74	0/2872	1.35	46/4478 (1.0%)
4	4	0.38	0/123	0.82	0/190
5	5	0.38	0/1762	1.10	10/2745 (0.4%)
6	B	0.44	0/2121	0.51	0/2852
7	C	0.43	0/1586	0.48	0/2134
8	D	0.40	0/1571	0.51	0/2113
9	E	0.32	0/1434	0.53	1/1926 (0.1%)
10	F	0.33	0/1333	0.47	0/1805
11	G	0.32	0/1122	0.53	0/1515
12	J	0.40	0/1152	0.46	0/1551
13	K	0.40	0/955	0.51	0/1279
14	L	0.38	0/1062	0.49	0/1413
15	M	0.40	0/1093	0.48	0/1460
16	N	0.41	0/964	0.52	0/1289
17	O	0.34	0/902	0.52	0/1209
18	P	0.40	0/929	0.47	0/1242
19	Q	0.43	0/960	0.46	0/1278
20	R	0.41	0/829	0.48	0/1107
21	S	0.38	0/864	0.47	0/1156
22	T	0.39	0/752	0.45	0/1005
23	U	0.39	0/796	0.48	1/1062 (0.1%)
24	V	0.37	0/766	0.46	0/1025
25	X	0.39	0/635	0.44	0/848
26	Y	0.30	0/502	0.42	0/667
27	Z	0.36	0/452	0.46	0/605
28	a	0.30	0/531	0.45	0/709
29	b	0.38	0/450	0.45	0/599
30	c	0.33	0/433	0.45	0/576
31	d	0.38	0/380	0.47	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.42	0/513	0.51	0/676
33	f	0.38	0/303	0.47	0/397
34	g	0.36	0/1791	0.60	0/2413
35	h	0.35	0/1663	0.51	0/2241
36	i	0.33	0/1665	0.46	0/2227
37	j	0.39	0/1165	0.51	0/1568
38	k	0.37	0/867	0.55	0/1171
39	l	0.30	0/1195	0.50	0/1602
40	m	0.37	0/989	0.49	0/1326
41	n	0.32	0/1034	0.54	0/1375
42	o	0.34	0/800	0.54	0/1082
43	p	0.35	0/893	0.48	0/1205
44	q	0.61	2/960 (0.2%)	0.57	1/1286 (0.1%)
45	r	0.28	0/909	0.47	0/1215
46	s	0.32	0/817	0.47	0/1088
47	t	0.36	0/722	0.48	0/964
48	u	0.33	0/659	0.50	0/884
49	v	0.34	0/657	0.48	0/881
50	w	0.35	0/553	0.50	0/743
51	x	0.30	0/680	0.48	0/915
52	y	0.32	0/675	0.46	0/895
53	z	0.32	0/597	0.53	0/792
54	W	0.41	0/642	0.45	0/848
All	All	0.69	6/156005 (0.0%)	0.95	409/233372 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	B	0	17
7	C	0	9
8	D	0	11
9	E	0	11
10	F	0	10
11	G	0	18
12	J	0	4
13	K	0	3
14	L	0	11
15	M	0	2
16	N	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
17	O	0	8
18	P	0	6
19	Q	0	5
20	R	0	6
21	S	0	2
22	T	0	2
23	U	0	8
24	V	0	5
25	X	0	6
26	Y	0	2
27	Z	0	2
28	a	0	10
29	b	0	1
30	c	0	2
32	e	0	5
33	f	0	3
34	g	0	17
35	h	0	18
36	i	0	7
37	j	0	15
38	k	0	9
39	l	0	3
40	m	0	3
41	n	0	7
42	o	0	3
43	p	0	6
44	q	0	9
45	r	0	5
46	s	0	1
47	t	0	2
48	u	0	10
49	v	0	5
50	w	0	3
51	x	0	6
53	z	0	2
54	W	0	2
All	All	0	306

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2030	A	O3'-P	-16.79	1.41	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	q	42	PRO	N-CA	13.41	1.70	1.47
2	2	1383	C	O3'-P	-11.46	1.47	1.61
2	2	1276	G	O3'-P	-8.09	1.51	1.61
44	q	41	THR	C-N	5.85	1.45	1.34
1	1	1244	A	N7-C5	-5.40	1.36	1.39

