



Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 12:39 PM EDT

PDB ID : 8CRX
EMDB ID : EMD-26959
Title : Cutibacterium acnes 70S ribosome with mRNA, P-site tRNA and Sarecycline bound
Authors : Lomakin, I.B.; Devarkar, S.C.; Bunick, C.G.
Deposited on : 2022-05-12
Resolution : 2.78 Å(reported)

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

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

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

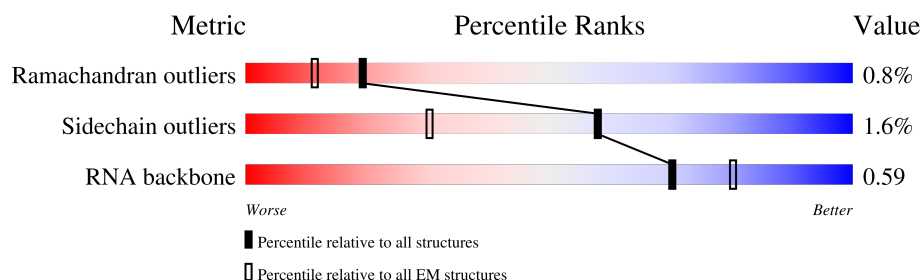
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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	A	1537	
2	D	201	
3	E	215	
4	F	96	
5	H	135	
6	K	135	
7	L	123	
8	O	87	

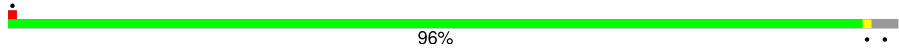
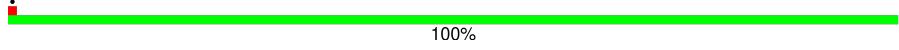
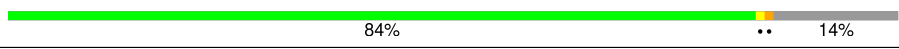
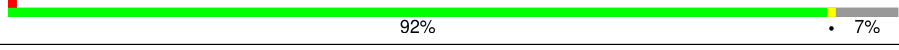



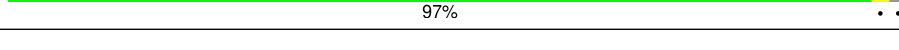
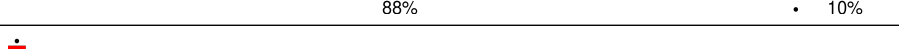
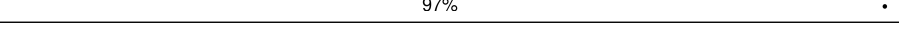
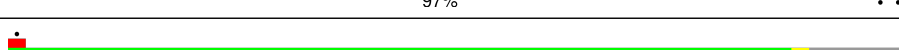
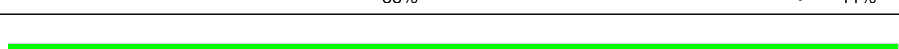


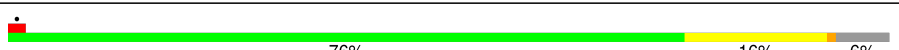




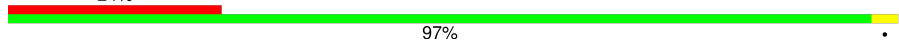

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	Q	90	
10	R	79	
11	T	88	
12	P	147	
13	X	33	
14	G	269	
15	I	156	
16	J	173	
17	M	103	
18	N	123	
19	S	61	
20	U	93	
21	B	283	
22	c	278	
23	d	223	
24	e	301	
25	f	210	
26	g	180	
27	i	147	
28	j	122	
29	k	146	
30	l	139	
31	m	187	
32	n	127	
33	o	117	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	p	123	
35	q	102	
36	r	153	
37	s	102	
38	t	122	
39	u	205	
40	v	89	
41	w	61	
42	x	77	
43	y	60	
44	z	63	
45	0	56	
46	1	44	
47	2	68	
48	4	69	
49	a	3086	
50	b	120	
51	V	24	
52	Y	22	
53	C	77	
54	3	37	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 144606 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 RNA (1537-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1505	Total	C	N	O	P	0	0
			32340	14408	5893	10534	1505		

- Molecule 2 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	200	Total	C	N	O	S	0	0
			1632	1021	313	297	1		

- Molecule 3 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	179	Total	C	N	O	S	0	0
			1309	816	244	245	4		

- Molecule 4 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	96	Total	C	N	O	S	0	0
			785	496	134	149	6		

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	134	Total	C	N	O	S	0	0
			1021	642	182	194	3		

- Molecule 6 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	117	Total	C	N	O	S	0	0
			858	532	168	154	4		

- Molecule 7 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	122	Total	C	N	O	S	0	0
			948	587	195	164	2		

- Molecule 8 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	87	Total	C	N	O	S	0	0
			708	440	140	125	3		

- Molecule 9 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	90	Total	C	N	O	S	0	0
			728	446	142	134	6		

- Molecule 10 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	67	Total	C	N	O	0	0
			527	334	103	90		

- Molecule 11 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	T	87	Total	C	N	O	0	0
			673	408	144	121		

- Molecule 12 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	128	Total	C	N	O	S	0	0
			994	621	185	187	1		

- Molecule 13 is a protein called 30S ribosomal protein bS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	X	32	Total	C	N	O	S	0	0
			277	170	71	35	1		

- Molecule 14 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	206	Total	C	N	O	S	0	0
			1613	1010	305	294	4		

- Molecule 15 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	155	Total	C	N	O	S	0	0
			1225	764	235	220	6		

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	134	Total	C	N	O	S	0	0
			1012	629	204	177	2		

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	98	Total	C	N	O	S	0	0
			786	496	146	141	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	122	Total	C	N	O		0	0
			976	598	205	173			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	60	Total	C	N	O	S	0	0
			474	298	98	73	5		

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	84	Total	C	N	O	S	0	0
			658	416	126	113	3		

- Molecule 21 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	233	Total	C	N	O	S	0	0
			1836	1163	326	338	9		