All (409) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1383	C	C2'-C3'-O3'	14.67	141.78	109.50
2	2	1383	C	P-O3'-C3'	12.38	134.55	119.70
5	5	13	C	N1-C2-O2	10.78	125.37	118.90
3	3	91	C	C6-N1-C2	-10.35	116.16	120.30
2	2	979	C	N3-C2-O2	-10.32	114.68	121.90
1	1	1313	U	N1-C2-O2	9.94	129.75	122.80
2	2	979	C	N1-C2-O2	9.65	124.69	118.90
3	3	91	C	C5-C6-N1	9.61	125.81	121.00
1	1	61	C	N1-C2-O2	9.56	124.64	118.90
1	1	1313	U	C2-N1-C1'	9.51	129.11	117.70
5	5	13	C	N3-C2-O2	-9.49	115.25	121.90
3	3	89	U	N1-C2-O2	9.46	129.43	122.80
1	1	1199	U	N1-C2-O2	9.39	129.37	122.80
3	3	93	C	C6-N1-C2	-9.28	116.59	120.30
1	1	61	C	N3-C2-O2	-9.19	115.47	121.90
1	1	1313	U	N3-C2-O2	-9.12	115.81	122.20
3	3	89	U	N3-C2-O2	-8.94	115.94	122.20
3	3	37	C	N1-C2-O2	8.69	124.11	118.90
1	1	2473	U	N1-C2-O2	8.64	128.85	122.80
1	1	2226	C	N1-C2-O2	8.61	124.07	118.90
3	3	68	C	N1-C2-O2	8.34	123.90	118.90
1	1	2161	C	N3-C2-O2	-8.27	116.11	121.90
5	5	13	C	C6-N1-C2	-8.27	116.99	120.30
3	3	71	C	N3-C2-O2	-8.10	116.23	121.90
1	1	2188	U	N3-C2-O2	-8.04	116.57	122.20
2	2	979	C	C6-N1-C2	-8.04	117.08	120.30
5	5	13	C	C2-N1-C1'	8.04	127.64	118.80
3	3	89	U	C2-N1-C1'	8.04	127.34	117.70
1	1	2161	C	N1-C2-O2	8.03	123.72	118.90
3	3	71	C	N1-C2-O2	8.02	123.71	118.90
3	3	92	C	C6-N1-C2	-8.00	117.10	120.30
1	1	1172	C	N1-C2-O2	7.96	123.68	118.90
1	1	1174	U	C2-N1-C1'	7.88	127.16	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	207	C	C2-N1-C1'	7.86	127.45	118.80
3	3	92	C	C5-C6-N1	7.86	124.93	121.00
1	1	2473	U	N3-C2-O2	-7.83	116.72	122.20
1	1	867	C	N1-C2-O2	7.81	123.59	118.90
3	3	37	C	N3-C2-O2	-7.77	116.46	121.90
2	2	58	C	C6-N1-C2	-7.74	117.20	120.30
1	1	1348	C	N1-C2-O2	7.72	123.53	118.90
2	2	618	C	N1-C2-O2	7.72	123.53	118.90
1	1	1174	U	N1-C2-O2	7.71	128.20	122.80
1	1	496	G	N3-C2-N2	-7.71	114.50	119.90
1	1	1172	C	N3-C2-O2	-7.59	116.59	121.90
2	2	1276	G	C4'-C3'-O3'	-7.55	93.55	109.40
1	1	1774	C	N3-C2-O2	-7.54	116.62	121.90
44	q	42	PRO	CA-N-CD	-7.50	101.00	111.50
2	2	979	C	C2-N1-C1'	7.46	127.01	118.80
1	1	1874	C	N1-C2-O2	7.45	123.37	118.90
1	1	2617	U	N3-C2-O2	-7.45	116.99	122.20
1	1	1774	C	C6-N1-C2	-7.42	117.33	120.30
2	2	1322	C	N1-C2-O2	7.38	123.33	118.90
1	1	1172	C	C2-N1-C1'	7.37	126.91	118.80
2	2	1158	C	C2-N1-C1'	7.35	126.89	118.80
1	1	1774	C	N1-C2-O2	7.34	123.31	118.90
1	1	1314	C	C2-N1-C1'	7.33	126.86	118.80
1	1	1172	C	C6-N1-C2	-7.32	117.37	120.30
2	2	207	C	C6-N1-C2	-7.24	117.41	120.30
3	3	68	C	N3-C2-O2	-7.22	116.84	121.90
1	1	2226	C	N3-C2-O2	-7.21	116.85	121.90
1	1	1411	U	C2-N1-C1'	7.21	126.35	117.70
3	3	8	C	N3-C2-O2	-7.18	116.87	121.90
1	1	485	C	N3-C2-O2	-7.09	116.93	121.90
1	1	2072	C	C2-N1-C1'	7.08	126.59	118.80
3	3	26	C	N1-C2-O2	7.04	123.12	118.90
1	1	1174	U	N3-C2-O2	-7.03	117.28	122.20
1	1	1159	U	N3-C2-O2	-7.03	117.28	122.20
1	1	847	U	N3-C2-O2	-7.02	117.29	122.20
2	2	1149	C	C5-C6-N1	6.97	124.49	121.00
2	2	496	A	C2-N3-C4	6.94	114.07	110.60
2	2	1395	C	C2-N1-C1'	6.94	126.43	118.80
1	1	234	U	N3-C2-O2	-6.93	117.35	122.20
1	1	1065	U	O4'-C1'-N1	6.92	113.74	108.20
1	1	847	U	N1-C2-O2	6.91	127.64	122.80
1	1	1313	U	C6-N1-C1'	-6.88	111.57	121.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	607	U	N3-C2-O2	-6.87	117.39	122.20
1	1	552	U	N3-C2-O2	-6.85	117.40	122.20
1	1	2063	C	C6-N1-C2	-6.82	117.57	120.30
2	2	58	C	C5-C6-N1	6.81	124.40	121.00
1	1	404	A	P-O3'-C3'	6.78	127.83	119.70
1	1	1101	U	N1-C2-O2	6.77	127.54	122.80
5	5	17	U	P-O3'-C3'	6.75	127.80	119.70
1	1	2473	U	C2-N1-C1'	6.75	125.80	117.70
2	2	1322	C	C2-N1-C1'	6.74	126.21	118.80
3	3	8	C	N1-C2-O2	6.74	122.94	118.90
1	1	1774	C	C2-N1-C1'	6.74	126.21	118.80
1	1	1199	U	N3-C2-O2	-6.73	117.49	122.20
2	2	1276	G	P-O3'-C3'	6.72	127.77	119.70
2	2	431	A	N1-C6-N6	-6.71	114.58	118.60
2	2	103	U	N3-C2-O2	-6.70	117.51	122.20
3	3	3	C	C5-C6-N1	6.69	124.34	121.00
1	1	1323	C	N1-C2-O2	6.68	122.91	118.90
2	2	618	C	N3-C2-O2	-6.66	117.24	121.90
1	1	12	U	N3-C2-O2	-6.66	117.54	122.20
3	3	103	U	C5-C6-N1	6.64	126.02	122.70
2	2	1132	C	C2-N1-C1'	6.63	126.10	118.80
1	1	1509	A	O4'-C1'-N9	6.61	113.49	108.20
1	1	867	C	N3-C2-O2	-6.60	117.28	121.90
1	1	1101	U	N3-C2-O2	-6.60	117.58	122.20
1	1	1199	U	C2-N1-C1'	6.59	125.61	117.70
1	1	1180	U	N1-C2-O2	6.58	127.41	122.80
5	5	30	C	C2-N1-C1'	6.58	126.04	118.80
1	1	487	C	N3-C2-O2	-6.58	117.30	121.90
1	1	2794	C	C2-N1-C1'	6.58	126.03	118.80
1	1	2188	U	N1-C2-O2	6.57	127.40	122.80
1	1	1267	U	N1-C2-O2	6.53	127.37	122.80
1	1	1267	U	N3-C2-O2	-6.51	117.64	122.20
1	1	495	G	C5-C6-O6	6.51	132.50	128.60
1	1	1656	C	C5-C6-N1	6.50	124.25	121.00
3	3	19	C	C5-C6-N1	6.47	124.23	121.00
1	1	1348	C	N3-C2-O2	-6.47	117.37	121.90
2	2	1071	C	C5-C6-N1	6.47	124.23	121.00
2	2	73	C	N1-C2-O2	6.46	122.78	118.90
1	1	2072	C	C5-C6-N1	6.46	124.23	121.00
2	2	110	C	N1-C2-O2	6.41	122.75	118.90
3	3	49	C	C6-N1-C2	-6.39	117.74	120.30
3	3	93	C	C5-C6-N1	6.39	124.19	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1294	U	N3-C2-O2	-6.38	117.74	122.20
2	2	1070	U	N3-C2-O2	-6.38	117.74	122.20
1	1	894	U	P-O3'-C3'	6.37	127.34	119.70
2	2	307	C	N1-C2-O2	6.36	122.72	118.90
2	2	29	U	N3-C2-O2	-6.33	117.77	122.20
1	1	500	G	C8-N9-C4	-6.32	103.87	106.40
1	1	1314	C	C6-N1-C2	-6.32	117.77	120.30
1	1	1920	C	C5-C6-N1	6.32	124.16	121.00
2	2	221	C	N1-C2-O2	6.32	122.69	118.90
2	2	221	C	N3-C2-O2	-6.31	117.48	121.90
2	2	1158	C	N1-C2-O2	6.30	122.68	118.90
1	1	2226	C	C2-N1-C1'	6.29	125.72	118.80
2	2	1149	C	N1-C2-O2	6.29	122.67	118.90
1	1	499	U	C5-C6-N1	6.29	125.84	122.70
1	1	2072	C	C6-N1-C2	-6.28	117.79	120.30
1	1	183	C	N3-C2-O2	-6.28	117.50	121.90
1	1	1931	U	N1-C2-O2	6.28	127.19	122.80
3	3	56	G	N3-C4-N9	6.27	129.76	126.00
3	3	71	C	C6-N1-C2	-6.27	117.79	120.30
2	2	582	C	N1-C2-O2	6.26	122.66	118.90
1	1	183	C	N1-C2-O2	6.25	122.65	118.90
1	1	2884	U	N3-C2-O2	-6.24	117.83	122.20
1	1	2666	C	N1-C2-O2	6.24	122.64	118.90
1	1	436	C	N3-C2-O2	-6.23	117.54	121.90
1	1	495	G	N3-C4-N9	-6.23	122.26	126.00
3	3	74	U	C5-C6-N1	6.21	125.81	122.70
1	1	500	G	C8-N9-C1'	6.21	135.07	127.00
2	2	610	U	N1-C2-O2	6.19	127.14	122.80
1	1	323	C	C2-N1-C1'	6.16	125.58	118.80
1	1	500	G	N9-C4-C5	6.14	107.86	105.40
1	1	243	U	N1-C2-O2	6.13	127.09	122.80
1	1	353	C	N1-C2-O2	6.13	122.58	118.90
2	2	610	U	N3-C2-O2	-6.13	117.91	122.20
1	1	417	C	C5-C6-N1	6.13	124.06	121.00
1	1	499	U	C6-N1-C2	-6.13	117.33	121.00
2	2	58	C	C2-N1-C1'	6.11	125.52	118.80
1	1	710	U	N1-C2-O2	6.10	127.07	122.80
2	2	110	C	N3-C2-O2	-6.09	117.63	121.90
2	2	210	C	N1-C2-O2	6.09	122.56	118.90
1	1	1584	U	C2-N1-C1'	6.09	125.01	117.70
3	3	70	C	N1-C2-O2	6.08	122.55	118.90
1	1	710	U	N3-C2-O2	-6.08	117.94	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2226	C	C6-N1-C2	-6.07	117.87	120.30
5	5	13	C	C5-C6-N1	6.06	124.03	121.00
1	1	1408	G	C4-N9-C1'	6.05	134.37	126.50
1	1	1159	U	N1-C2-O2	6.05	127.04	122.80
1	1	1294	U	N1-C2-O2	6.05	127.03	122.80
1	1	500	G	O4'-C1'-N9	6.05	113.04	108.20
1	1	1776	G	C4-N9-C1'	6.05	134.36	126.50
2	2	183	C	N1-C2-O2	6.05	122.53	118.90
2	2	1279	G	C4-N9-C1'	6.03	134.34	126.50
1	1	1931	U	C2-N1-C1'	6.02	124.92	117.70
3	3	3	C	C6-N1-C2	-6.02	117.89	120.30
1	1	496	G	N1-C2-N2	6.01	121.61	116.20
1	1	1874	C	N3-C2-O2	-6.01	117.69	121.90
2	2	1128	C	N1-C2-O2	6.00	122.50	118.90
1	1	702	U	N3-C2-O2	-6.00	118.00	122.20
1	1	1314	C	C5-C6-N1	5.99	124.00	121.00
2	2	960	U	N1-C2-O2	5.98	126.98	122.80
1	1	138	U	C2-N1-C1'	5.96	124.85	117.70
1	1	2063	C	C2-N1-C1'	5.94	125.34	118.80
2	2	458	U	N3-C2-O2	-5.91	118.06	122.20
1	1	1188	U	N1-C2-O2	5.91	126.94	122.80
2	2	458	U	N1-C2-O2	5.91	126.93	122.80
1	1	1956	U	N3-C2-O2	-5.90	118.07	122.20
1	1	1245	G	N3-C2-N2	-5.90	115.77	119.90
1	1	2425	A	P-O3'-C3'	5.90	126.78	119.70
2	2	1262	C	N1-C2-O2	5.90	122.44	118.90
2	2	328	C	N1-C2-O2	5.89	122.44	118.90
1	1	669	G	N3-C4-N9	5.88	129.53	126.00
1	1	2354	C	C6-N1-C2	-5.88	117.95	120.30
1	1	2617	U	N1-C2-O2	5.88	126.91	122.80
1	1	640	C	C5-C6-N1	5.87	123.94	121.00
2	2	479	U	N1-C2-O2	5.87	126.91	122.80
1	1	1956	U	N1-C2-O2	5.87	126.91	122.80
1	1	1043	C	N1-C2-O2	5.85	122.41	118.90
2	2	1149	C	C6-N1-C2	-5.85	117.96	120.30
1	1	2554	U	N3-C2-O2	-5.85	118.10	122.20
1	1	1920	C	C6-N1-C2	-5.85	117.96	120.30
1	1	1180	U	N3-C2-O2	-5.84	118.11	122.20
2	2	368	U	C2-N1-C1'	5.84	124.70	117.70
2	2	754	C	C2-N1-C1'	5.83	125.22	118.80
1	1	552	U	N1-C2-O2	5.83	126.88	122.80
2	2	618	C	C6-N1-C2	-5.82	117.97	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	60	C	N1-C2-O2	5.81	122.39	118.90
1	1	702	U	N1-C2-O2	5.81	126.86	122.80
1	1	2716	C	C2-N1-C1'	5.80	125.18	118.80
1	1	1243	C	C6-N1-C2	-5.80	117.98	120.30
2	2	1158	C	N3-C2-O2	-5.78	117.85	121.90
1	1	1644	C	N3-C2-O2	-5.76	117.86	121.90
1	1	2793	C	C2-N1-C1'	5.76	125.14	118.80
1	1	1584	U	N1-C2-O2	5.76	126.83	122.80
2	2	207	C	C5-C6-N1	5.75	123.87	121.00
1	1	542	C	N3-C2-O2	-5.73	117.89	121.90
1	1	275	C	N3-C2-O2	-5.73	117.89	121.90
1	1	1776	G	N3-C4-N9	5.73	129.44	126.00
1	1	1584	U	N3-C2-O2	-5.72	118.19	122.20
5	5	47	U	P-O3'-C3'	5.72	126.57	119.70
1	1	275	C	N1-C2-O2	5.71	122.33	118.90
1	1	495	G	N1-C6-O6	-5.71	116.47	119.90
3	3	26	C	N3-C2-O2	-5.71	117.91	121.90
1	1	545	U	C2-N1-C1'	5.70	124.54	117.70
2	2	1070	U	N1-C2-O2	5.70	126.79	122.80
2	2	1395	C	C6-N1-C2	-5.70	118.02	120.30
1	1	1590	A	C6-N1-C2	-5.69	115.19	118.60
1	1	243	U	N3-C2-O2	-5.69	118.22	122.20
1	1	1855	U	N3-C2-O2	-5.69	118.22	122.20
1	1	1047	G	O4'-C1'-N9	5.68	112.74	108.20
1	1	2179	C	C6-N1-C2	-5.68	118.03	120.30
1	1	885	C	C6-N1-C2	-5.67	118.03	120.30
1	1	1412	U	C5-C6-N1	5.66	125.53	122.70
1	1	1993	U	N3-C2-O2	-5.65	118.24	122.20
1	1	847	U	C2-N1-C1'	5.65	124.48	117.70
1	1	2656	U	N1-C2-O2	5.65	126.75	122.80
3	3	70	C	C2-N1-C1'	5.65	125.01	118.80
1	1	2334	U	C2-N1-C1'	5.64	124.47	117.70
2	2	1317	C	N1-C2-O2	5.62	122.27	118.90
1	1	495	G	N9-C4-C5	5.62	107.65	105.40
1	1	2556	C	N1-C2-O2	5.61	122.27	118.90
2	2	582	C	N3-C2-O2	-5.60	117.98	121.90
2	2	1146	A	C5-C6-N6	-5.60	119.22	123.70
1	1	1962	5MC	OP1-P-O3'	5.60	117.51	105.20
2	2	1406	U	N3-C2-O2	-5.60	118.28	122.20
3	3	19	C	C6-N1-C2	-5.60	118.06	120.30
1	1	2394	C	N1-C2-O2	5.60	122.26	118.90
1	1	2286	G	P-O3'-C3'	5.59	126.41	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1408	G	C8-N9-C1'	-5.59	119.74	127.00
3	3	55	U	N3-C2-O2	-5.58	118.29	122.20
1	1	2554	U	N1-C2-O2	5.58	126.71	122.80
2	2	611	C	N1-C2-O2	5.57	122.25	118.90
2	2	1322	C	C6-N1-C1'	-5.57	114.12	120.80
1	1	1776	G	C8-N9-C1'	-5.55	119.79	127.00
1	1	1507	C	C5-C6-N1	5.54	123.77	121.00
2	2	1109	C	C3'-C2'-C1'	5.54	105.93	101.50
1	1	2794	C	C6-N1-C2	-5.53	118.09	120.30
5	5	30	C	C6-N1-C2	-5.53	118.09	120.30
1	1	999	U	N3-C2-O2	-5.52	118.33	122.20
1	1	2063	C	N3-C2-O2	-5.52	118.03	121.90
2	2	998	C	N3-C2-O2	-5.52	118.04	121.90
1	1	1585	C	N1-C2-O2	5.49	122.20	118.90
1	1	1931	U	N3-C2-O2	-5.49	118.36	122.20
1	1	1114	C	C6-N1-C2	-5.49	118.11	120.30
2	2	1038	C	C2-N1-C1'	5.48	124.83	118.80
23	U	52	LEU	CA-CB-CG	5.47	127.89	115.30
2	2	368	U	N1-C2-O2	5.47	126.63	122.80
1	1	1171	G	N3-C4-N9	5.46	129.28	126.00
1	1	2562	U	N1-C2-O2	5.46	126.62	122.80
2	2	618	C	C2-N1-C1'	5.46	124.80	118.80
3	3	26	C	C6-N1-C2	-5.46	118.12	120.30
2	2	1520	C	C2-N1-C1'	5.45	124.80	118.80
1	1	2043	C	C2-N1-C1'	5.44	124.79	118.80
2	2	1406	U	N1-C2-O2	5.44	126.61	122.80
2	2	1322	C	N3-C2-O2	-5.44	118.09	121.90
2	2	439	U	N3-C2-O2	-5.44	118.39	122.20
3	3	71	C	C2-N1-C1'	5.43	124.78	118.80
1	1	114	U	C2-N1-C1'	5.43	124.22	117.70
1	1	1114	C	C6-N1-C1'	5.43	127.31	120.80
1	1	1862	G	C4-N9-C1'	5.43	133.55	126.50
1	1	2122	U	N3-C2-O2	-5.43	118.40	122.20
1	1	717	C	N1-C2-O2	5.42	122.15	118.90
3	3	74	U	C6-N1-C2	-5.42	117.75	121.00
2	2	421	U	C2-N1-C1'	5.41	124.20	117.70
3	3	79	G	C6-C5-N7	-5.41	127.15	130.40
1	1	1395	A	O4'-C1'-N9	5.41	112.53	108.20
1	1	2248	C	N1-C2-O2	5.41	122.14	118.90
1	1	1323	C	N3-C2-O2	-5.41	118.12	121.90
2	2	1262	C	N3-C2-O2	-5.40	118.12	121.90
1	1	2820	A	OP1-P-O3'	5.40	117.08	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1038	C	C6-N1-C2	-5.39	118.14	120.30
1	1	257	C	N1-C2-O2	5.39	122.13	118.90
1	1	1875	G	N3-C4-N9	5.39	129.23	126.00
1	1	353	C	N3-C2-O2	-5.38	118.14	121.90
3	3	48	U	N3-C2-O2	-5.37	118.44	122.20
1	1	784	G	P-O3'-C3'	5.37	126.14	119.70
1	1	1348	C	C2-N1-C1'	5.37	124.70	118.80
1	1	2161	C	C6-N1-C2	-5.36	118.15	120.30
1	1	485	C	C6-N1-C2	-5.36	118.16	120.30
1	1	2188	U	C6-N1-C2	-5.36	117.79	121.00
1	1	1605	C	N3-C2-O2	-5.34	118.16	121.90
2	2	960	U	N3-C2-O2	-5.34	118.46	122.20
1	1	729	G	N3-C2-N2	-5.34	116.16	119.90
1	1	500	G	N9-C1'-C2'	-5.34	106.13	112.00
1	1	1379	U	C5-C6-N1	5.34	125.37	122.70
1	1	475	C	C5-C6-N1	5.33	123.67	121.00
1	1	2248	C	C2-N1-C1'	5.33	124.66	118.80
1	1	1605	C	N1-C2-O2	5.33	122.10	118.90
1	1	2334	U	N3-C2-O2	-5.32	118.47	122.20
3	3	25	U	N1-C2-O2	5.32	126.52	122.80
1	1	2354	C	C5-C6-N1	5.31	123.66	121.00
2	2	1132	C	N1-C2-O2	5.31	122.09	118.90
1	1	12	U	N1-C2-O2	5.31	126.52	122.80
1	1	2586	U	N3-C2-O2	-5.31	118.48	122.20
1	1	140	C	N1-C2-O2	5.31	122.08	118.90
1	1	2901	C	N1-C2-O2	5.31	122.08	118.90
1	1	1656	C	C6-N1-C2	-5.30	118.18	120.30
1	1	709	U	N1-C2-O2	5.30	126.51	122.80
1	1	2329	U	C5-C6-N1	5.29	125.35	122.70
2	2	103	U	N1-C2-O2	5.29	126.50	122.80
1	1	2656	U	N3-C2-O2	-5.29	118.50	122.20
1	1	1174	U	C6-N1-C1'	-5.29	113.80	121.20
1	1	2636	C	N1-C2-O2	5.29	122.07	118.90
2	2	439	U	C2-N1-C1'	5.29	124.04	117.70
1	1	487	C	C6-N1-C2	-5.28	118.19	120.30
1	1	234	U	N1-C2-O2	5.28	126.49	122.80
1	1	669	G	C4-N9-C1'	5.27	133.35	126.50
2	2	5	U	N1-C2-O2	5.27	126.49	122.80
2	2	1298	U	N3-C2-O2	-5.27	118.51	122.20
1	1	323	C	C5-C6-N1	5.26	123.63	121.00
1	1	2393	U	N3-C2-O2	-5.26	118.52	122.20
1	1	2179	C	N1-C2-O2	5.26	122.06	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	143	C	C2-N1-C1'	5.26	124.58	118.80
1	1	2562	U	N3-C2-O2	-5.25	118.52	122.20
1	1	1760	C	N1-C2-O2	5.25	122.05	118.90
2	2	214	C	N1-C2-O2	5.25	122.05	118.90
2	2	1135	U	N1-C2-O2	5.25	126.48	122.80
1	1	1043	C	N3-C2-O2	-5.25	118.23	121.90
3	3	55	U	C6-N1-C2	-5.25	117.85	121.00
1	1	912	C	C2-N1-C1'	5.25	124.57	118.80
1	1	1398	C	N1-C2-O2	5.25	122.05	118.90
1	1	475	C	C6-N1-C2	-5.24	118.20	120.30
1	1	974	G	O4'-C1'-N9	5.24	112.39	108.20
1	1	436	C	N1-C2-O2	5.24	122.04	118.90
1	1	2666	C	N3-C2-O2	-5.23	118.24	121.90
1	1	370	G	O4'-C1'-N9	-5.23	104.02	108.20
3	3	60	C	N3-C2-O2	-5.23	118.24	121.90
1	1	1669	A	C4-N9-C1'	5.22	135.70	126.30
1	1	2043	C	C6-N1-C2	-5.22	118.21	120.30
2	2	1136	C	N1-C2-O2	5.22	122.03	118.90
1	1	1042	G	O4'-C1'-N9	5.22	112.37	108.20
2	2	1471	U	N3-C2-O2	-5.22	118.55	122.20
1	1	66	C	C6-N1-C2	-5.21	118.22	120.30
1	1	1962	5MC	P-O3'-C3'	5.21	125.95	119.70
2	2	1128	C	N3-C2-O2	-5.20	118.26	121.90
1	1	860	U	N1-C2-O2	5.20	126.44	122.80
1	1	1409	U	N1-C2-O2	5.19	126.43	122.80
1	1	2656	U	C2-N1-C1'	5.19	123.92	117.70
2	2	54	C	N1-C2-O2	5.19	122.01	118.90
2	2	563	A	C4-N9-C1'	5.19	135.63	126.30
1	1	2586	U	N1-C2-O2	5.18	126.43	122.80
2	2	463	U	N1-C2-O2	5.18	126.43	122.80
1	1	2011	U	N3-C2-O2	-5.18	118.57	122.20
2	2	207	C	N1-C2-O2	5.18	122.01	118.90
2	2	1158	C	C6-N1-C1'	-5.18	114.59	120.80
1	1	1042	G	N3-C4-N9	-5.17	122.90	126.00
1	1	2556	C	N3-C2-O2	-5.16	118.29	121.90
2	2	183	C	C2-N1-C1'	5.15	124.47	118.80
1	1	1199	U	C6-N1-C1'	-5.15	113.99	121.20
1	1	2393	U	N1-C2-O2	5.14	126.40	122.80
1	1	1267	U	C2-N1-C1'	5.13	123.86	117.70
2	2	1148	U	N1-C2-O2	5.13	126.39	122.80
1	1	102	U	C2-N1-C1'	5.12	123.85	117.70
1	1	607	U	N1-C2-O2	5.12	126.39	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1737	G	C8-N9-C4	-5.12	104.35	106.40
2	2	1174	G	N3-C4-N9	5.12	129.07	126.00
1	1	2354	C	C2-N1-C1'	5.12	124.43	118.80
1	1	2782	G	C6-C5-N7	-5.12	127.33	130.40
3	3	26	C	C2-N1-C1'	5.12	124.43	118.80
2	2	74	A	O4'-C1'-N9	5.11	112.29	108.20
1	1	122	G	O5'-P-OP2	-5.11	101.10	105.70
2	2	610	U	C2-N1-C1'	5.11	123.83	117.70
2	2	1149	C	C2-N1-C1'	5.11	124.42	118.80
3	3	27	C	N1-C2-O2	5.10	121.96	118.90
2	2	993	G	N3-C4-N9	5.10	129.06	126.00
1	1	2793	C	N1-C2-O2	5.10	121.96	118.90
5	5	31	C	C6-N1-C2	-5.10	118.26	120.30
1	1	1379	U	P-O3'-C3'	5.09	125.81	119.70
1	1	1188	U	N3-C2-O2	-5.09	118.64	122.20
1	1	2342	C	N3-C2-O2	-5.09	118.33	121.90
1	1	2179	C	C5-C6-N1	5.08	123.54	121.00
1	1	1669	A	C8-N9-C4	-5.08	103.77	105.80
2	2	467	U	N1-C2-O2	5.07	126.35	122.80
3	3	55	U	C5-C6-N1	5.07	125.23	122.70
2	2	632	U	C2-N1-C1'	5.05	123.76	117.70
1	1	343	C	N3-C2-O2	-5.05	118.37	121.90
1	1	2334	U	N1-C2-O2	5.05	126.33	122.80
3	3	89	U	C6-N1-C1'	-5.05	114.13	121.20
2	2	368	U	N3-C2-O2	-5.05	118.67	122.20
1	1	783	A	C2-N3-C4	5.04	113.12	110.60
3	3	68	C	C2-N1-C1'	5.04	124.35	118.80
1	1	1172	C	C5-C6-N1	5.04	123.52	121.00
2	2	1038	C	C5-C6-N1	5.04	123.52	121.00
1	1	500	G	C4-N9-C1'	-5.04	119.95	126.50
1	1	139	U	C2-N1-C1'	5.04	123.74	117.70
9	E	103	LEU	CA-CB-CG	5.04	126.88	115.30
1	1	235	U	N3-C2-O2	-5.03	118.68	122.20
3	3	68	C	C6-N1-C2	-5.03	118.29	120.30
2	2	476	U	N1-C2-O2	5.02	126.32	122.80
1	1	1855	U	N1-C2-O2	5.02	126.31	122.80
2	2	684	U	N3-C2-O2	-5.01	118.69	122.20
1	1	373	U	N1-C2-O2	5.00	126.30	122.80
1	1	1202	G	N3-C4-N9	5.00	129.00	126.00
2	2	439	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (306) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	107	PRO	Peptide
6	B	109	GLY	Peptide
6	B	119	GLY	Peptide
6	B	121	ASP	Peptide
6	B	132	MET	Peptide
6	B	157	SER	Peptide
6	B	160	THR	Peptide
6	B	18	LYS	Peptide
6	B	195	VAL	Peptide
6	B	197	ASN	Peptide
6	B	203	ARG	Peptide
6	B	3	VAL	Peptide
6	B	31	ALA	Peptide
6	B	34	LEU	Peptide
6	B	4	VAL	Peptide
6	B	68	LYS	Peptide
6	B	69	ARG	Peptide
7	C	158	GLY	Peptide
7	C	18	ASP	Peptide
7	C	186	LEU	Peptide
7	C	19	GLY	Peptide
7	C	191	GLY	Peptide
7	C	208	LYS	Peptide
7	C	54	ALA	Peptide
7	C	76	GLY	Peptide
7	C	93	GLY	Peptide
8	D	11	ALA	Peptide
8	D	149	ILE	Peptide
8	D	17	THR	Peptide
8	D	18	THR	Peptide
8	D	41	GLN	Peptide
8	D	45	ALA	Peptide
8	D	50	ALA	Peptide
8	D	63	LYS	Peptide
8	D	64	GLY	Peptide
8	D	8	ALA	Peptide
8	D	82	GLY	Peptide
9	E	108	VAL	Peptide
9	E	11	GLU	Peptide
9	E	121	SER	Peptide
9	E	123	ASP	Peptide
9	E	126	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
9	E	150	ARG	Peptide
9	E	174	ASP	Peptide
9	E	177	PHE	Peptide
9	E	61	SER	Peptide
9	E	65	PRO	Peptide
9	E	72	LYS	Peptide
10	F	101	ASN	Peptide
10	F	106	SER	Peptide
10	F	118	PRO	Peptide
10	F	26	ILE	Peptide
10	F	28	GLY	Peptide
10	F	41	VAL	Peptide
10	F	45	HIS	Peptide
10	F	46	ALA	Peptide
10	F	54	PRO	Peptide
10	F	90	VAL	Peptide
11	G	106	ALA	Peptide
11	G	113	SER	Peptide
11	G	120	GLY	Peptide
11	G	135	HIS	Peptide
11	G	137	GLU	Peptide
11	G	26	ALA	Peptide
11	G	31	VAL	Peptide
11	G	32	PRO	Peptide
11	G	40	THR	Peptide
11	G	7	ASP	Peptide
11	G	72	ILE	Peptide
11	G	78	VAL	Peptide
11	G	85	GLY	Peptide
11	G	86	ASP	Peptide
11	G	88	GLY	Peptide
11	G	9	VAL	Peptide
11	G	90	LEU	Peptide
11	G	92	GLY	Peptide
12	J	24	THR	Peptide
12	J	57	LEU	Peptide
12	J	75	TYR	Peptide
12	J	82	GLY	Peptide
13	K	1	MET	Peptide
13	K	108	ARG	Peptide
13	K	68	GLY	Peptide
14	L	102	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
14	L	111	ILE	Peptide
14	L	138	ALA	Peptide
14	L	15	ALA	Peptide
14	L	28	GLY	Peptide
14	L	35	HIS	Peptide
14	L	37	GLY	Peptide
14	L	51	GLU	Peptide
14	L	53	GLY	Peptide
14	L	86	GLU	Peptide
14	L	88	GLY	Peptide
15	M	107	GLY	Peptide
15	M	83	GLY	Peptide
16	N	1	MET	Peptide
16	N	115	LEU	Peptide
16	N	82	GLU	Peptide
16	N	94	TYR	Peptide
17	O	100	HIS	Peptide
17	O	113	ALA	Peptide
17	O	114	GLY	Peptide
17	O	33	ARG	Peptide
17	O	58	ILE	Peptide
17	O	64	TYR	Peptide
17	O	91	SER	Peptide
17	O	94	ARG	Peptide
18	P	104	THR	Peptide
18	P	15	GLN	Peptide
18	P	26	VAL	Peptide
18	P	34	GLU	Peptide
18	P	81	VAL	Peptide
18	P	96	LYS	Peptide
19	Q	100	VAL	Peptide
19	Q	117	LEU	Peptide
19	Q	2	ALA	Peptide
19	Q	91	ASP	Peptide
19	Q	92	ARG	Peptide
20	R	17	GLY	Peptide
20	R	18	GLN	Peptide
20	R	30	GLY	Peptide
20	R	43	ASN	Peptide
20	R	45	GLU	Peptide
20	R	51	VAL	Peptide
21	S	4	ILE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	S	72	THR	Peptide
22	T	13	ALA	Peptide
22	T	49	LYS	Peptide
23	U	18	ASP	Peptide
23	U	26	LYS	Peptide
23	U	35	ILE	Peptide
23	U	36	VAL	Peptide
23	U	57	GLY	Peptide
23	U	6	ARG	Peptide
23	U	7	ARG	Peptide
23	U	98	SER	Peptide
24	V	13	GLY	Peptide
24	V	34	LYS	Peptide
24	V	43	ASP	Peptide
24	V	6	ALA	Peptide
24	V	87	GLN	Peptide
54	W	41	ARG	Peptide
54	W	80	ILE	Peptide
25	X	11	ARG	Peptide
25	X	16	ASN	Peptide
25	X	24	ALA	Peptide
25	X	43	GLU	Peptide
25	X	61	LYS	Peptide
25	X	63	GLY	Peptide
26	Y	62	GLY	Peptide
26	Y	8	GLU	Peptide
27	Z	2	ALA	Peptide
27	Z	58	GLU	Peptide
28	a	17	SER	Peptide
28	a	19	GLY	Peptide
28	a	31	ASP	Peptide
28	a	4	ASP	Peptide
28	a	45	THR	Peptide
28	a	51	VAL	Peptide
28	a	52	ALA	Peptide
28	a	54	GLY	Peptide
28	a	61	ASN	Peptide
28	a	9	TYR	Peptide
29	b	24	ALA	Peptide
30	c	16	GLY	Peptide
30	c	24	THR	Peptide
32	e	17	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
32	e	20	GLY	Peptide
32	e	31	HIS	Peptide
32	e	38	THR	Peptide
32	e	64	TYR	Peptide
33	f	10	LEU	Peptide
33	f	21	GLY	Peptide
33	f	29	ALA	Peptide
34	g	123	ASP	Peptide
34	g	124	GLY	Peptide
34	g	126	PHE	Peptide
34	g	127	ASP	Peptide
34	g	153	ASP	Peptide
34	g	193	PRO	Peptide
34	g	205	ASP	Peptide
34	g	206	ALA	Peptide
34	g	4	VAL	Peptide
34	g	5	SER	Peptide
34	g	71	GLY	Peptide
34	g	72	THR	Peptide
34	g	74	ARG	Peptide
34	g	75	ALA	Peptide
34	g	89	GLN	Peptide
34	g	98	GLY	Peptide
34	g	99	GLY	Peptide
35	h	104	ALA	Peptide
35	h	126	ARG	Peptide
35	h	144	LEU	Peptide
35	h	155	GLY	Peptide
35	h	156	ARG	Peptide
35	h	184	TYR	Peptide
35	h	186	THR	Peptide
35	h	19	ASN	Peptide
35	h	2	GLY	Peptide
35	h	47	LEU	Peptide
35	h	59	ARG	Peptide
35	h	60	PRO	Peptide
35	h	61	ALA	Peptide
35	h	62	LYS	Peptide
35	h	68	ILE	Peptide
35	h	78	GLY	Peptide
35	h	79	LYS	Peptide
35	h	98	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
36	i	146	ARG	Peptide
36	i	171	LEU	Peptide
36	i	173	VAL	Peptide
36	i	205	SER	Peptide
36	i	22	LYS	Peptide
36	i	5	LEU	Peptide
36	i	6	GLY	Peptide
37	j	108	GLY	Peptide
37	j	119	GLY	Peptide
37	j	12	GLN	Peptide
37	j	14	LYS	Peptide
37	j	164	ILE	Peptide
37	j	21	VAL	Peptide
37	j	27	GLY	Peptide
37	j	28	GLY	Peptide
37	j	29	ARG	Peptide
37	j	30	ILE	Peptide
37	j	31	PHE	Peptide
37	j	69	ARG	Peptide
37	j	75	ALA	Peptide
37	j	77	ASN	Peptide
37	j	88	VAL	Peptide
38	k	33	GLU	Peptide
38	k	34	GLY	Peptide
38	k	35	LYS	Peptide
38	k	50	PRO	Peptide
38	k	54	LEU	Peptide
38	k	6	ILE	Peptide
38	k	61	LEU	Peptide
38	k	94	HIS	Peptide
38	k	95	ALA	Peptide
39	l	131	LYS	Peptide
39	l	18	PHE	Peptide
39	l	54	SER	Peptide
40	m	119	ALA	Peptide
40	m	79	SER	Peptide
40	m	88	ARG	Peptide
41	n	12	ARG	Peptide
41	n	17	ALA	Peptide
41	n	21	ILE	Peptide
41	n	4	ASN	Peptide
41	n	55	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
41	n	56	ASP	Peptide
41	n	8	GLY	Peptide
42	o	35	GLN	Peptide
42	o	57	VAL	Peptide
42	o	63	ASP	Peptide
43	p	103	ALA	Peptide
43	p	13	ARG	Peptide
43	p	53	ARG	Peptide
43	p	90	GLY	Peptide
43	p	91	PRO	Peptide
43	p	92	GLY	Peptide
44	q	105	SER	Peptide
44	q	14	ARG	Peptide
44	q	15	LYS	Peptide
44	q	2	ALA	Peptide
44	q	24	LEU	Peptide
44	q	25	GLU	Peptide
44	q	26	ALA	Peptide
44	q	79	VAL	Peptide
44	q	84	GLY	Peptide
45	r	104	THR	Peptide
45	r	112	PRO	Peptide
45	r	46	SER	Peptide
45	r	47	GLU	Peptide
45	r	65	VAL	Peptide
46	s	53	ARG	Peptide
47	t	19	ALA	Peptide
47	t	20	ASN	Peptide
48	u	10	GLY	Peptide
48	u	11	ALA	Peptide
48	u	24	SER	Peptide
48	u	25	ARG	Peptide
48	u	27	ALA	Peptide
48	u	30	GLY	Peptide
48	u	36	VAL	Peptide
48	u	5	ARG	Peptide
48	u	53	ASP	Peptide
48	u	8	ARG	Peptide
49	v	31	HIS	Peptide
49	v	47	HIS	Peptide
49	v	70	THR	Peptide
49	v	79	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
49	v	81	LYS	Peptide
50	w	13	PHE	Peptide
50	w	16	GLU	Peptide
50	w	74	HIS	Peptide
51	x	25	SER	Peptide
51	x	28	LYS	Peptide
51	x	53	ASN	Peptide
51	x	55	ARG	Peptide
51	x	66	MET	Peptide
51	x	81	ARG	Peptide
53	z	59	LYS	Peptide
53	z	69	ARG	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B	269/273 (98%)	256 (95%)	10 (4%)	3 (1%)	12	39
7	C	207/209 (99%)	200 (97%)	6 (3%)	1 (0%)	25	58
8	D	199/201 (99%)	192 (96%)	5 (2%)	2 (1%)	13	42
9	E	175/179 (98%)	158 (90%)	12 (7%)	5 (3%)	3	20
10	F	173/177 (98%)	162 (94%)	9 (5%)	2 (1%)	11	38
11	G	147/149 (99%)	131 (89%)	11 (8%)	5 (3%)	3	17
12	J	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	19	51
13	K	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16	48
14	L	142/144 (99%)	135 (95%)	6 (4%)	1 (1%)	19	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
16	N	117/127 (92%)	111 (95%)	5 (4%)	1 (1%)	14	45
17	O	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
18	P	112/115 (97%)	106 (95%)	5 (4%)	1 (1%)	14	45
19	Q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
20	R	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	3	19
21	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
22	T	92/100 (92%)	88 (96%)	4 (4%)	0	100	100
23	U	101/104 (97%)	95 (94%)	5 (5%)	1 (1%)	13	42
24	V	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
25	X	75/78 (96%)	73 (97%)	1 (1%)	1 (1%)	10	36
26	Y	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
27	Z	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	7	29
28	a	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
29	b	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
30	c	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
31	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
32	e	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	8	31
33	f	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	20
34	g	223/241 (92%)	207 (93%)	11 (5%)	5 (2%)	5	24
35	h	206/233 (88%)	190 (92%)	13 (6%)	3 (2%)	8	33
36	i	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
37	j	154/167 (92%)	143 (93%)	8 (5%)	3 (2%)	6	27
38	k	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	13	42
39	l	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	19	51
40	m	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
41	n	125/130 (96%)	116 (93%)	6 (5%)	3 (2%)	5	22
42	o	97/103 (94%)	89 (92%)	6 (6%)	2 (2%)	5	25
43	p	115/129 (89%)	109 (95%)	5 (4%)	1 (1%)	14	45
44	q	120/124 (97%)	109 (91%)	7 (6%)	4 (3%)	3	17
45	r	114/118 (97%)	108 (95%)	3 (3%)	3 (3%)	4	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	s	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
47	t	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	11	38
48	u	80/82 (98%)	75 (94%)	3 (4%)	2 (2%)	4	22
49	v	78/84 (93%)	71 (91%)	5 (6%)	2 (3%)	4	21
50	w	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
51	x	81/92 (88%)	76 (94%)	5 (6%)	0	100	100
52	y	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
53	z	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
54	W	82/85 (96%)	76 (93%)	5 (6%)	1 (1%)	11	38
All	All	5616/5913 (95%)	5316 (95%)	237 (4%)	63 (1%)	15	39

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	18	THR
9	E	123	ASP
11	G	91	PHE
13	K	109	SER
20	R	80	ARG
27	Z	3	LYS
34	g	88	ASP
35	h	61	ALA
37	j	70	ASN
39	l	56	LYS
41	n	13	LYS
44	q	27	CYS
49	v	80	GLU
8	D	71	GLY
9	E	62	GLY
9	E	174	ASP
11	G	93	SER
14	L	112	LEU
18	P	35	GLY
20	R	44	GLY
34	g	99	GLY
34	g	125	THR
34	g	128	LYS
37	j	78	ASN
41	n	109	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	o	39	PRO
44	q	15	LYS
45	r	47	GLU
47	t	22	THR
49	v	32	PRO
35	h	62	LYS
41	n	54	LEU
6	B	155	ALA
7	C	150	GLN
11	G	89	LYS
12	J	58	ASN
25	X	44	LYS
37	j	90	THR
42	o	32	THR
44	q	102	LEU
45	r	105	ASN
48	u	12	LYS
48	u	36	VAL
54	W	43	THR
6	B	143	ASN
6	B	161	TYR
10	F	118	PRO
20	R	37	GLU
33	f	10	LEU
35	h	108	LYS
38	k	33	GLU
44	q	42	PRO
10	F	47	ASP
11	G	32	PRO
34	g	127	ASP
43	p	120	GLY
9	E	109	PRO
32	e	32	ILE
9	E	108	VAL
16	N	7	GLY
23	U	39	ILE
45	r	65	VAL
11	G	31	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B	216/218 (99%)	216 (100%)	0	100	100
7	C	164/164 (100%)	164 (100%)	0	100	100
8	D	165/165 (100%)	165 (100%)	0	100	100
9	E	148/150 (99%)	148 (100%)	0	100	100
10	F	136/138 (99%)	136 (100%)	0	100	100
11	G	114/114 (100%)	114 (100%)	0	100	100
12	J	116/116 (100%)	116 (100%)	0	100	100
13	K	104/104 (100%)	103 (99%)	1 (1%)	73	86
14	L	103/103 (100%)	103 (100%)	0	100	100
15	M	109/109 (100%)	109 (100%)	0	100	100
16	N	99/103 (96%)	99 (100%)	0	100	100
17	O	86/87 (99%)	86 (100%)	0	100	100
18	P	99/100 (99%)	99 (100%)	0	100	100
19	Q	89/90 (99%)	89 (100%)	0	100	100
20	R	84/84 (100%)	84 (100%)	0	100	100
21	S	93/93 (100%)	93 (100%)	0	100	100
22	T	81/84 (96%)	81 (100%)	0	100	100
23	U	84/85 (99%)	84 (100%)	0	100	100
24	V	78/78 (100%)	78 (100%)	0	100	100
25	X	67/68 (98%)	67 (100%)	0	100	100
26	Y	54/55 (98%)	54 (100%)	0	100	100
27	Z	48/49 (98%)	48 (100%)	0	100	100
28	a	59/62 (95%)	59 (100%)	0	100	100
29	b	47/48 (98%)	47 (100%)	0	100	100
30	c	47/49 (96%)	47 (100%)	0	100	100
31	d	38/38 (100%)	38 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	e	51/52 (98%)	51 (100%)	0	100	100
33	f	34/34 (100%)	34 (100%)	0	100	100
34	g	187/199 (94%)	187 (100%)	0	100	100
35	h	171/190 (90%)	170 (99%)	1 (1%)	84	91
36	i	172/173 (99%)	172 (100%)	0	100	100
37	j	119/126 (94%)	118 (99%)	1 (1%)	79	89
38	k	91/116 (78%)	90 (99%)	1 (1%)	70	84
39	l	124/147 (84%)	124 (100%)	0	100	100
40	m	104/105 (99%)	104 (100%)	0	100	100
41	n	105/107 (98%)	104 (99%)	1 (1%)	73	86
42	o	86/90 (96%)	86 (100%)	0	100	100
43	p	90/99 (91%)	90 (100%)	0	100	100
44	q	102/103 (99%)	99 (97%)	3 (3%)	37	65
45	r	94/96 (98%)	93 (99%)	1 (1%)	70	84
46	s	83/84 (99%)	83 (100%)	0	100	100
47	t	76/77 (99%)	75 (99%)	1 (1%)	65	82
48	u	65/65 (100%)	65 (100%)	0	100	100
49	v	74/78 (95%)	74 (100%)	0	100	100
50	w	57/65 (88%)	57 (100%)	0	100	100
51	x	72/79 (91%)	72 (100%)	0	100	100
52	y	65/66 (98%)	65 (100%)	0	100	100
53	z	60/61 (98%)	60 (100%)	0	100	100
54	W	62/63 (98%)	62 (100%)	0	100	100
All	All	4672/4829 (97%)	4662 (100%)	10 (0%)	91	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	K	17	ARG
35	h	47	LEU
37	j	93	ARG
38	k	62	MET
41	n	106	ARG
44	q	44	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	q	63	VAL
44	q	90	LEU
45	r	9	ILE
47	t	88	ARG

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

Mol	Chain	Res	Type
6	B	86	ASN
6	B	90	ASN
6	B	117	GLN
6	B	128	ASN
6	B	153	GLN
7	C	150	GLN
8	D	41	GLN
8	D	90	GLN
9	E	63	GLN
10	F	128	GLN
11	G	43	ASN
11	G	66	ASN
16	N	62	ASN
17	O	34	HIS
17	O	98	GLN
18	P	12	GLN
21	S	7	HIS
21	S	15	GLN
21	S	60	HIS
21	S	61	ASN
22	T	72	GLN
24	V	24	ASN
24	V	49	ASN
26	Y	38	GLN
27	Z	20	HIS
29	b	5	GLN
35	h	6	HIS
35	h	140	ASN
36	i	54	GLN
36	i	74	ASN
36	i	164	GLN
37	j	146	ASN
38	k	46	GLN
38	k	81	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	o	35	GLN
44	q	46	ASN
44	q	112	GLN
45	r	14	HIS
47	t	37	ASN
47	t	40	GLN
47	t	80	GLN
49	v	45	HIS
51	x	56	GLN
52	y	61	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2900/2904 (99%)	551 (19%)	12 (0%)
2	2	1528/1534 (99%)	279 (18%)	4 (0%)
3	3	119/120 (99%)	33 (27%)	0
4	4	4/5 (80%)	0	0
5	5	75/76 (98%)	25 (33%)	2 (2%)
All	All	4626/4639 (99%)	888 (19%)	18 (0%)