- Molecule 22 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	274	Total	C	N	O	S	0	0
			2091	1289	425	372	5		

- Molecule 23 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	214	Total	C	N	O	S	0	0
			1586	984	304	291	7		

- Molecule 24 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	210	Total	C	N	O	S	0	0
			1577	979	301	295	2		

- Molecule 25 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	184	Total	C	N	O	S	0	0
			1468	924	269	266	9		

- Molecule 26 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	177	Total	C	N	O	S	0	0
			1376	867	250	258	1		

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	146	Total	C	N	O	S	0	0
			1139	718	213	205	3		

- Molecule 28 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	122	Total	C	N	O	S	0	0
			946	596	177	169	4		

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	k	144	Total	C	N	O	S	0	0
			1072	675	196	199	2		

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	136	Total	C	N	O	S	0	0
			1082	685	210	181	6		

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	m	120	Total	C	N	O	S	0	0
			936	583	188	163	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	102	ILE	ASN	conflict	UNP A0A085AZY3

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	126	Total	C	N	O	S	0	0
			952	583	190	176	3		

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	114	Total	C	N	O	S	0	0
			896	559	174	162	1		

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	p	119	Total	C	N	O	S	0	0
			958	589	196	171	2		

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q	102	Total	C	N	O	S	0	0
			778	487	140	150	1		

- Molecule 36 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	r	132	Total	C	N	O	S	0	0
			1017	624	204	182	7		

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	95	Total	C	N	O	S	0	0
			751	474	138	138	1		

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	107	Total	C	N	O	S	0	0
			833	516	163	153	1		

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	179	Total	C	N	O	S	0	0
			1376	865	240	268	3		

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	v	78	Total	C	N	O	0	0
			591	355	127	109		

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	60	Total	C	N	O	S	0	0
			474	290	102	77	5		

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	x	69	Total	C	N	O		0	0
			564	348	108	108			

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	58	Total	C	N	O	S	0	0
			467	290	91	83	3		

- Molecule 44 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	62	Total	C	N	O	S	0	0
			477	287	102	83	5		

- Molecule 45 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	0	50	Total	C	N	O	S	0	0
			423	253	91	73	6		

- Molecule 46 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	44	Total	C	N	O	S	0	0
			362	213	91	56	2		

- Molecule 47 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	67	Total	C	N	O	S	0	0
			513	315	110	87	1		

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	66	Total	C	N	O	S	0	0
			512	313	97	97	5		

- Molecule 49 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	a	2903	Total	C	N	O	P	6	0
			62531	27850	11406	20366	2909		

- Molecule 50 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	b	120	Total	C	N	O	P	0	0
			2567	1145	466	836	120		

- Molecule 51 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	V	23	Total	C	N	O	0	0
			183	106	50	27		

- Molecule 52 is a RNA chain called 32MF mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Y	10	Total	C	N	O	P	0	0
			211	95	35	71	10		

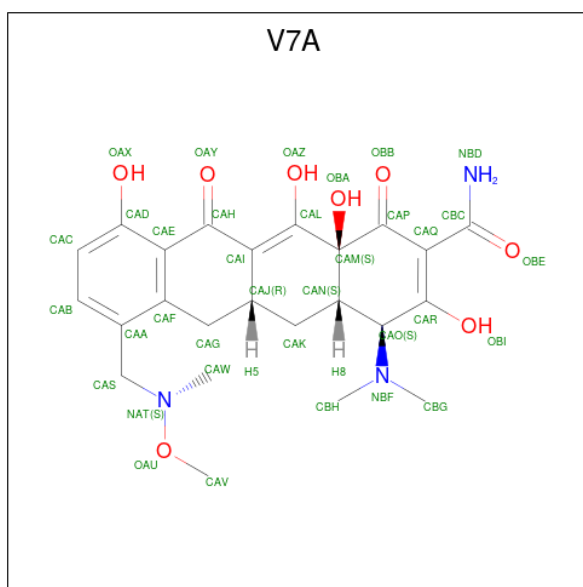
- Molecule 53 is a RNA chain called P-site initiator tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	C	76	Total	C	N	O	P	0	0
			1625	725	294	529	76	1	

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	37	Total	C	N	O	S	0	0
			302	184	66	47	5		

- Molecule 55 is Sarecycline (three-letter code: V7A) (formula: C₂₄H₂₉N₃O₈).



Mol	Chain	Residues	Atoms				AltConf
55	A	1	Total 35	C 24	N 3	O 8	0
55	a	1	Total 35	C 24	N 3	O 8	0

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

Mol	Chain	Residues	Atoms	AltConf
56	A	82	Total Mg 82 82	0
56	c	3	Total Mg 3 3	0
56	d	1	Total Mg 1 1	0
56	k	2	Total Mg 2 2	0
56	1	1	Total Mg 1 1	0
56	a	294	Total Mg 294 294	0
56	b	2	Total Mg 2 2	0
56	C	1	Total Mg 1 1	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	S	1	Total 1	Zn 1	0
57	w	1	Total 1	Zn 1	0
57	z	1	Total 1	Zn 1	0
57	0	1	Total 1	Zn 1	0
57	4	1	Total 1	Zn 1	0