All (888) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	58	G
1	1	60	G
1	1	63	A
1	1	71	A
1	1	74	A
1	1	75	G
1	1	80	G
1	1	84	A
1	1	85	G
1	1	102	U
1	1	103	A
1	1	118	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	119	A
1	1	120	U
1	1	125	A
1	1	136	G
1	1	137	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	143	C
1	1	144	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	248	G
1	1	249	C
1	1	250	G
1	1	261	G
1	1	264	C
1	1	265	A
1	1	266	G
1	1	275	C
1	1	276	U
1	1	279	A
1	1	285	G
1	1	308	G
1	1	311	A
1	1	322	A
1	1	329	G
1	1	330	A
1	1	353	C
1	1	354	A
1	1	361	G
1	1	362	A
1	1	371	A
1	1	372	G
1	1	386	G
1	1	396	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	399	U
1	1	404	A
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	451	U
1	1	457	A
1	1	459	U
1	1	477	A
1	1	479	A
1	1	481	G
1	1	483	A
1	1	491	G
1	1	492	A
1	1	493	G
1	1	495	G
1	1	496	G
1	1	497	A
1	1	500	G
1	1	501	A
1	1	503	A
1	1	505	A
1	1	508	A
1	1	509	C
1	1	518	G
1	1	529	A
1	1	531	C
1	1	532	A
1	1	533	G
1	1	537	G
1	1	538	A
1	1	539	G
1	1	540	C
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	549	G
1	1	551	G
1	1	563	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	568	U
1	1	570	G
1	1	571	U
1	1	573	U
1	1	575	A
1	1	603	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	621	A
1	1	627	A
1	1	634	C
1	1	637	A
1	1	645	C
1	1	647	G
1	1	653	U
1	1	654	A
1	1	655	A
1	1	668	A
1	1	686	U
1	1	709	U
1	1	710	U
1	1	717	C
1	1	726	G
1	1	729	G
1	1	730	A
1	1	734	A
1	1	747	5MU
1	1	752	A
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	789	A
1	1	805	G
1	1	806	C
1	1	811	U
1	1	812	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	819	A
1	1	827	U
1	1	828	U
1	1	831	G
1	1	845	A
1	1	846	U
1	1	856	G
1	1	858	G
1	1	859	G
1	1	869	G
1	1	877	A
1	1	878	A
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	890	C
1	1	891	G
1	1	893	C
1	1	895	U
1	1	896	A
1	1	907	G
1	1	910	A
1	1	914	G
1	1	915	C
1	1	931	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1009	A
1	1	1012	U
1	1	1013	C
1	1	1022	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1025	G
1	1	1026	G
1	1	1028	A
1	1	1029	A
1	1	1030	C
1	1	1033	U
1	1	1042	G
1	1	1043	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1060	U
1	1	1061	U
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1083	U
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1095	A
1	1	1096	A
1	1	1097	U
1	1	1107	G
1	1	1111	A
1	1	1112	G
1	1	1116	G
1	1	1122	G
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1142	A
1	1	1156	A
1	1	1169	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1170	C
1	1	1171	G
1	1	1172	C
1	1	1173	U
1	1	1175	A
1	1	1176	U
1	1	1179	G
1	1	1180	U
1	1	1186	G
1	1	1198	U
1	1	1199	U
1	1	1200	C
1	1	1201	U
1	1	1204	A
1	1	1206	G
1	1	1212	G
1	1	1236	G
1	1	1238	G
1	1	1244	A
1	1	1248	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1300	G
1	1	1301	A
1	1	1321	A
1	1	1332	G
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1408	G
1	1	1409	U
1	1	1410	G
1	1	1411	U
1	1	1416	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1417	C
1	1	1419	A
1	1	1427	A
1	1	1428	C
1	1	1434	A
1	1	1437	C
1	1	1452	G
1	1	1453	A
1	1	1460	U
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1497	U
1	1	1502	A
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1523	U
1	1	1524	G
1	1	1529	G
1	1	1531	C
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1558	C
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1582	C
1	1	1583	A
1	1	1584	U
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1610	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1619	G
1	1	1646	C
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1660	G
1	1	1672	A
1	1	1674	G
1	1	1715	G
1	1	1716	U
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1757	A
1	1	1764	C
1	1	1773	A
1	1	1800	C
1	1	1801	A
1	1	1802	A
1	1	1807	G
1	1	1808	A
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1835	2MG
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1862	G
1	1	1864	U
1	1	1866	A
1	1	1867	G
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1878	G
1	1	1896	G
1	1	1906	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1907	G
1	1	1912	A
1	1	1913	A
1	1	1914	C
1	1	1916	A
1	1	1923	U
1	1	1924	C
1	1	1927	A
1	1	1929	G
1	1	1930	G
1	1	1931	U
1	1	1937	A
1	1	1938	A
1	1	1955	U
1	1	1963	U
1	1	1964	G
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2020	A
1	1	2022	U
1	1	2023	C
1	1	2030	A
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2072	C
1	1	2093	G
1	1	2097	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2099	U
1	1	2102	G
1	1	2110	G
1	1	2111	U
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2122	U
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2143	C
1	1	2146	C
1	1	2147	A
1	1	2157	G
1	1	2158	A
1	1	2162	G
1	1	2164	C
1	1	2167	U
1	1	2171	A
1	1	2172	U
1	1	2182	U
1	1	2183	A
1	1	2189	U
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2203	U
1	1	2204	G
1	1	2211	A
1	1	2212	A
1	1	2225	A
1	1	2226	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2266	A
1	1	2278	A
1	1	2279	G
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2305	U
1	1	2309	A
1	1	2319	G
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2335	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2354	C
1	1	2361	G
1	1	2365	G
1	1	2383	G
1	1	2385	C
1	1	2396	G
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2425	A
1	1	2426	A
1	1	2428	G
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2447	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2448	A
1	1	2470	G
1	1	2476	A
1	1	2478	A
1	1	2484	G
1	1	2491	U
1	1	2494	G
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2525	G
1	1	2529	G
1	1	2535	G
1	1	2554	U
1	1	2562	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2585	U
1	1	2586	U
1	1	2602	A
1	1	2603	G
1	1	2609	U
1	1	2613	U
1	1	2629	U
1	1	2630	G
1	1	2636	C
1	1	2646	C
1	1	2663	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2725	A
1	1	2726	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2732	G
1	1	2733	A
1	1	2739	U
1	1	2744	G
1	1	2748	A
1	1	2757	A
1	1	2765	A
1	1	2769	U
1	1	2777	G
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2796	U
1	1	2797	U
1	1	2798	U
1	1	2799	A
1	1	2818	U
1	1	2820	A
1	1	2821	A
1	1	2825	G
1	1	2835	A
1	1	2861	U
1	1	2867	G
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2903	U
2	2	4	U
2	2	6	G
2	2	7	A
2	2	9	G
2	2	39	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	58	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	68	G
2	2	69	G
2	2	72	A
2	2	74	A
2	2	77	A
2	2	81	A
2	2	82	G
2	2	83	C
2	2	84	U
2	2	87	C
2	2	88	U
2	2	92	U
2	2	94	G
2	2	95	C
2	2	108	G
2	2	120	A
2	2	122	G
2	2	129	A
2	2	131	A
2	2	141	G
2	2	144	G
2	2	160	A
2	2	177	G
2	2	181	A
2	2	182	A
2	2	183	C
2	2	197	A
2	2	202	G
2	2	204	G
2	2	208	U
2	2	209	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	222	C
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	262	A
2	2	266	G
2	2	267	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	279	A
2	2	289	G
2	2	306	A
2	2	321	A
2	2	328	C
2	2	330	C
2	2	332	G
2	2	347	G
2	2	351	G
2	2	352	C
2	2	354	G
2	2	356	A
2	2	363	A
2	2	367	U
2	2	372	C
2	2	384	G
2	2	388	G
2	2	390	U
2	2	398	U
2	2	406	G
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	436	C
2	2	439	U
2	2	452	A
2	2	456	A
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	477	C
2	2	478	A
2	2	479	U
2	2	481	G
2	2	484	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	485	U
2	2	486	U
2	2	496	A
2	2	509	A
2	2	510	A
2	2	511	C
2	2	515	G
2	2	517	G
2	2	518	C
2	2	519	C
2	2	521	G
2	2	527	7MG
2	2	532	A
2	2	533	A
2	2	547	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	615	G
2	2	633	G
2	2	639	G
2	2	650	G
2	2	653	U
2	2	665	A
2	2	666	G
2	2	700	G
2	2	702	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	755	G
2	2	777	A
2	2	793	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	794	A
2	2	814	A
2	2	815	A
2	2	817	C
2	2	819	A
2	2	821	G
2	2	828	U
2	2	829	G
2	2	841	C
2	2	843	U
2	2	844	G
2	2	846	G
2	2	851	G
2	2	902	G
2	2	914	A
2	2	934	C
2	2	935	A
2	2	958	A
2	2	960	U
2	2	966	2MG
2	2	968	A
2	2	969	A
2	2	971	G
2	2	975	A
2	2	976	G
2	2	982	U
2	2	989	U
2	2	992	U
2	2	993	G
2	2	996	A
2	2	1004	A
2	2	1008	U
2	2	1009	U
2	2	1010	U
2	2	1017	U
2	2	1018	G
2	2	1020	G
2	2	1021	A
2	2	1026	G
2	2	1027	C
2	2	1028	C
2	2	1029	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1030	U
2	2	1031	C
2	2	1043	G
2	2	1044	A
2	2	1046	A
2	2	1065	U
2	2	1066	C
2	2	1071	C
2	2	1085	U
2	2	1086	U
2	2	1094	G
2	2	1095	U
2	2	1099	G
2	2	1101	A
2	2	1104	G
2	2	1108	G
2	2	1124	G
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1145	A
2	2	1151	A
2	2	1152	A
2	2	1154	G
2	2	1158	C
2	2	1159	U
2	2	1167	A
2	2	1174	G
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1226	C
2	2	1227	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1228	C
2	2	1236	A
2	2	1238	A
2	2	1239	A
2	2	1240	U
2	2	1257	A
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1277	C
2	2	1279	G
2	2	1280	A
2	2	1285	A
2	2	1286	U
2	2	1287	A
2	2	1299	A
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1319	A
2	2	1320	C
2	2	1322	C
2	2	1328	C
2	2	1331	G
2	2	1340	A
2	2	1346	A
2	2	1353	G
2	2	1363	A
2	2	1368	A
2	2	1370	G
2	2	1378	C
2	2	1379	G
2	2	1381	U
2	2	1383	C
2	2	1384	C
2	2	1396	A
2	2	1398	A
2	2	1404	C
2	2	1419	G
2	2	1429	A
2	2	1432	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1441	A
2	2	1446	A
2	2	1452	C
2	2	1453	G
2	2	1492	A
2	2	1493	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	8	C
3	3	13	G
3	3	16	G
3	3	32	U
3	3	35	C
3	3	45	A
3	3	48	U
3	3	51	G
3	3	52	A
3	3	53	A
3	3	56	G
3	3	60	C
3	3	66	A
3	3	68	C
3	3	70	C
3	3	71	C
3	3	73	A
3	3	74	U
3	3	78	A
3	3	79	G
3	3	88	C
3	3	89	U
3	3	90	C
3	3	92	C
3	3	93	C
3	3	94	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	99	A
3	3	105	G
3	3	108	A
3	3	109	A
3	3	113	C
3	3	119	A
5	5	4	G
5	5	8	U
5	5	9	A
5	5	11	C
5	5	12	U
5	5	13	C
5	5	15	U
5	5	16	U
5	5	17	U
5	5	18	G
5	5	19	G
5	5	20	U
5	5	21	A
5	5	22	G
5	5	47	U
5	5	48	C
5	5	49	G
5	5	55	PSU
5	5	58	A
5	5	60	U
5	5	69	C
5	5	71	G
5	5	74	C
5	5	75	C
5	5	76	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	784	G
1	1	894	U
1	1	1379	U
1	1	1962	5MC
1	1	2030	A
1	1	2189	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2193	G
1	1	2225	A
1	1	2286	G
1	1	2425	A
1	1	2756	U
2	2	428	G
2	2	496	A
2	2	516	PSU
2	2	1383	C
5	5	17	U
5	5	47	U

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

34 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	$\# Z > 2$
1	G7M	1	2069	1	20,26,27	2.26	8 (40%)	16,39,42	1.33	2 (12%)
1	PSU	1	2504	1	18,21,22	4.19	7 (38%)	21,30,33	1.99	5 (23%)
1	PSU	1	1911	1	18,21,22	4.32	7 (38%)	21,30,33	1.97	5 (23%)
1	2MG	1	2445	1	18,26,27	2.35	7 (38%)	16,38,41	2.08	6 (37%)
1	OMU	1	2552	1	19,22,23	2.83	8 (42%)	25,31,34	2.01	5 (20%)
2	2MG	2	1207	2	18,26,27	2.46	7 (38%)	16,38,41	1.60	4 (25%)
1	2MG	1	1835	1	18,26,27	2.34	7 (38%)	16,38,41	1.42	3 (18%)
2	4OC	2	1402	2	20,23,24	3.03	8 (40%)	25,32,35	1.03	3 (12%)
1	PSU	1	746	1	18,21,22	4.26	8 (44%)	21,30,33	1.90	5 (23%)
1	OMG	1	2251	5,1	19,26,27	2.28	8 (42%)	21,38,41	1.44	4 (19%)
1	6MZ	1	1618	1	17,25,26	1.57	1 (5%)	15,36,39	3.61	6 (40%)
2	2MG	2	1516	2	18,26,27	2.45	7 (38%)	16,38,41	1.87	5 (31%)
44	0TD	q	89	44	8,9,10	3.58	2 (25%)	6,11,13	2.23	3 (50%)
2	MA6	2	1519	2	19,26,27	1.68	3 (15%)	18,38,41	3.37	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MA6	2	1518	2	19,26,27	1.69	3 (15%)	18,38,41	3.29	3 (16%)
2	PSU	2	516	2	18,21,22	4.24	7 (38%)	21,30,33	1.90	5 (23%)
1	PSU	1	955	1	18,21,22	4.11	7 (38%)	21,30,33	2.15	5 (23%)
1	OMC	1	2498	1	19,22,23	0.82	0	25,31,34	1.02	1 (4%)
1	PSU	1	2605	1	18,21,22	4.12	7 (38%)	21,30,33	2.07	5 (23%)
1	PSU	1	2580	1	18,21,22	4.15	8 (44%)	21,30,33	2.18	6 (28%)
1	2MA	1	2503	1	18,25,26	3.23	7 (38%)	20,37,40	1.57	2 (10%)
2	7MG	2	527	2	23,26,27	1.35	3 (13%)	27,39,42	2.71	8 (29%)
1	5MC	1	1962	1	19,22,23	3.55	8 (42%)	26,32,35	1.15	1 (3%)
2	5MC	2	967	2	19,22,23	3.70	8 (42%)	26,32,35	1.04	1 (3%)
1	5MU	1	747	1	19,22,23	4.77	7 (36%)	27,32,35	3.77	10 (37%)
2	2MG	2	966	2	18,26,27	2.47	7 (38%)	16,38,41	1.58	4 (25%)
5	5MU	5	54	5	19,22,23	5.06	7 (36%)	27,32,35	3.62	9 (33%)
1	PSU	1	2457	1	18,21,22	4.09	8 (44%)	21,30,33	2.39	6 (28%)
1	PSU	1	1917	1	18,21,22	4.16	7 (38%)	21,30,33	1.96	4 (19%)
1	1MG	1	745	1	19,26,27	3.12	7 (36%)	18,39,42	1.69	4 (22%)
2	5MC	2	1407	2	19,22,23	3.58	8 (42%)	26,32,35	0.99	2 (7%)
2	UR3	2	1498	2	19,22,23	2.73	6 (31%)	26,32,35	1.59	4 (15%)
5	PSU	5	55	5	18,21,22	4.44	7 (38%)	21,30,33	1.91	5 (23%)
1	5MU	1	1939	1	19,22,23	4.72	7 (36%)	27,32,35	3.90	10 (37%)

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
1	G7M	1	2069	1	-	0/3/25/26	0/3/3/3
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
2	4OC	2	1402	2	-	1/9/29/30	0/2/2/2
1	PSU	1	746	1	-	4/7/25/26	0/2/2/2
1	OMG	1	2251	5,1	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	1	1618	1	-	4/5/27/28	0/3/3/3
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
44	0TD	q	89	44	-	1/7/12/14	-
2	MA6	2	1519	2	-	4/7/29/30	0/3/3/3
2	MA6	2	1518	2	-	1/7/29/30	0/3/3/3
2	PSU	2	516	2	-	3/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	1	-	0/9/27/28	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
1	2MA	1	2503	1	-	1/3/25/26	0/3/3/3
2	7MG	2	527	2	-	3/7/37/38	0/3/3/3
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
2	2MG	2	966	2	-	2/5/27/28	0/3/3/3
5	5MU	5	54	5	-	0/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	2/7/25/26	0/2/2/2
5	PSU	5	55	5	-	2/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2

All (217) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	54	5MU	C2-N1	11.97	1.57	1.38
5	5	55	PSU	C6-C5	11.77	1.48	1.35
1	1	1911	PSU	C6-C5	11.71	1.48	1.35
2	2	516	PSU	C6-C5	11.22	1.47	1.35
1	1	2504	PSU	C6-C5	11.16	1.47	1.35
5	5	54	5MU	C6-N1	11.03	1.56	1.38
1	1	746	PSU	C6-C5	11.01	1.47	1.35
1	1	955	PSU	C6-C5	10.81	1.47	1.35
1	1	747	5MU	C2-N1	10.79	1.55	1.38
1	1	2580	PSU	C6-C5	10.76	1.47	1.35
1	1	2605	PSU	C6-C5	10.76	1.47	1.35
1	1	1917	PSU	C6-C5	10.66	1.47	1.35
1	1	2457	PSU	C6-C5	10.57	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1939	5MU	C2-N1	10.54	1.55	1.38
1	1	747	5MU	C6-N1	10.29	1.55	1.38
5	5	54	5MU	C4-C5	10.25	1.61	1.44
1	1	1939	5MU	C6-N1	10.16	1.55	1.38
5	5	55	PSU	C2-N1	9.90	1.49	1.36
44	q	89	0TD	CB-CA	-9.69	1.51	1.54
2	2	516	PSU	C2-N1	9.54	1.49	1.36
1	1	746	PSU	C2-N1	9.53	1.49	1.36
1	1	1911	PSU	C2-N1	9.53	1.49	1.36
1	1	747	5MU	C4-C5	9.46	1.60	1.44
1	1	2457	PSU	C2-N1	9.44	1.49	1.36
1	1	1939	5MU	C4-C5	9.43	1.60	1.44
1	1	1917	PSU	C2-N1	9.42	1.48	1.36
1	1	955	PSU	C2-N1	9.24	1.48	1.36
1	1	2605	PSU	C2-N1	9.22	1.48	1.36
1	1	2504	PSU	C2-N1	9.18	1.48	1.36
1	1	2580	PSU	C2-N1	9.07	1.48	1.36
1	1	745	1MG	C2-N2	8.81	1.49	1.34
2	2	967	5MC	C6-C5	8.78	1.48	1.34
1	1	1962	5MC	C6-C5	8.73	1.48	1.34
2	2	1407	5MC	C6-C5	8.64	1.48	1.34
1	1	2503	2MA	C4-N3	8.24	1.48	1.35
1	1	747	5MU	C4-N3	-7.79	1.24	1.38
1	1	1939	5MU	C4-N3	-7.79	1.24	1.38
5	5	55	PSU	C2-N3	7.67	1.50	1.37
5	5	54	5MU	C4-N3	-7.32	1.25	1.38
1	1	1911	PSU	C2-N3	7.32	1.49	1.37
1	1	2580	PSU	C2-N3	7.31	1.49	1.37
1	1	746	PSU	C2-N3	7.28	1.49	1.37
1	1	1917	PSU	C2-N3	7.25	1.49	1.37
1	1	2504	PSU	C2-N3	7.20	1.49	1.37
1	1	2605	PSU	C2-N3	7.15	1.49	1.37
1	1	2503	2MA	C2-N3	7.04	1.46	1.34
1	1	955	PSU	C2-N3	6.99	1.49	1.37
2	2	516	PSU	C2-N3	6.90	1.48	1.37
1	1	2457	PSU	C2-N3	6.87	1.48	1.37
2	2	967	5MC	C4-N3	6.78	1.45	1.34
5	5	54	5MU	C6-C5	6.73	1.45	1.34
2	2	1402	4OC	C4-N3	6.60	1.43	1.32
2	2	1498	UR3	C6-C5	6.53	1.50	1.35
2	2	1498	UR3	C2-N1	6.36	1.47	1.38
1	1	2552	OMU	C2-N1	6.34	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1962	5MC	C4-N3	6.29	1.44	1.34
2	2	1407	5MC	C4-N3	6.25	1.44	1.34
1	1	747	5MU	C6-C5	6.21	1.44	1.34
2	2	967	5MC	C5-C4	6.16	1.48	1.44
1	1	1939	5MU	C6-C5	6.16	1.44	1.34
1	1	2552	OMU	C2-N3	6.15	1.48	1.38
2	2	1402	4OC	C6-C5	6.13	1.49	1.35
2	2	967	5MC	C2-N3	6.09	1.48	1.36
1	1	745	1MG	C2-N3	6.06	1.43	1.33
2	2	1402	4OC	C2-N3	5.97	1.48	1.36
2	2	1407	5MC	C2-N3	5.80	1.47	1.36
1	1	1962	5MC	C2-N3	5.80	1.47	1.36
2	2	966	2MG	C2-N2	5.68	1.45	1.33
2	2	1407	5MC	C5-C4	5.65	1.48	1.44
2	2	1207	2MG	C2-N2	5.57	1.45	1.33
2	2	1516	2MG	C2-N2	5.48	1.44	1.33
1	1	1835	2MG	C2-N2	5.47	1.44	1.33
1	1	2552	OMU	C6-C5	5.45	1.47	1.35
1	1	1962	5MC	C5-C4	5.39	1.48	1.44
2	2	1498	UR3	C2-N3	5.31	1.49	1.39
5	5	55	PSU	C6-N1	5.25	1.44	1.36
1	1	2251	OMG	C2-N3	5.24	1.46	1.33
1	1	2445	2MG	C2-N2	5.23	1.44	1.33
2	2	966	2MG	C4-N3	5.16	1.49	1.37
1	1	2503	2MA	C2-N1	5.09	1.42	1.34
1	1	746	PSU	C6-N1	5.01	1.44	1.36
1	1	1618	6MZ	C6-C5	-4.98	1.37	1.44
1	1	2503	2MA	C6-N1	4.97	1.42	1.33
2	2	516	PSU	C6-N1	4.94	1.44	1.36
2	2	1207	2MG	C4-N3	4.89	1.49	1.37
1	1	1911	PSU	C6-N1	4.89	1.44	1.36
1	1	1835	2MG	C4-N3	4.85	1.48	1.37
1	1	1917	PSU	C6-N1	4.84	1.44	1.36
1	1	2504	PSU	C6-N1	4.79	1.44	1.36
1	1	2605	PSU	C6-N1	4.75	1.44	1.36
2	2	1519	MA6	C6-C5	-4.73	1.37	1.44
1	1	2580	PSU	C6-N1	4.72	1.44	1.36
1	1	2069	G7M	C2-N3	4.63	1.44	1.33
1	1	955	PSU	C6-N1	4.63	1.43	1.36
2	2	1518	MA6	C6-C5	-4.60	1.37	1.44
1	1	745	1MG	C4-N3	4.59	1.48	1.37
2	2	1516	2MG	C2-N1	4.58	1.44	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1516	2MG	C4-N3	4.57	1.48	1.37
1	1	2457	PSU	C6-N1	4.56	1.43	1.36
1	1	2069	G7M	C2-N2	4.53	1.44	1.34
1	1	2445	2MG	C4-N3	4.53	1.48	1.37
2	2	1207	2MG	C2-N1	4.49	1.43	1.36
2	2	1518	MA6	C6-N6	4.46	1.47	1.37
1	1	745	1MG	C2-N1	4.43	1.45	1.37
2	2	1402	4OC	C4-N4	4.42	1.45	1.36
2	2	966	2MG	C2-N1	4.41	1.43	1.36
2	2	967	5MC	C4-N4	4.38	1.45	1.34
1	1	2251	OMG	C4-N3	4.36	1.47	1.37
2	2	1407	5MC	C6-N1	4.31	1.45	1.38
1	1	2069	G7M	C4-N3	4.30	1.47	1.37
2	2	1407	5MC	C4-N4	4.23	1.44	1.34
1	1	2445	2MG	C2-N1	4.22	1.43	1.36
1	1	1962	5MC	C6-N1	4.19	1.45	1.38
1	1	1962	5MC	C4-N4	4.15	1.44	1.34
2	2	1519	MA6	C6-N6	4.13	1.47	1.37
2	2	967	5MC	C6-N1	4.12	1.45	1.38
1	1	1835	2MG	C2-N1	4.10	1.43	1.36
2	2	1402	4OC	C2-N1	4.08	1.48	1.40
2	2	1407	5MC	C2-N1	4.02	1.48	1.40
1	1	1962	5MC	C2-N1	3.97	1.48	1.40
2	2	967	5MC	C2-N1	3.95	1.48	1.40
1	1	2251	OMG	C2-N2	3.88	1.43	1.34
5	5	55	PSU	C4-N3	3.80	1.46	1.38
1	1	745	1MG	O6-C6	-3.74	1.14	1.22
1	1	2552	OMU	C4-N3	3.61	1.44	1.38
2	2	516	PSU	O4-C4	-3.50	1.16	1.23
1	1	746	PSU	C4-N3	3.45	1.45	1.38
1	1	2580	PSU	C4-N3	3.44	1.45	1.38
1	1	1917	PSU	C4-N3	3.44	1.45	1.38
1	1	2605	PSU	C4-N3	3.40	1.45	1.38
1	1	2504	PSU	C4-N3	3.40	1.45	1.38
1	1	1911	PSU	C4-N3	3.39	1.45	1.38
1	1	2069	G7M	C6-N1	3.37	1.43	1.37
2	2	1516	2MG	C6-N1	3.33	1.42	1.37
2	2	1402	4OC	C5-C4	3.26	1.48	1.41
2	2	527	7MG	C5-C4	3.23	1.47	1.37
2	2	1207	2MG	C6-N1	3.22	1.42	1.37
1	1	1939	5MU	O4-C4	-3.21	1.17	1.23
2	2	516	PSU	C4-N3	3.21	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	747	5MU	O4-C4	-3.20	1.17	1.23
1	1	2552	OMU	O4-C4	-3.19	1.18	1.24
2	2	1402	4OC	O2-C2	-3.15	1.17	1.23
2	2	1207	2MG	C5-C6	3.14	1.53	1.47
1	1	955	PSU	C4-N3	3.14	1.44	1.38
2	2	966	2MG	C6-N1	3.14	1.42	1.37
1	1	2457	PSU	C4-N3	3.12	1.44	1.38
2	2	1407	5MC	O2-C2	-3.11	1.17	1.23
1	1	2251	OMG	C5-C4	-3.05	1.35	1.43
1	1	2445	2MG	C5-C4	-3.04	1.35	1.43
1	1	1962	5MC	O2-C2	-2.99	1.18	1.23
2	2	1516	2MG	C5-C4	-2.96	1.35	1.43
2	2	967	5MC	O2-C2	-2.96	1.18	1.23
2	2	1402	4OC	C6-N1	2.95	1.45	1.38
1	1	747	5MU	O2-C2	-2.94	1.17	1.23
2	2	1516	2MG	C5-C6	2.92	1.53	1.47
1	1	2251	OMG	C6-N1	2.92	1.42	1.37
1	1	2445	2MG	C6-N1	2.91	1.42	1.37
5	5	54	5MU	O4-C4	-2.91	1.18	1.23
1	1	1939	5MU	O2-C2	-2.91	1.17	1.23
2	2	1498	UR3	C6-N1	2.90	1.45	1.38
1	1	1835	2MG	C5-C4	-2.89	1.35	1.43
1	1	2069	G7M	C5-C6	2.89	1.52	1.45
1	1	2552	OMU	O2-C2	-2.87	1.18	1.23
2	2	527	7MG	C4-N9	-2.86	1.34	1.37
1	1	746	PSU	O4-C4	-2.86	1.18	1.23
1	1	1917	PSU	O4-C4	-2.85	1.18	1.23
2	2	966	2MG	C5-C6	2.84	1.53	1.47
1	1	2457	PSU	O4-C4	-2.81	1.18	1.23
1	1	2445	2MG	C5-C6	2.79	1.52	1.47
1	1	955	PSU	O4-C4	-2.78	1.18	1.23
2	2	1207	2MG	C5-C4	-2.76	1.36	1.43
1	1	2580	PSU	O4-C4	-2.73	1.18	1.23
1	1	2605	PSU	O4-C4	-2.71	1.18	1.23
1	1	2504	PSU	O4-C4	-2.69	1.18	1.23
1	1	746	PSU	O4'-C1'	-2.68	1.40	1.43
1	1	2580	PSU	O4'-C1'	-2.65	1.40	1.43
1	1	1911	PSU	O4-C4	-2.63	1.18	1.23
2	2	966	2MG	C5-C4	-2.59	1.36	1.43
1	1	745	1MG	C5-C4	-2.56	1.36	1.43
5	5	55	PSU	O4-C4	-2.55	1.18	1.23
1	1	955	PSU	O2-C2	-2.54	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2069	G7M	C2-N1	2.47	1.43	1.37
1	1	1835	2MG	C6-N1	2.46	1.41	1.37
5	5	54	5MU	O2-C2	-2.45	1.18	1.23
1	1	2457	PSU	O2-C2	-2.44	1.18	1.23
1	1	2504	PSU	O2-C2	-2.44	1.18	1.23
1	1	2580	PSU	O2-C2	-2.43	1.18	1.23
1	1	2251	OMG	O6-C6	-2.43	1.17	1.23
1	1	2605	PSU	O2-C2	-2.43	1.18	1.23
1	1	1835	2MG	C5-C6	2.41	1.52	1.47
1	1	2552	OMU	C6-N1	2.41	1.43	1.38
1	1	2251	OMG	C5-C6	2.40	1.52	1.47
1	1	1911	PSU	O2-C2	-2.34	1.18	1.23
1	1	2503	2MA	C6-C5	2.31	1.52	1.43
1	1	2445	2MG	O6-C6	-2.28	1.18	1.23
2	2	1498	UR3	O2-C2	-2.28	1.18	1.22
1	1	1917	PSU	O2-C2	-2.27	1.18	1.23
2	2	516	PSU	O2-C2	-2.27	1.18	1.23
2	2	527	7MG	C6-N1	-2.27	1.34	1.38
1	1	2069	G7M	O6-C6	-2.25	1.18	1.23
1	1	2457	PSU	O4'-C1'	-2.24	1.40	1.43
2	2	1519	MA6	C2-N3	2.24	1.35	1.32
1	1	1835	2MG	O6-C6	-2.22	1.18	1.23
2	2	1518	MA6	C2-N3	2.21	1.35	1.32
2	2	1498	UR3	C4-N3	2.20	1.45	1.40
1	1	2552	OMU	C5-C4	2.19	1.48	1.43
1	1	2251	OMG	C2-N1	2.17	1.42	1.37
44	q	89	0TD	CB-SB	2.16	1.84	1.82
2	2	1516	2MG	O6-C6	-2.14	1.18	1.23
5	5	55	PSU	O2-C2	-2.13	1.18	1.23
1	1	746	PSU	O2-C2	-2.08	1.19	1.23
1	1	745	1MG	C5-C6	2.07	1.53	1.47
2	2	966	2MG	O6-C6	-2.07	1.18	1.23
1	1	2503	2MA	C6-N6	-2.07	1.26	1.34
1	1	2503	2MA	C5-N7	-2.06	1.32	1.39
1	1	2069	G7M	C5-C4	-2.04	1.34	1.39
2	2	1207	2MG	O6-C6	-2.02	1.18	1.23

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1939	5MU	C5-C4-N3	12.59	126.27	115.32
5	5	54	5MU	C5-C4-N3	12.08	125.82	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	747	5MU	C5-C4-N3	11.83	125.61	115.32
2	2	1519	MA6	N1-C6-N6	-11.72	103.29	116.83
2	2	1518	MA6	N1-C6-N6	-11.57	103.47	116.83
1	1	1618	6MZ	C1'-N9-C4	-11.01	107.29	126.64
1	1	1939	5MU	C5-C6-N1	-10.83	111.54	123.31
1	1	747	5MU	C5-C6-N1	-10.59	111.81	123.31
5	5	54	5MU	C5-C6-N1	-9.34	113.17	123.31
2	2	527	7MG	N9-C4-N3	9.10	138.79	125.46
1	1	1618	6MZ	N3-C2-N1	-6.69	119.59	128.67
2	2	1519	MA6	N3-C2-N1	-6.67	119.62	128.67
1	1	2552	OMU	C4-N3-C2	-6.47	118.57	126.61
2	2	1518	MA6	N3-C2-N1	-6.32	120.10	128.67
1	1	1939	5MU	C4-N3-C2	-5.68	119.90	127.34
1	1	2457	PSU	C4-N3-C2	-5.65	118.59	126.37
2	2	527	7MG	C5-C4-N3	-5.53	117.76	128.13
1	1	2457	PSU	N1-C2-N3	5.50	120.97	115.17
1	1	1939	5MU	O4-C4-C5	-5.46	118.67	124.92
2	2	527	7MG	N9-C8-N7	-5.31	95.85	103.37
1	1	747	5MU	O4-C4-C5	-5.26	118.90	124.92
1	1	747	5MU	C4-N3-C2	-5.24	120.47	127.34
1	1	955	PSU	C4-N3-C2	-5.19	119.22	126.37
1	1	955	PSU	N1-C2-N3	5.04	120.48	115.17
2	2	1498	UR3	C4-N3-C2	-5.02	120.54	124.58
1	1	2605	PSU	C4-N3-C2	-5.00	119.49	126.37
5	5	54	5MU	O4-C4-C5	-4.99	119.21	124.92
2	2	516	PSU	C4-N3-C2	-4.94	119.56	126.37
1	1	2503	2MA	C2-N3-C4	4.94	119.45	115.46
1	1	746	PSU	C4-N3-C2	-4.92	119.60	126.37
1	1	2445	2MG	N1-C2-N2	4.83	121.50	116.56
1	1	1917	PSU	C4-N3-C2	-4.82	119.73	126.37
1	1	2580	PSU	C4-N3-C2	-4.78	119.79	126.37
1	1	1939	5MU	N3-C2-N1	4.76	121.09	114.89
1	1	2580	PSU	N1-C2-N3	4.74	120.17	115.17
1	1	747	5MU	N3-C2-N1	4.73	121.05	114.89
1	1	2504	PSU	C4-N3-C2	-4.71	119.89	126.37
1	1	2504	PSU	N1-C2-N3	4.70	120.13	115.17
1	1	1911	PSU	C4-N3-C2	-4.70	119.89	126.37
1	1	2605	PSU	N1-C2-N3	4.68	120.10	115.17
5	5	55	PSU	C4-N3-C2	-4.67	119.94	126.37
1	1	1911	PSU	N1-C2-N3	4.64	120.06	115.17
5	5	54	5MU	C4-N3-C2	-4.61	121.29	127.34
1	1	745	1MG	C5-C6-N1	4.60	120.61	113.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1917	PSU	N1-C2-N3	4.52	119.93	115.17
2	2	527	7MG	C2-N3-C4	4.46	119.99	112.30
1	1	2552	OMU	N3-C2-N1	4.45	120.68	114.89
1	1	2457	PSU	C6-C5-C4	4.35	121.11	118.17
5	5	55	PSU	N1-C2-N3	4.31	119.71	115.17
2	2	1516	2MG	N1-C2-N2	4.30	120.95	116.56
5	5	54	5MU	N3-C2-N1	4.28	120.46	114.89
2	2	516	PSU	N1-C2-N3	4.04	119.43	115.17
1	1	746	PSU	N1-C2-N3	4.01	119.40	115.17
1	1	2552	OMU	C5-C4-N3	3.95	120.33	114.80
2	2	1518	MA6	C2-N1-C6	3.93	120.69	116.84
1	1	747	5MU	C5M-C5-C6	-3.91	117.56	122.85
5	5	54	5MU	C5M-C5-C4	3.88	122.92	118.78
2	2	1519	MA6	C2-N1-C6	3.87	120.63	116.84
1	1	2580	PSU	C6-N1-C2	-3.84	119.13	122.69
1	1	1917	PSU	C6-N1-C2	-3.82	119.14	122.69
1	1	2504	PSU	C6-N1-C2	-3.78	119.19	122.69
5	5	54	5MU	C5M-C5-C6	-3.76	117.77	122.85
1	1	1939	5MU	C5M-C5-C6	-3.73	117.80	122.85
1	1	1911	PSU	C6-N1-C2	-3.68	119.28	122.69
1	1	955	PSU	C6-N1-C2	-3.54	119.41	122.69
2	2	1498	UR3	C5-C4-N3	3.47	119.61	115.04
1	1	2605	PSU	C6-N1-C2	-3.44	119.49	122.69
1	1	2445	2MG	CM2-N2-C2	-3.44	116.26	123.65
1	1	2251	OMG	C2-N1-C6	-3.42	118.86	125.11
1	1	2445	2MG	C5-C6-N1	3.40	120.56	114.07
1	1	1962	5MC	C5-C6-N1	-3.38	119.65	123.31
1	1	745	1MG	C8-N7-C5	3.36	108.27	102.55
2	2	966	2MG	C5-C6-N1	3.34	120.43	114.07
2	2	1207	2MG	C5-C6-N1	3.32	120.40	114.07
1	1	1618	6MZ	C2-N1-C6	3.32	119.17	116.60
1	1	2580	PSU	C6-C5-C4	3.31	120.41	118.17
1	1	2457	PSU	C6-N1-C2	-3.31	119.62	122.69
1	1	2498	OMC	C2'-C1'-N1	-3.31	107.97	114.24
1	1	2069	G7M	C2-N1-C6	-3.29	119.08	125.11
2	2	1207	2MG	C8-N7-C5	3.27	108.11	102.55
1	1	2457	PSU	O2-C2-N1	-3.24	119.45	122.79
44	q	89	0TD	OD1-CG-CB	-3.21	115.71	122.44
1	1	2251	OMG	C5-C6-N1	3.21	120.20	114.07
1	1	2503	2MA	N3-C2-N1	-3.20	120.16	125.77
2	2	1516	2MG	C5-C6-N1	3.20	120.18	114.07
1	1	2251	OMG	C8-N7-C5	3.19	107.99	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	967	5MC	C5-C6-N1	-3.19	119.85	123.31
1	1	2445	2MG	C8-N7-C5	3.18	107.96	102.55
1	1	955	PSU	C6-C5-C4	3.17	120.31	118.17
2	2	1516	2MG	C8-N7-C5	3.16	107.93	102.55
5	5	55	PSU	C6-N1-C2	-3.13	119.79	122.69
44	q	89	0TD	OD2-CG-CB	3.10	119.85	113.15
1	1	1939	5MU	O2-C2-N1	-3.08	118.79	122.80
1	1	1939	5MU	C5M-C5-C4	3.08	122.07	118.78
44	q	89	0TD	O-C-CA	-3.03	116.97	124.77
1	1	2605	PSU	C6-C5-C4	3.03	120.22	118.17
1	1	2580	PSU	O2-C2-N1	-3.00	119.69	122.79
1	1	1835	2MG	C5-C6-N1	3.00	119.79	114.07
1	1	747	5MU	C5M-C5-C4	3.00	121.98	118.78
1	1	2605	PSU	O2-C2-N1	-2.98	119.71	122.79
1	1	1835	2MG	C8-N7-C5	2.98	107.62	102.55
2	2	966	2MG	C8-N7-C5	2.97	107.61	102.55
1	1	747	5MU	C6-C5-C4	2.97	120.46	118.02
2	2	1207	2MG	N1-C2-N2	2.96	119.58	116.56
1	1	955	PSU	O2-C2-N1	-2.86	119.84	122.79
2	2	1498	UR3	C6-N1-C2	-2.82	119.50	121.80
2	2	1516	2MG	CM2-N2-C2	-2.81	117.62	123.65
5	5	55	PSU	C6-C5-C4	2.79	120.06	118.17
2	2	516	PSU	C6-N1-C2	-2.78	120.11	122.69
1	1	746	PSU	C6-C5-C4	2.77	120.04	118.17
1	1	1917	PSU	O2-C2-N1	-2.76	119.94	122.79
2	2	527	7MG	C5-C6-N1	2.74	115.77	110.94
1	1	746	PSU	C6-N1-C2	-2.74	120.15	122.69
5	5	54	5MU	O4-C4-N3	-2.74	114.97	120.11
2	2	966	2MG	N1-C2-N2	2.72	119.34	116.56
1	1	1939	5MU	O4-C4-N3	-2.69	115.06	120.11
1	1	747	5MU	O2-C2-N1	-2.68	119.31	122.80
1	1	746	PSU	O2-C2-N1	-2.67	120.04	122.79
1	1	2552	OMU	O4-C4-C5	-2.64	120.60	125.16
1	1	2552	OMU	O2-C2-N1	-2.63	119.37	122.80
1	1	1911	PSU	O2-C2-N1	-2.63	120.08	122.79
1	1	2504	PSU	O2-C2-N1	-2.63	120.08	122.79
5	5	55	PSU	O2-C2-N1	-2.63	120.08	122.79
1	1	745	1MG	O6-C6-C5	-2.59	119.92	124.18
1	1	2580	PSU	O4'-C1'-C2'	2.58	108.72	105.15
1	1	1939	5MU	C6-C5-C4	2.56	120.13	118.02
2	2	1498	UR3	C1'-N1-C2	2.56	121.23	117.04
1	1	2504	PSU	C6-C5-C4	2.54	119.89	118.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1407	5MC	C5-C6-N1	-2.53	120.57	123.31
1	1	747	5MU	O4-C4-N3	-2.46	115.49	120.11
2	2	966	2MG	O6-C6-C5	-2.46	119.45	124.32
5	5	54	5MU	C1'-N1-C2	2.40	121.91	117.59
1	1	2445	2MG	N2-C2-N3	-2.40	117.45	120.51
2	2	527	7MG	O4'-C1'-N9	2.37	112.52	109.30
1	1	1618	6MZ	C9-N6-C6	-2.37	120.66	122.85
1	1	745	1MG	CM1-N1-C6	2.33	120.71	117.54
2	2	1402	4OC	C6-C5-C4	2.32	119.79	117.00
1	1	2445	2MG	O6-C6-C5	-2.31	119.74	124.32
1	1	2069	G7M	N2-C2-N1	2.30	121.62	116.76
1	1	1911	PSU	C6-C5-C4	2.29	119.72	118.17
2	2	527	7MG	O6-C6-C5	-2.27	122.05	127.62
2	2	1516	2MG	O6-C6-C5	-2.26	119.84	124.32
2	2	527	7MG	C5-C4-N9	-2.25	103.45	106.33
1	1	2251	OMG	O6-C6-C5	-2.24	119.88	124.32
1	1	1618	6MZ	O4'-C1'-N9	-2.24	105.77	108.75
1	1	2457	PSU	O4'-C1'-C2'	2.23	108.23	105.15
2	2	1402	4OC	O2-C2-N3	-2.23	118.82	122.33
2	2	516	PSU	O3'-C3'-C4'	2.22	117.46	111.08
1	1	1618	6MZ	C6-C5-C4	2.14	119.95	117.68
2	2	516	PSU	C5-C4-N3	2.10	121.17	116.55
2	2	1207	2MG	O6-C6-C5	-2.10	120.16	124.32
2	2	1402	4OC	CM4-N4-C4	-2.09	118.37	122.45
2	2	1407	5MC	O2-C2-N3	-2.04	119.11	122.33
1	1	1835	2MG	CM2-N2-C2	-2.00	119.34	123.65