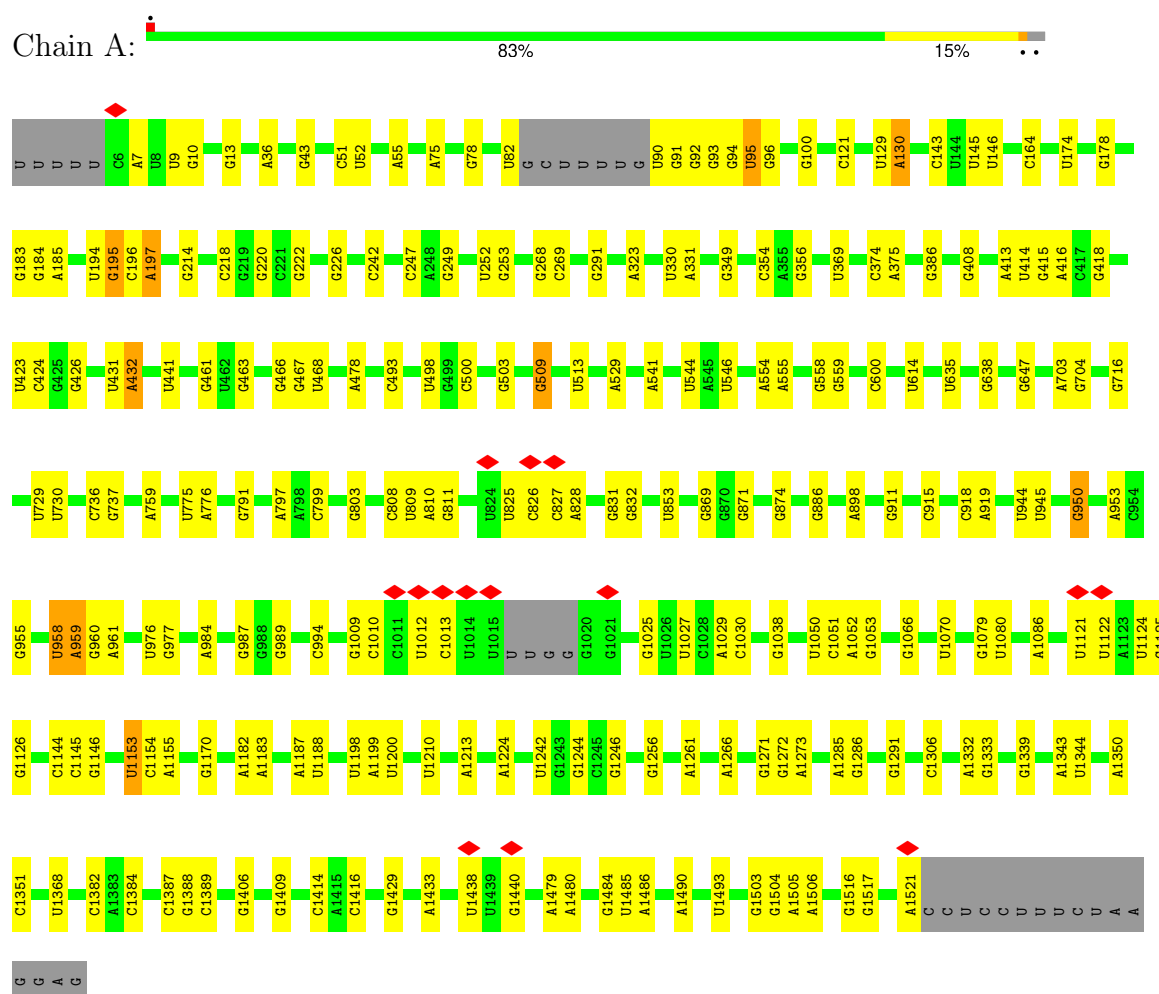
- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	A	1	Total 1	O 1	0
58	d	1	Total 1	O 1	0
58	s	1	Total 1	O 1	0
58	a	123	Total 123	O 123	0
58	b	3	Total 3	O 3	0

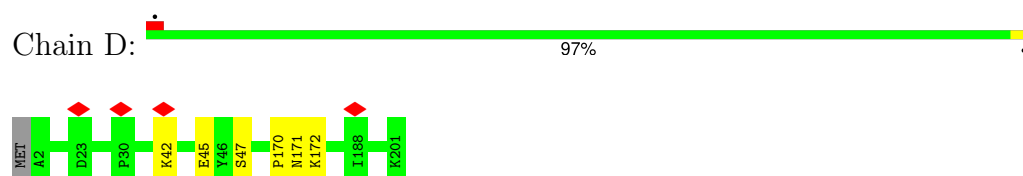
3 Residue-property plots

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: RNA (1537-MER)

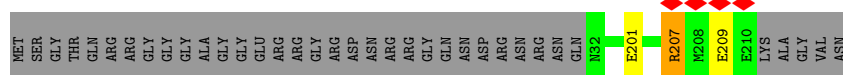


• Molecule 2: 30S ribosomal protein S4



- Molecule 3: 30S ribosomal protein S5

Chain E:  82% 17%



- Molecule 4: 30S ribosomal protein S6

Chain F:  99%




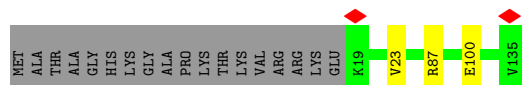
- Molecule 5: 30S ribosomal protein S8

Chain H:  98%



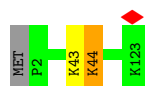
- Molecule 6: 30S ribosomal protein S11

Chain K:  84% 13%



- Molecule 7: 30S ribosomal protein S12

Chain L:  98%




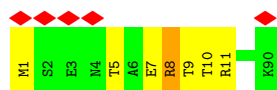
- Molecule 8: 30S ribosomal protein S15

Chain O:  99%

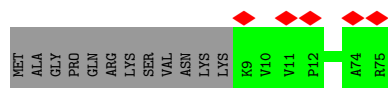
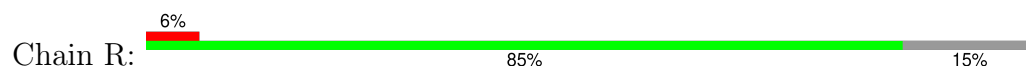


- Molecule 9: 30S ribosomal protein S17

Chain Q:  6% 92% 7%



- Molecule 10: 30S ribosomal protein S18



- Molecule 11: 30S ribosomal protein S20



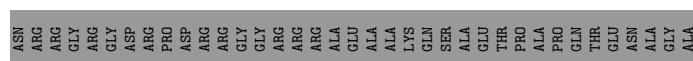
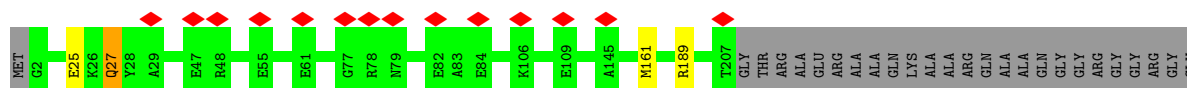
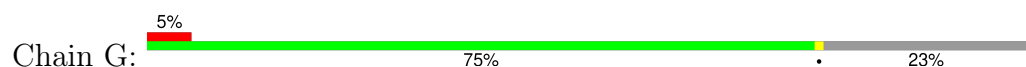
- Molecule 12: 30S ribosomal protein S16



- Molecule 13: 30S ribosomal protein bS22



- Molecule 14: 30S ribosomal protein S3

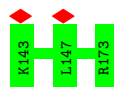
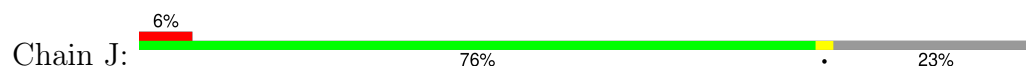


- Molecule 15: 30S ribosomal protein S7

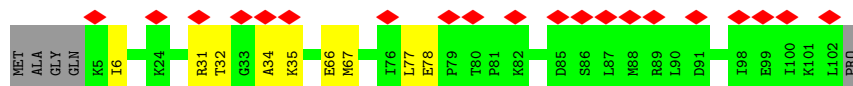
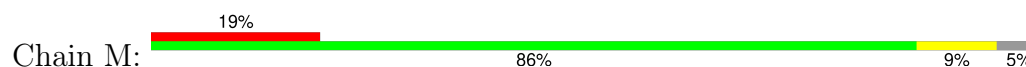




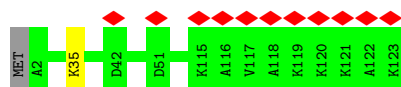
- Molecule 16: 30S ribosomal protein S9



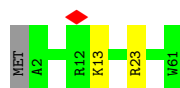
- Molecule 17: 30S ribosomal protein S10



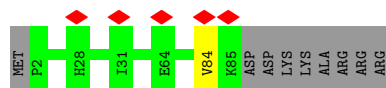
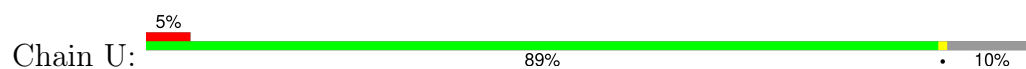
- Molecule 18: 30S ribosomal protein S13



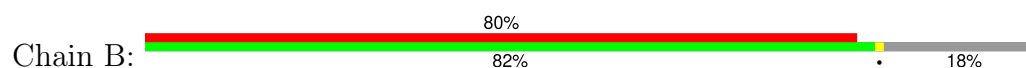
- Molecule 19: 30S ribosomal protein S14 type Z