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	746	PSU	C2'-C1'-C5-C4
1	1	746	PSU	C2'-C1'-C5-C6
1	1	1618	6MZ	C5-C6-N6-C9
1	1	1618	6MZ	N1-C6-N6-C9
1	1	2504	PSU	O4'-C4'-C5'-O5'
2	2	516	PSU	C2'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
2	2	527	7MG	C3'-C4'-C5'-O5'
2	2	1498	UR3	O4'-C4'-C5'-O5'
5	5	55	PSU	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
2	2	527	7MG	O4'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
2	2	1498	UR3	C3'-C4'-C5'-O5'
5	5	55	PSU	O4'-C4'-C5'-O5'
44	q	89	0TD	CG-CB-SB-CSB
2	2	1519	MA6	C5-C6-N6-C9
1	1	746	PSU	O4'-C1'-C5-C4
2	2	1519	MA6	C3'-C4'-C5'-O5'
2	2	527	7MG	C4'-C5'-O5'-P
2	2	1519	MA6	N1-C6-N6-C10
1	1	2503	2MA	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
1	1	746	PSU	O4'-C1'-C5-C6

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](#)

1 ligand is 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
55	KKL	1	3301	-	20,25,25	7.11	17 (85%)	27,34,34	1.48	5 (18%)

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
55	KKL	1	3301	-	-	0/10/14/14	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1	3301	KKL	N14-N13	18.38	1.73	1.37
55	1	3301	KKL	C05-C04	12.61	1.59	1.38
55	1	3301	KKL	C16-C15	10.79	1.60	1.39
55	1	3301	KKL	C07-N09	10.09	1.65	1.35
55	1	3301	KKL	C18-C21	8.86	1.63	1.44
55	1	3301	KKL	C05-C06	-7.85	1.27	1.39
55	1	3301	KKL	C17-C16	-5.81	1.29	1.38
55	1	3301	KKL	C01-C06	-4.62	1.32	1.39
55	1	3301	KKL	C02-C01	4.40	1.45	1.38
55	1	3301	KKL	C04-C03	-4.23	1.31	1.40
55	1	3301	KKL	C20-C19	3.84	1.45	1.38
55	1	3301	KKL	C17-C18	3.54	1.46	1.39
55	1	3301	KKL	O08-C07	-3.07	1.16	1.23
55	1	3301	KKL	C21-C22	-2.72	1.08	1.18
55	1	3301	KKL	C03-N23	2.69	1.47	1.38
55	1	3301	KKL	C06-C07	2.20	1.55	1.50
55	1	3301	KKL	C02-C03	-2.18	1.35	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1	3301	KKL	C17-C18-C21	-3.40	115.68	120.66
55	1	3301	KKL	C10-N09-C07	-2.67	120.32	126.58
55	1	3301	KKL	C05-C06-C01	2.45	121.69	118.57
55	1	3301	KKL	C02-C03-N23	-2.41	116.46	120.90
55	1	3301	KKL	C05-C04-C03	-2.32	117.83	120.66

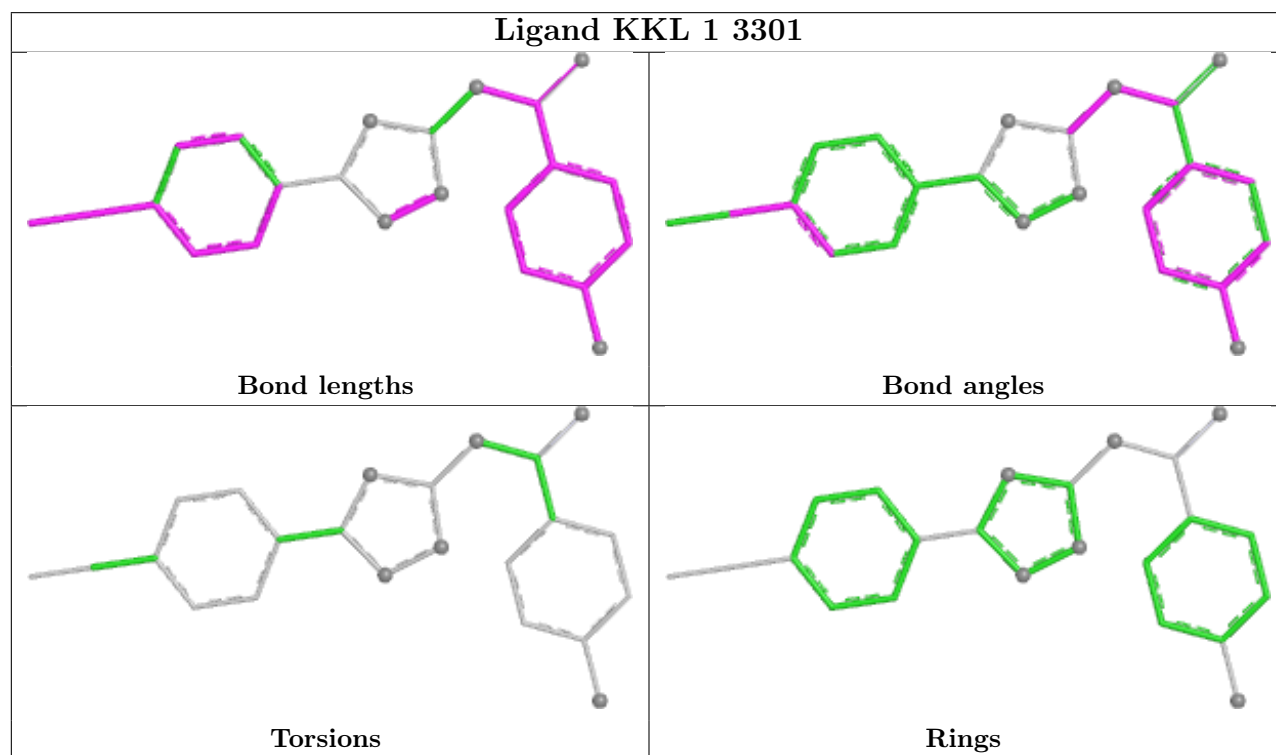
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

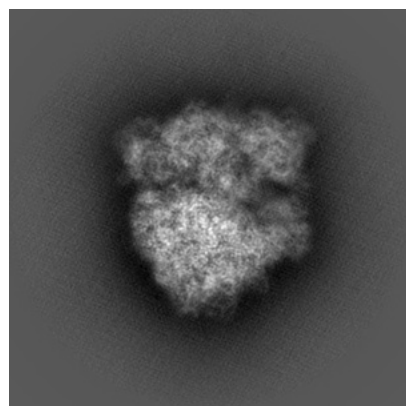
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20121. These allow visual inspection of the internal detail of the map and identification of artifacts.

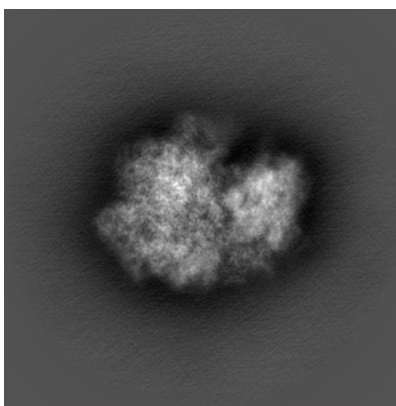
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

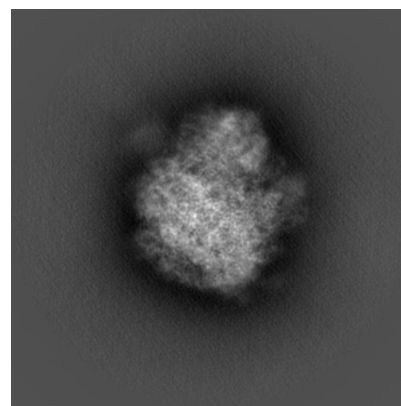
6.1.1 Primary map



X

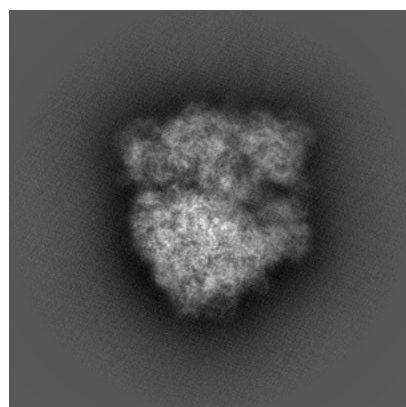


Y

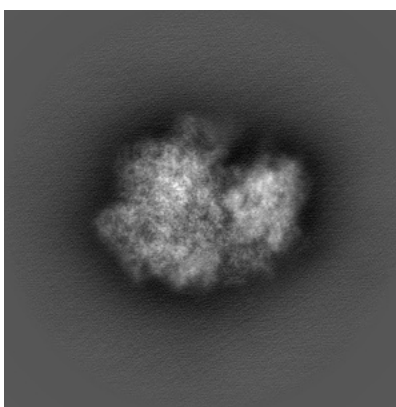


Z

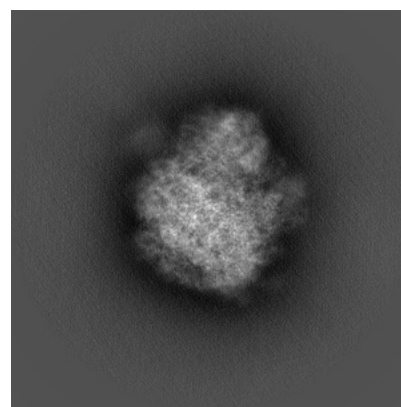
6.1.2 Raw map



X



Y

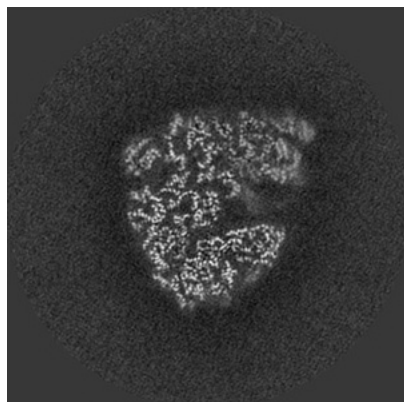


Z

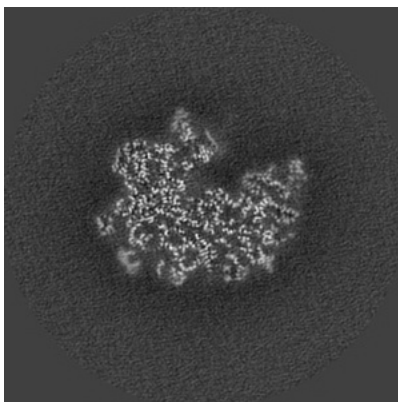
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

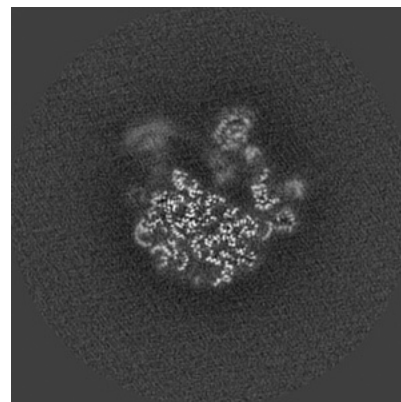
6.2.1 Primary map



X Index: 192

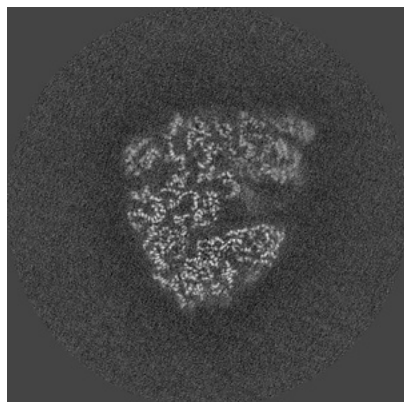


Y Index: 192

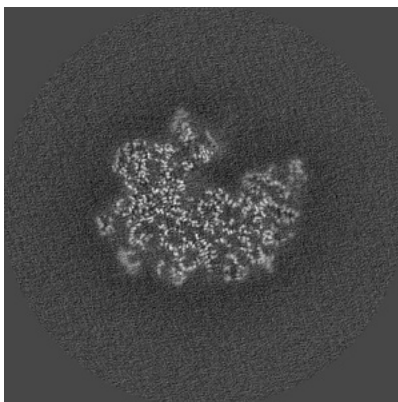


Z Index: 192

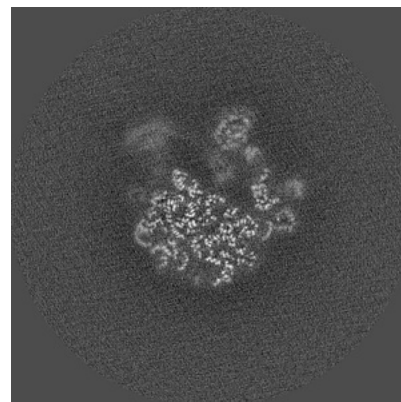
6.2.2 Raw map



X Index: 192



Y Index: 192

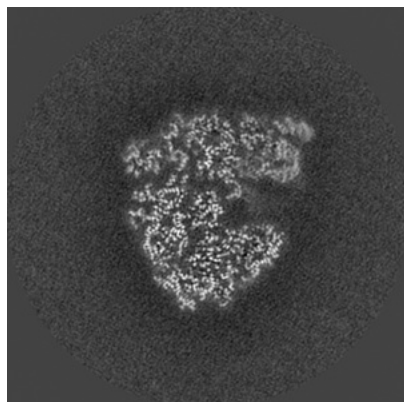


Z Index: 192

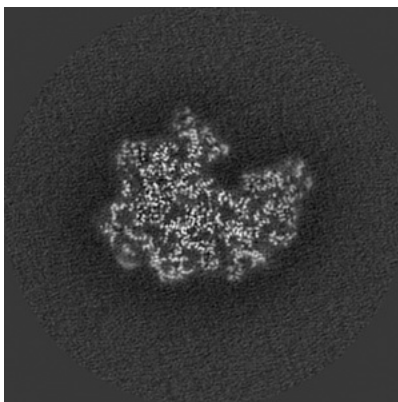
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