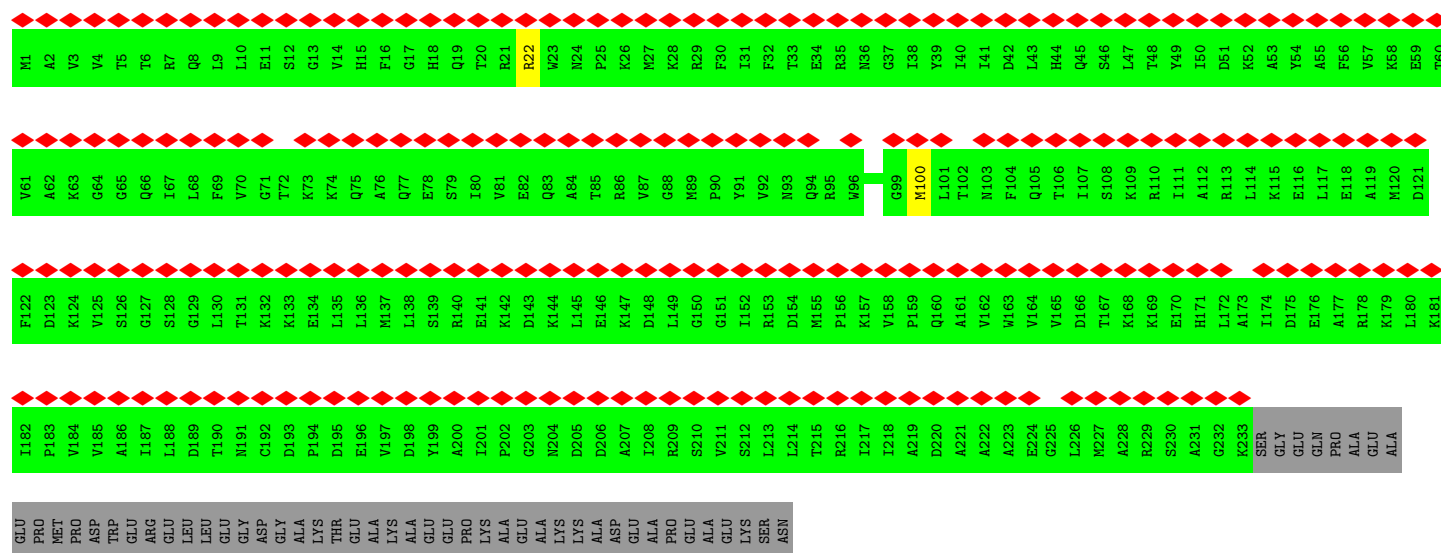


- Molecule 20: 30S ribosomal protein S19



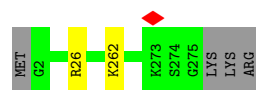
- Molecule 21: 30S ribosomal protein S2





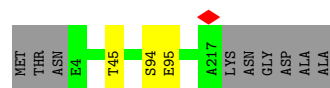
• Molecule 22: 50S ribosomal protein L2

Chain c:  98%



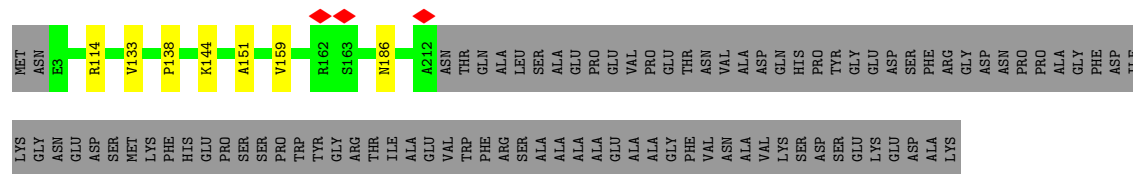
• Molecule 23: 50S ribosomal protein L3

Chain d:  95%




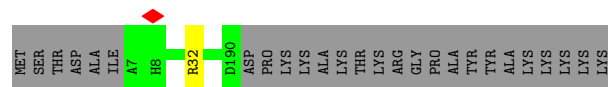
• Molecule 24: 50S ribosomal protein L4

Chain e:  67%



• Molecule 25: 50S ribosomal protein L5

Chain f:  87%



• Molecule 26: 50S ribosomal protein L6

Chain g:  93% 5%



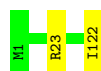
- Molecule 27: 50S ribosomal protein L13

Chain i:  99%



- Molecule 28: 50S ribosomal protein L14

Chain j:  98%

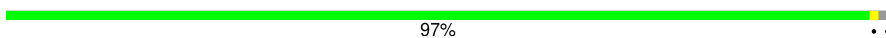


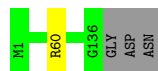
- Molecule 29: 50S ribosomal protein L15

Chain k:  98%



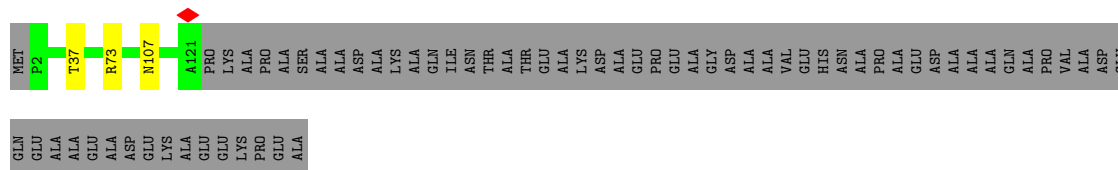
- Molecule 30: 50S ribosomal protein L16

Chain l:  97%



- Molecule 31: 50S ribosomal protein L17

Chain m:  63% 36%



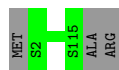
- Molecule 32: 50S ribosomal protein L18

Chain n:  98%



- Molecule 33: 50S ribosomal protein L19

Chain o: 97%



- Molecule 34: 50S ribosomal protein L20

Chain p: 96%



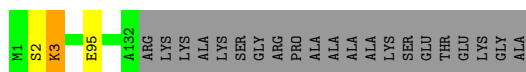
- Molecule 35: 50S ribosomal protein L21

Chain q: 100%



- Molecule 36: 50S ribosomal protein L22

Chain r: 84%



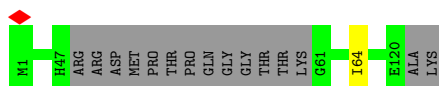
- Molecule 37: 50S ribosomal protein L23

Chain s: 92%

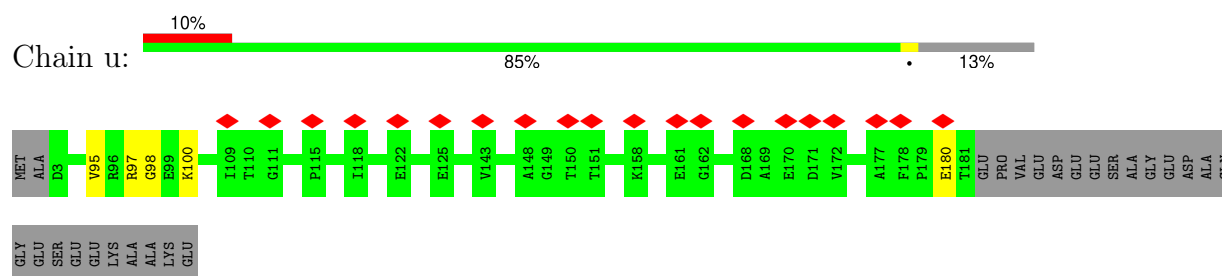


- Molecule 38: 50S ribosomal protein L24

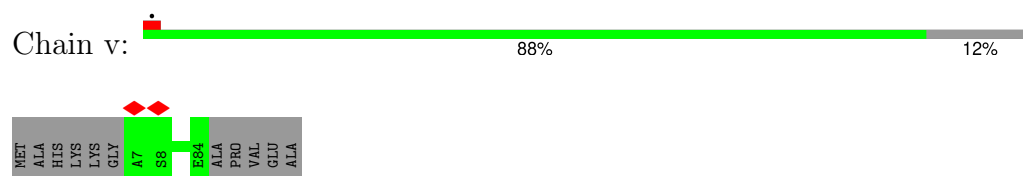
Chain t: 87%



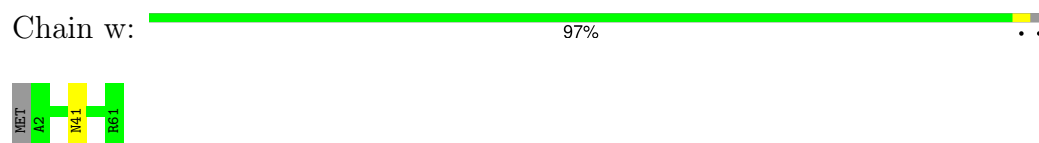
- Molecule 39: 50S ribosomal protein L25