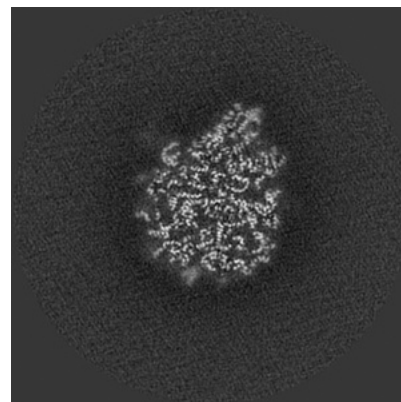
6.3.1 Primary map



X Index: 190

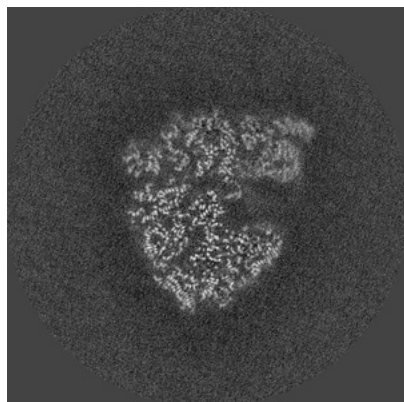


Y Index: 187

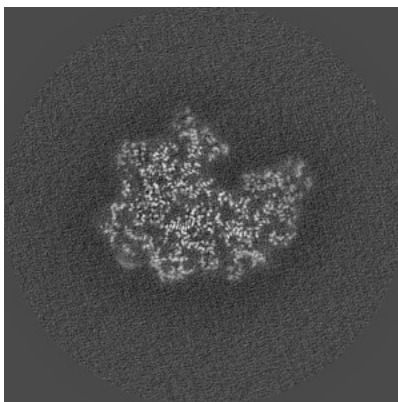


Z Index: 156

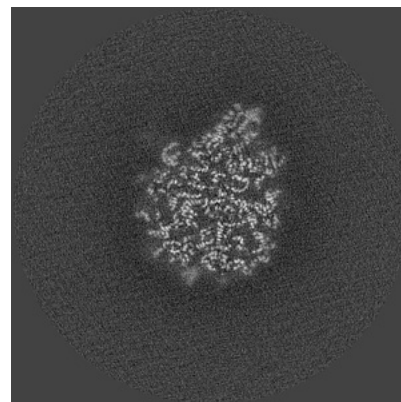
6.3.2 Raw map



X Index: 189



Y Index: 187

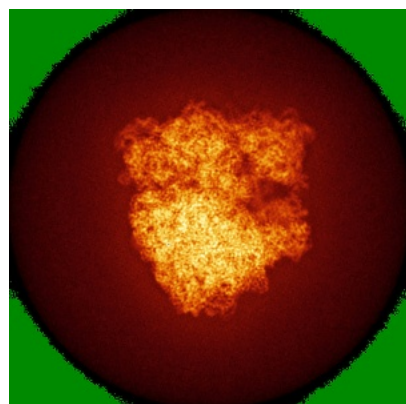


Z Index: 156

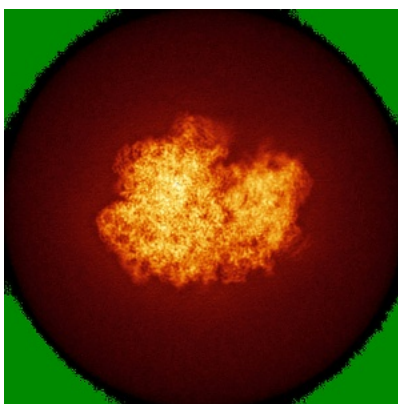
The images above show the largest variance slices of the map in three orthogonal directions.

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

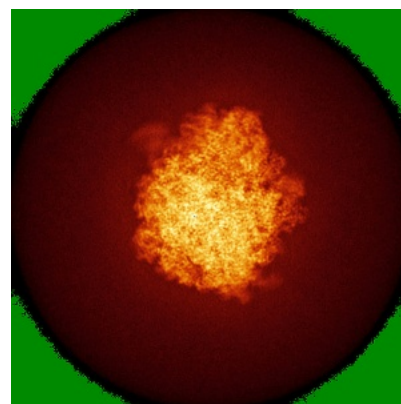
6.4.1 Primary map



X

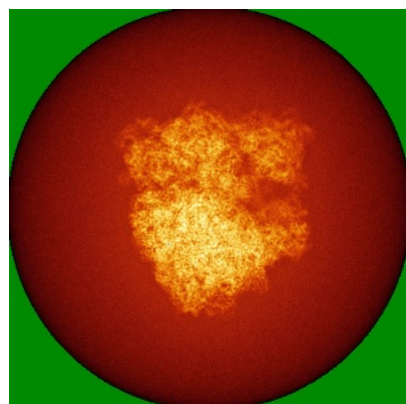


Y

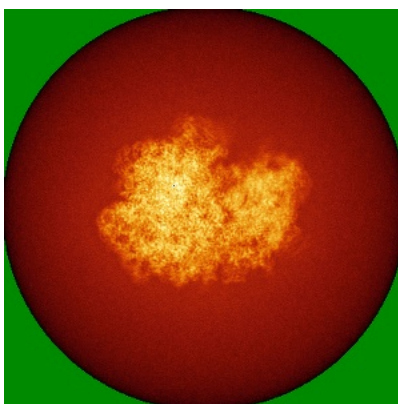


Z

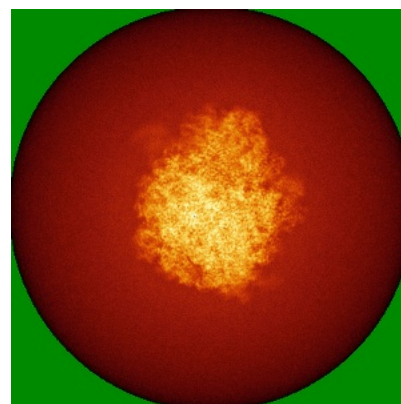
6.4.2 Raw map



X



Y

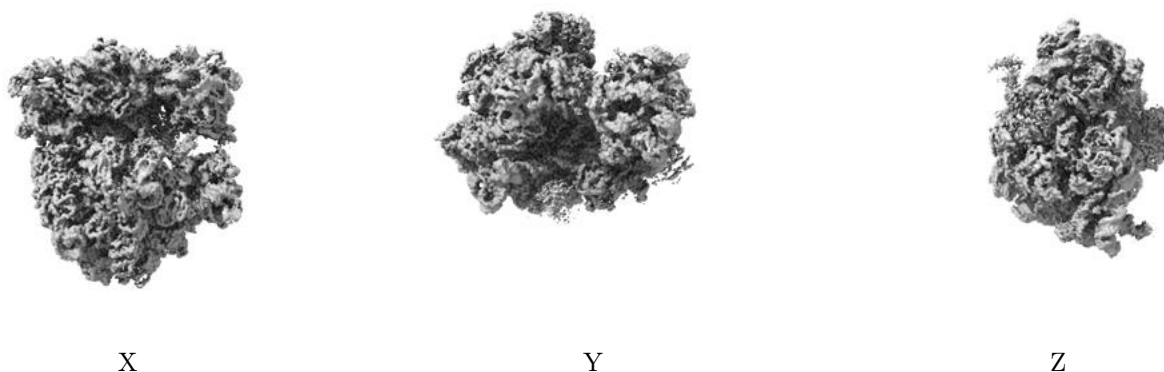


Z

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

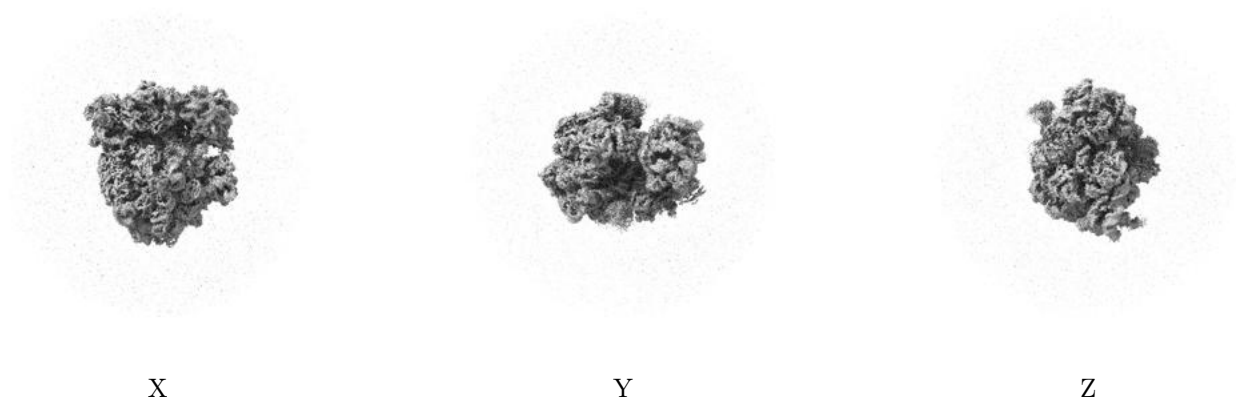
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

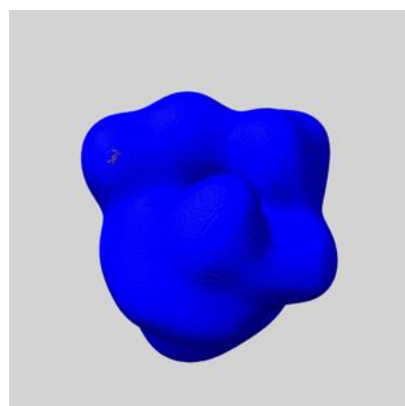
6.6 Mask visualisation [i](#)

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

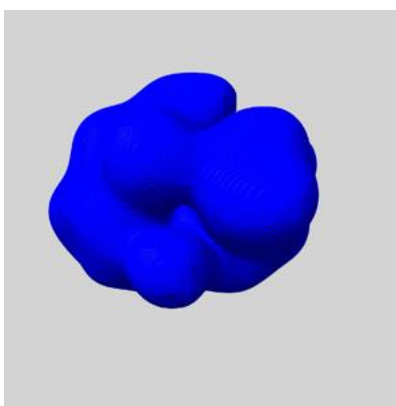
A mask typically either:

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

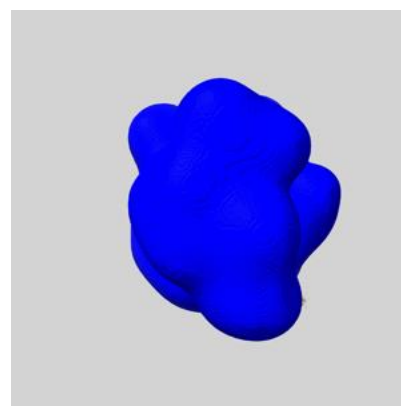
6.6.1 emd_20121_msk_1.map [i](#)



X



Y

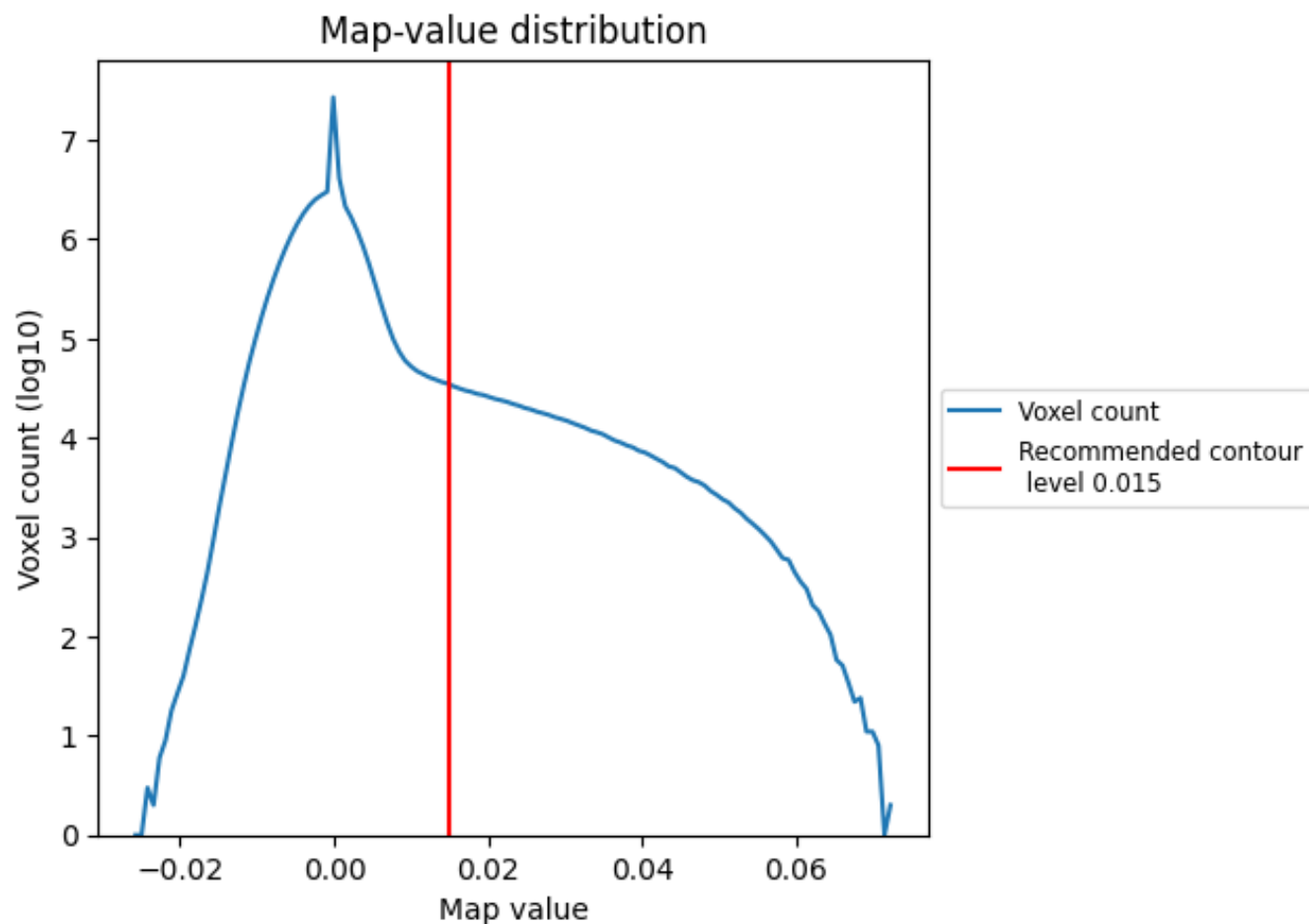


Z

7 Map analysis [i](#)

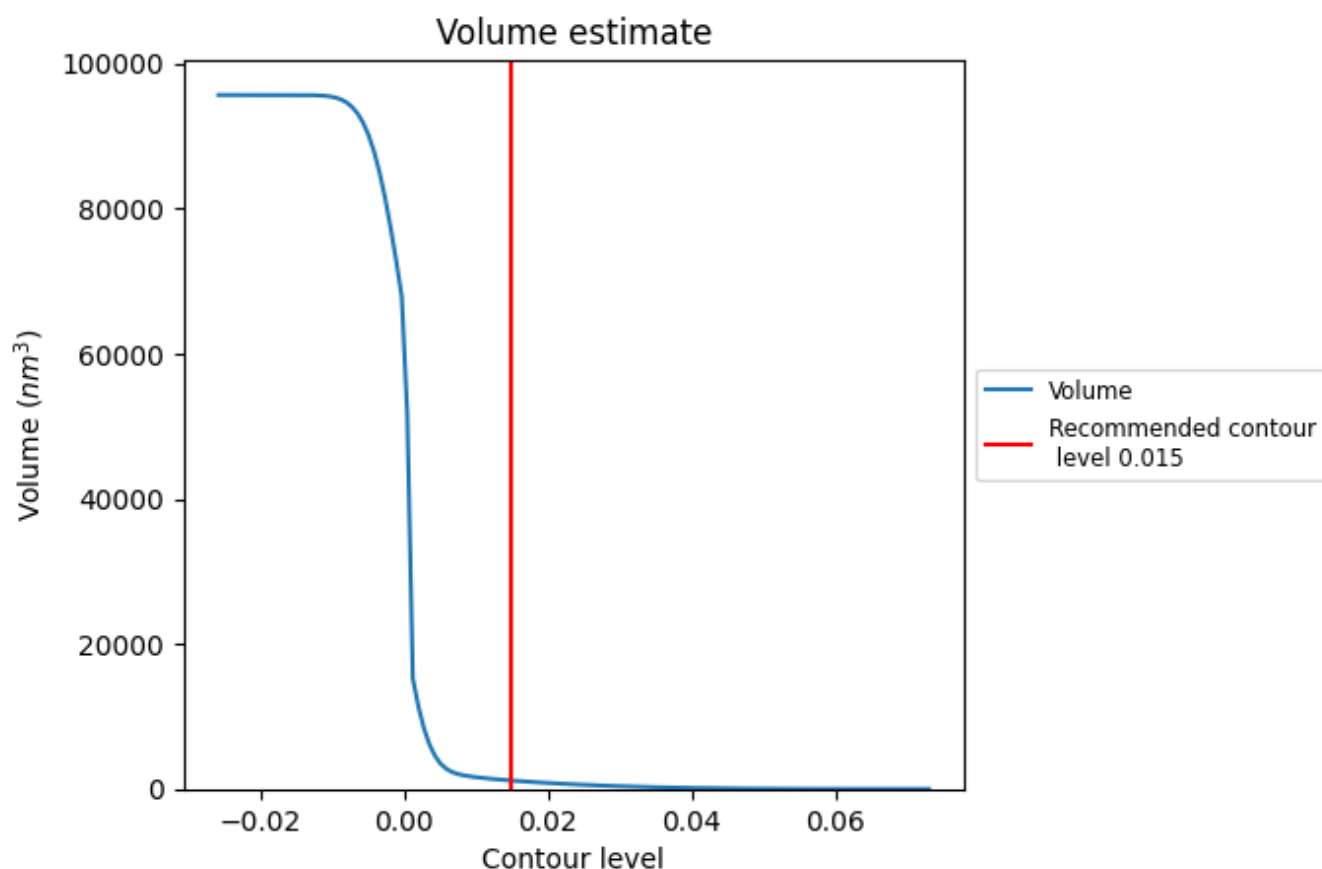
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

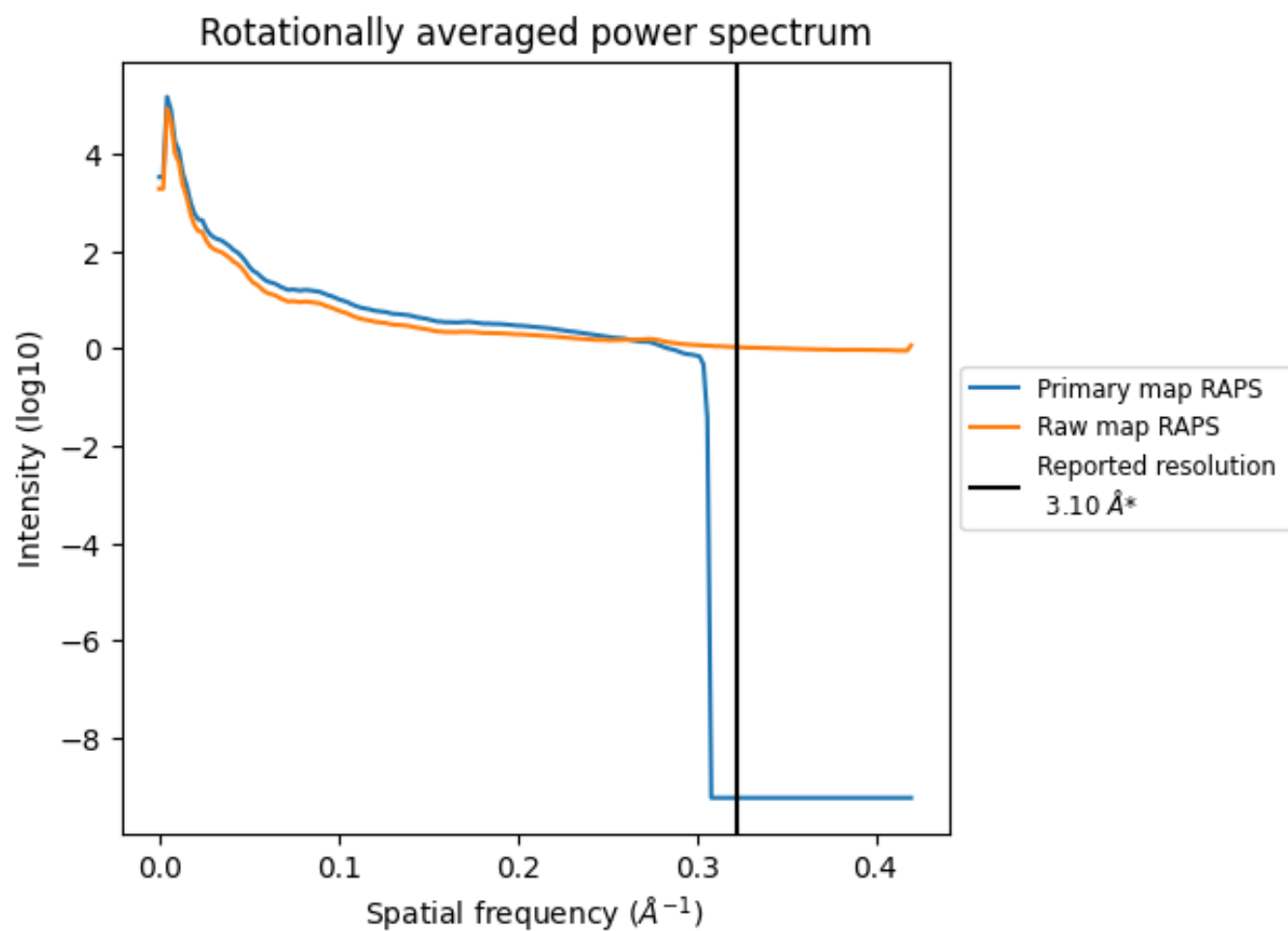
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1158 nm³; this corresponds to an approximate mass of 1046 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

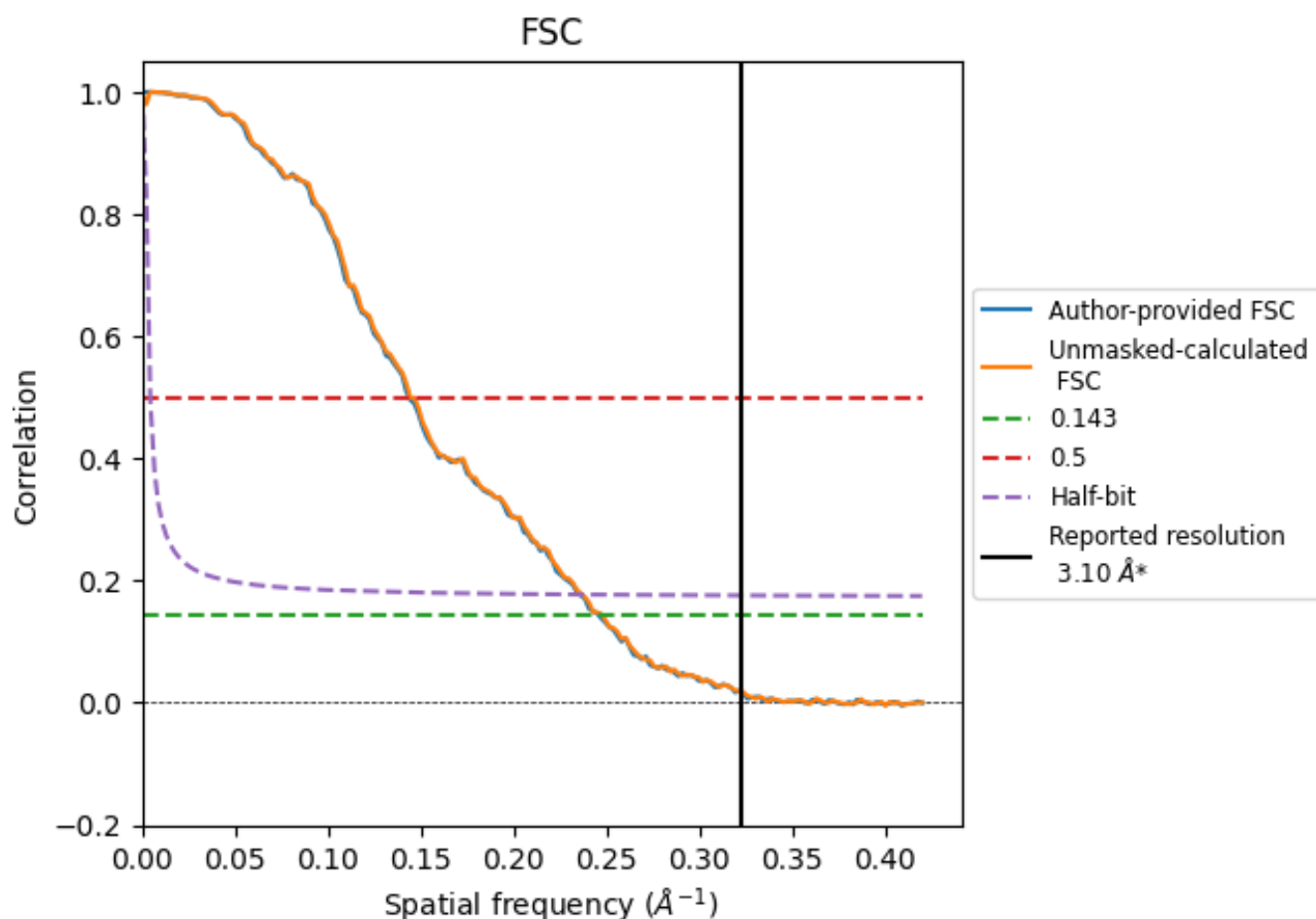


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	4.07	6.96	4.25
Unmasked-calculated*	4.04	6.93	4.22

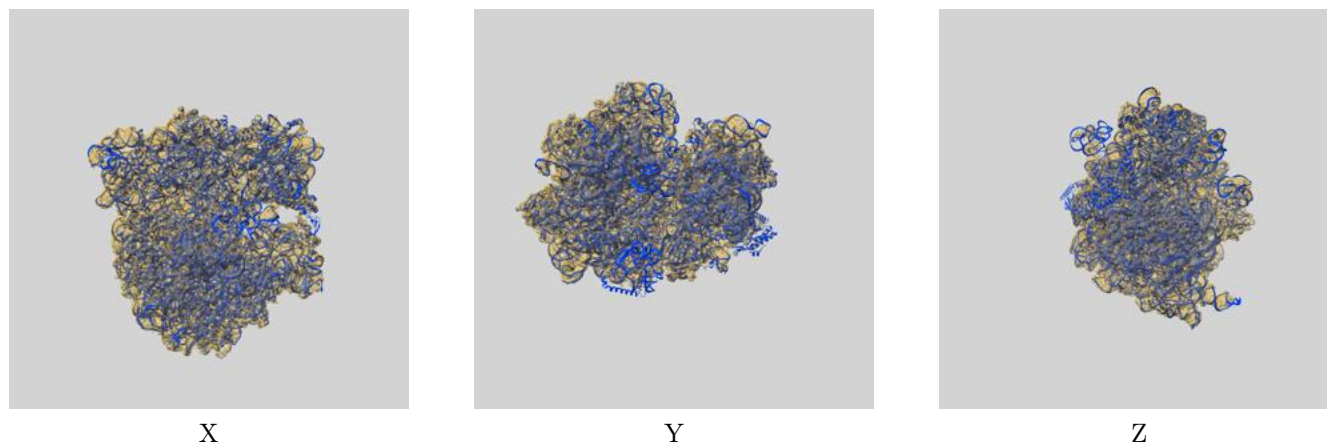
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.04 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

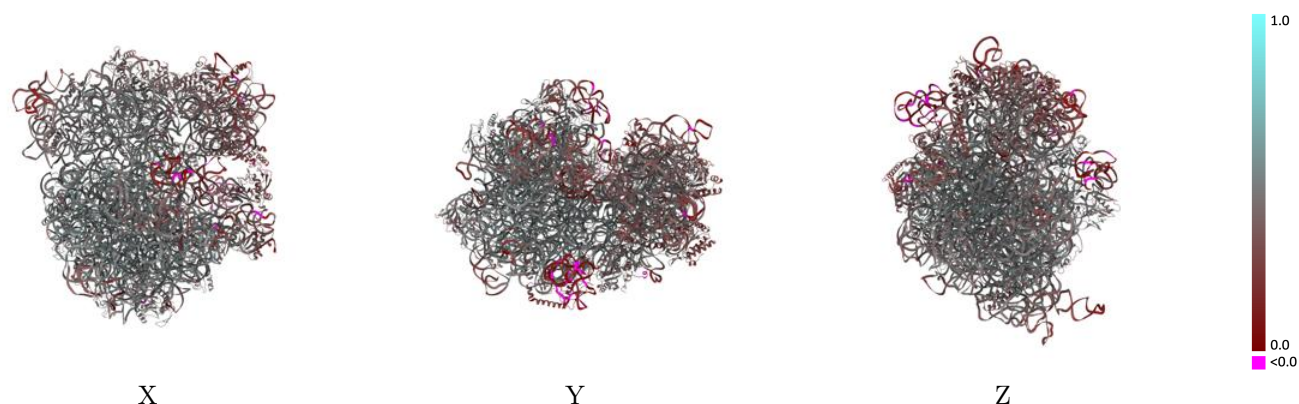
This section contains information regarding the fit between EMDB map EMD-20121 and PDB model 6OM6. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



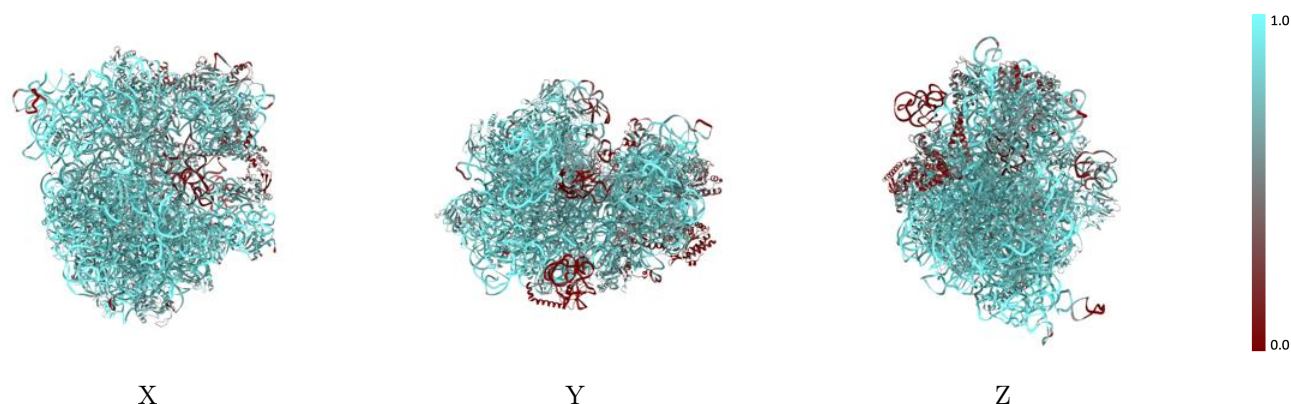
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



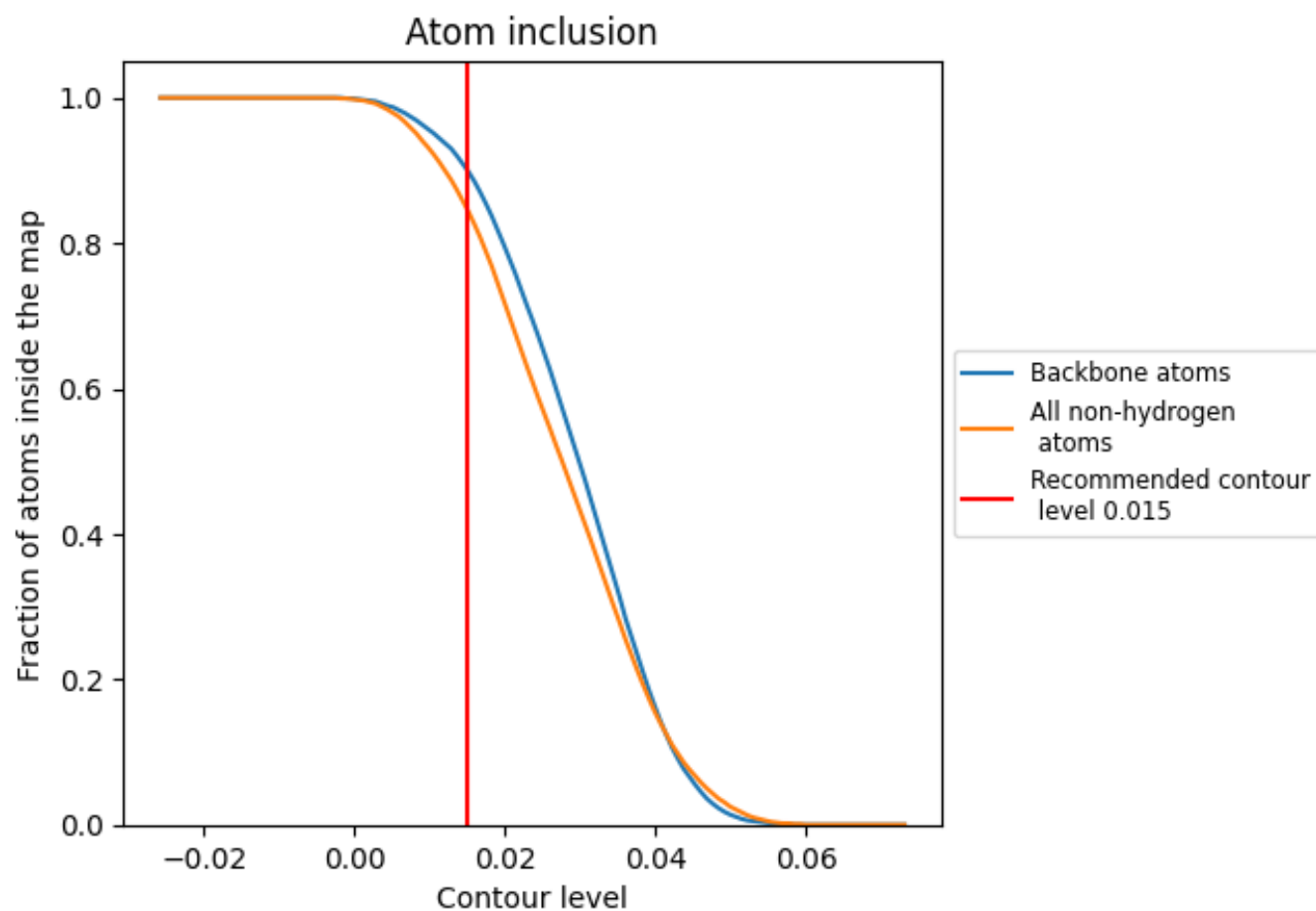
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.4400
1	 0.9250	 0.4580
2	 0.9340	 0.4320
3	 0.8930	 0.3130
4	 0.6360	 0.4200
5	 0.1700	 0.2800
B	 0.8590	 0.5210
C	 0.8440	 0.5120
D	 0.7550	 0.4720
E	 0.6070	 0.3490
F	 0.7090	 0.4190
G	 0.1130	 0.2760
J	 0.8320	 0.5060
K	 0.8020	 0.5000
L	 0.8160	 0.4880
M	 0.8410	 0.5030
N	 0.8810	 0.5150
O	 0.7680	 0.4150
P	 0.8010	 0.4920
Q	 0.8590	 0.4950
R	 0.7990	 0.4870
S	 0.8190	 0.5050
T	 0.7700	 0.4810
U	 0.7600	 0.4500
V	 0.7750	 0.4620
W	 0.7780	 0.4810
X	 0.8520	 0.4900
Y	 0.7420	 0.4340
Z	 0.8030	 0.4990
a	 0.0040	 0.2160
b	 0.8270	 0.5040
c	 0.6630	 0.4600
d	 0.8700	 0.5210
e	 0.8640	 0.5180
f	 0.8080	 0.4910



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.1780	 0.3300
h	 0.6130	 0.3990
i	 0.6670	 0.4080
j	 0.7640	 0.4470
k	 0.6540	 0.4050
l	 0.5700	 0.3460
m	 0.7630	 0.4520
n	 0.6080	 0.3470
o	 0.5020	 0.3450
p	 0.7570	 0.4410
q	 0.7420	 0.4560
r	 0.5910	 0.3380
s	 0.6460	 0.3620
t	 0.7740	 0.4330
u	 0.7540	 0.4600
v	 0.7310	 0.4330
w	 0.5850	 0.3720
x	 0.5750	 0.3220
y	 0.7480	 0.3990
z	 0.3000	 0.3490