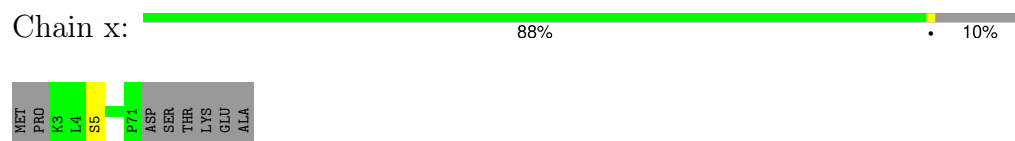
- Molecule 40: 50S ribosomal protein L27



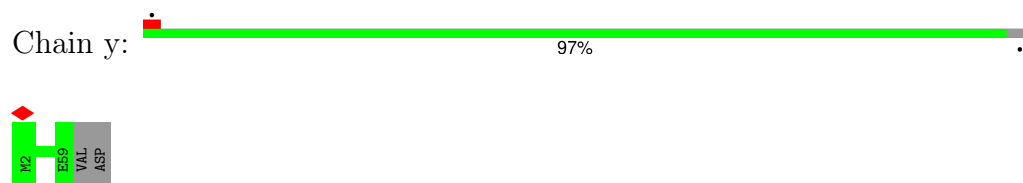
- Molecule 41: 50S ribosomal protein L28



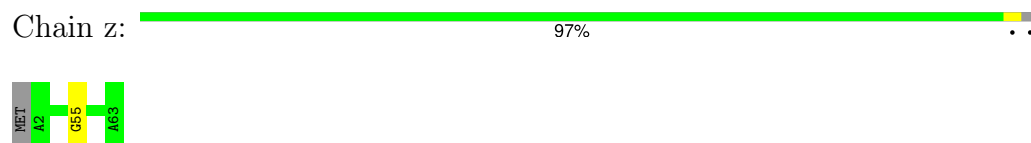
- Molecule 42: 50S ribosomal protein L29



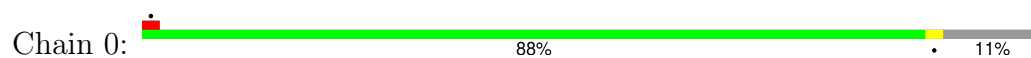
- Molecule 43: 50S ribosomal protein L30

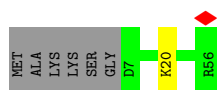


- Molecule 44: 50S ribosomal protein L32



- Molecule 45: 50S ribosomal protein L33





- Molecule 46: 50S ribosomal protein L34

Chain 1: 100%

There are no outlier residues recorded for this chain.

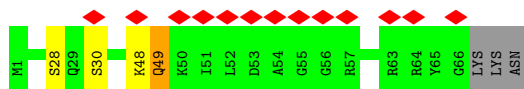
- Molecule 47: 50S ribosomal protein L35

Chain 2: 97%



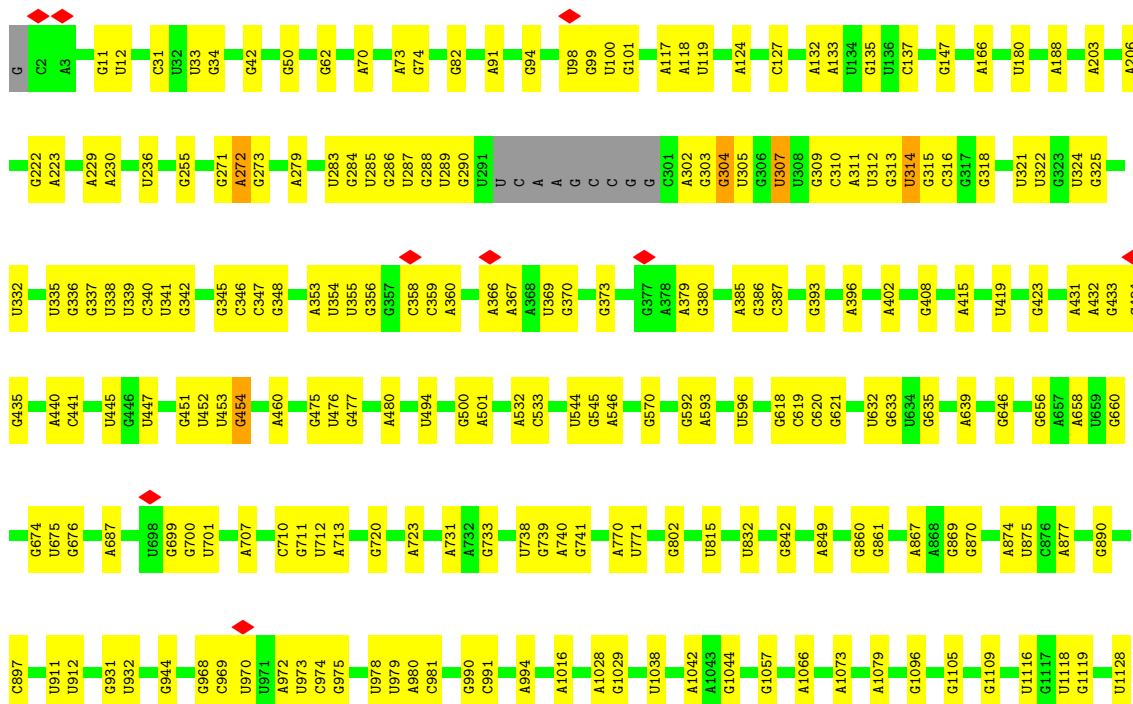
- Molecule 48: 50S ribosomal protein L31

Chain 4: 90%



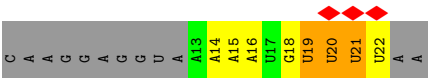
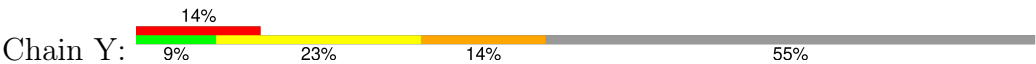
- Molecule 49: 23S ribosomal RNA

Chain a: 76%

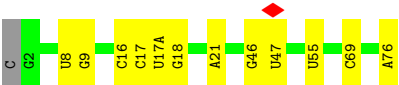
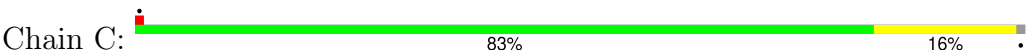




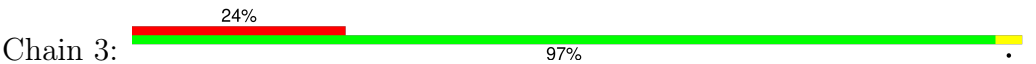
• Molecule 52: 32MF mRNA



• Molecule 53: P-site initiator tRNA



• Molecule 54: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.56	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.518	Depositor
Minimum map value	-0.551	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	363.12, 363.12, 363.12	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, OMC, V7A, MA6, PSU, H2U, 3TD, OMG, 5MC, 2MG, 4SU, ZN, 4OC, MG, G7M, 5MU, OMU, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	2/35898 (0.0%)	0.73	19/56012 (0.0%)
2	D	0.33	0/1662	0.57	0/2239
3	E	0.32	0/1325	0.58	0/1789
4	F	0.29	0/794	0.55	0/1069
5	H	0.31	0/1036	0.52	0/1395
6	K	0.30	0/874	0.59	0/1177
7	L	0.34	0/960	0.60	0/1283
8	O	0.27	0/718	0.56	0/959
9	Q	0.34	0/734	0.60	0/978
10	R	0.28	0/532	0.60	0/713
11	T	0.29	0/676	0.52	0/897
12	P	0.41	0/1013	0.66	0/1370
13	X	0.25	0/277	0.64	0/355
14	G	0.30	0/1638	0.58	0/2201
15	I	0.28	0/1246	0.56	0/1679
16	J	0.29	0/1027	0.61	0/1376
17	M	0.35	0/800	0.63	0/1080
18	N	0.28	0/985	0.63	0/1317
19	S	0.36	0/484	0.58	0/644
20	U	0.31	0/675	0.54	0/908
21	B	0.25	0/1864	0.52	0/2509
22	c	0.33	0/2132	0.59	0/2871
23	d	0.35	0/1611	0.58	0/2172
24	e	0.35	0/1600	0.62	0/2165
25	f	0.28	0/1493	0.56	0/2001
26	g	0.32	0/1398	0.56	0/1884
27	i	0.34	0/1164	0.50	0/1574
28	j	0.33	0/957	0.59	0/1282
29	k	0.35	0/1090	0.58	0/1465
30	l	0.32	0/1108	0.56	0/1488
31	m	0.32	0/949	0.58	0/1277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	n	0.27	0/959	0.59	0/1281
33	o	0.30	0/909	0.57	0/1216
34	p	0.31	0/969	0.53	0/1292
35	q	0.32	0/785	0.57	0/1050
36	r	0.34	0/1028	0.60	0/1379
37	s	0.31	0/759	0.57	0/1022
38	t	0.29	0/840	0.58	0/1123
39	u	0.29	0/1396	0.56	0/1896
40	v	0.33	0/598	0.61	0/800
41	w	0.31	0/483	0.58	0/648
42	x	0.29	0/567	0.57	0/759
43	y	0.29	0/471	0.58	0/627
44	z	0.33	0/487	0.52	0/654
45	0	0.34	0/429	0.63	0/569
46	1	0.29	0/365	0.67	0/478
47	2	0.30	0/519	0.58	0/682
48	4	0.36	0/521	0.64	0/700
49	a	0.50	1/69579 (0.0%)	0.78	93/108567 (0.1%)
50	b	0.40	0/2871	0.68	0/4475
51	V	0.28	0/184	0.66	0/236
52	Y	0.53	0/235	1.19	4/363 (1.1%)
53	C	0.20	0/1725	0.67	0/2689
54	3	0.25	0/305	0.56	0/401
All	All	0.44	3/155704 (0.0%)	0.72	116/233036 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	L	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1153	U	C1'-N1	5.86	1.57	1.48
1	A	1154	C	C1'-N1	5.83	1.57	1.48
49	a	445	U	C1'-N1	5.70	1.57	1.48

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	a	127	C	C5-C6-N1	15.97	128.99	121.00
49	a	127	C	C4-C5-C6	13.26	124.03	117.40
49	a	1349	U	P-O3'-C3'	-11.91	105.41	119.70
49	a	315	G	P-O3'-C3'	-11.90	105.42	119.70
49	a	2711	G	P-O3'-C3'	-11.60	105.78	119.70
49	a	2661	G	P-O3'-C3'	-11.46	105.95	119.70
49	a	2653	C	P-O3'-C3'	-11.26	106.19	119.70
49	a	2940	A	P-O3'-C3'	-11.06	106.43	119.70
49	a	660	G	P-O3'-C3'	-10.76	106.79	119.70
1	A	853	U	P-O3'-C3'	-10.51	107.09	119.70
49	a	2937	C	P-O3'-C3'	10.29	132.05	119.70
49	a	2052	G	P-O3'-C3'	-10.22	107.44	119.70
49	a	2249	C	P-O3'-C3'	-10.16	107.50	119.70
49	a	441	C	P-O3'-C3'	-10.00	107.70	119.70
49	a	314	U	P-O3'-C3'	-9.96	107.75	119.70
49	a	2652	G	P-O3'-C3'	-9.79	107.96	119.70
49	a	1189	G	P-O3'-C3'	-9.65	108.12	119.70
49	a	1118	U	P-O3'-C3'	-9.64	108.14	119.70
49	a	2657	C	P-O3'-C3'	-9.62	108.15	119.70
49	a	2051	U	P-O3'-C3'	-9.62	108.16	119.70
1	A	810	A	P-O3'-C3'	-9.51	108.29	119.70
49	a	2050	G	P-O3'-C3'	-9.50	108.30	119.70
1	A	432	A	P-O3'-C3'	-9.48	108.32	119.70
49	a	2939	A	P-O3'-C3'	-9.45	108.36	119.70
49	a	2654	G	P-O3'-C3'	-9.34	108.49	119.70
49	a	2719	U	P-O3'-C3'	-9.32	108.51	119.70
49	a	712	U	P-O3'-C3'	-9.27	108.58	119.70
49	a	2588	U	P-O3'-C3'	-9.26	108.59	119.70
52	Y	18	G	P-O3'-C3'	-9.17	108.70	119.70
49	a	2714	G	P-O3'-C3'	-9.10	108.78	119.70
52	Y	19	U	P-O3'-C3'	-9.07	108.81	119.70
49	a	990	G	P-O3'-C3'	-9.03	108.86	119.70
49	a	2053	U	P-O3'-C3'	-9.01	108.89	119.70
1	A	195	G	P-O3'-C3'	-8.98	108.92	119.70
49	a	2722	C	P-O3'-C3'	-8.96	108.95	119.70
49	a	2721	C	P-O3'-C3'	-8.92	108.99	119.70
49	a	911	U	P-O3'-C3'	-8.91	109.01	119.70
1	A	958	U	P-O3'-C3'	-8.80	109.13	119.70
49	a	127	C	C6-N1-C2	8.70	123.78	120.30
49	a	2710	U	P-O3'-C3'	-8.69	109.28	119.70
49	a	2887	A	P-O3'-C3'	-8.65	109.32	119.70
49	a	2662	C	P-O3'-C3'	-8.62	109.36	119.70
49	a	2655	C	P-O3'-C3'	-8.59	109.40	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	a	711	G	P-O3'-C3'	-8.46	109.55	119.70
49	a	2886	C	P-O3'-C3'	-8.33	109.71	119.70
49	a	2894	U	P-O3'-C3'	-8.30	109.74	119.70
49	a	304	G	P-O3'-C3'	-8.29	109.75	119.70
49	a	2153	A	P-O3'-C3'	-8.23	109.83	119.70
49	a	2525	U	P-O3'-C3'	-8.22	109.83	119.70
1	A	196	C	P-O3'-C3'	-8.19	109.87	119.70
49	a	2055	U	P-O3'-C3'	-8.19	109.88	119.70
1	A	1343	A	P-O3'-C3'	-8.18	109.89	119.70
1	A	129	U	P-O3'-C3'	-8.12	109.95	119.70
49	a	2717	G	P-O3'-C3'	-8.10	109.98	119.70
49	a	1637	G	P-O3'-C3'	-8.10	109.98	119.70
49	a	1832	C	P-O3'-C3'	-8.07	110.02	119.70
49	a	2651	A	P-O3'-C3'	-8.05	110.04	119.70
49	a	2658	A	P-O3'-C3'	-8.02	110.08	119.70
52	Y	20	U	P-O3'-C3'	-7.99	110.11	119.70
1	A	959	A	P-O3'-C3'	-7.99	110.11	119.70
49	a	2054	A	P-O3'-C3'	-7.88	110.24	119.70
49	a	2720	C	P-O3'-C3'	-7.86	110.26	119.70
49	a	303	G	P-O3'-C3'	-7.85	110.28	119.70
49	a	2056	G	P-O3'-C3'	-7.82	110.31	119.70
49	a	454	G	P-O3'-C3'	-7.78	110.36	119.70
49	a	1914	C	C2-N1-C1'	7.76	127.34	118.80
49	a	2718	G	P-O3'-C3'	-7.72	110.43	119.70
1	A	809	U	P-O3'-C3'	-7.64	110.53	119.70
49	a	2961	U	O4'-C1'-N1	7.55	114.24	108.20
49	a	272	A	P-O3'-C3'	-7.46	110.75	119.70
49	a	2587	U	P-O3'-C3'	-7.46	110.75	119.70
52	Y	21	U	P-O3'-C3'	-7.36	110.87	119.70
49	a	2712	G	P-O3'-C3'	-7.35	110.89	119.70
49	a	2250	G	P-O3'-C3'	-7.22	111.04	119.70
49	a	1348	G	P-O3'-C3'	-7.20	111.06	119.70
49	a	2612	A	P-O3'-C3'	-7.19	111.07	119.70
49	a	1914	C	N1-C2-O2	7.17	123.20	118.90
49	a	2049	A	P-O3'-C3'	-7.04	111.25	119.70
1	A	1344	U	P-O3'-C3'	-6.88	111.44	119.70
49	a	2961	U	N1-C1'-C2'	6.80	122.83	114.00
49	a	1638	U	P-O3'-C3'	-6.79	111.55	119.70
49	a	1389	U	C2-N1-C1'	6.72	125.76	117.70
49	a	1833	G	P-O3'-C3'	-6.69	111.67	119.70
49	a	452	U	P-O3'-C3'	-6.57	111.82	119.70
49	a	272	A	C1'-O4'-C4'	-6.55	104.66	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	a	738	U	P-O3'-C3'	-6.52	111.87	119.70
49	a	302	A	P-O3'-C3'	-6.39	112.03	119.70
49	a	271	G	C3'-C2'-C1'	-6.38	96.39	101.50
49	a	932	U	C2-N1-C1'	6.38	125.35	117.70
49	a	1730	U	C1'-O4'-C4'	6.05	114.74	109.90
49	a	307	U	C2-N1-C1'	5.92	124.80	117.70
49	a	2715	U	P-O3'-C3'	-5.88	112.64	119.70
1	A	736	C	C2-N1-C1'	5.82	125.20	118.80
1	A	197	A	P-O3'-C3'	-5.72	112.83	119.70
1	A	1144	C	C2-N1-C1'	5.72	125.09	118.80
49	a	2611	G	P-O3'-C3'	-5.71	112.84	119.70
49	a	1914	C	C6-N1-C1'	-5.69	113.97	120.80
1	A	130	A	P-O3'-C3'	-5.67	112.89	119.70
49	a	271	G	C2'-C3'-O3'	5.67	122.76	113.70
1	A	96	G	P-O3'-C3'	-5.61	112.97	119.70
49	a	2709	C	P-O3'-C3'	-5.60	112.98	119.70
49	a	2708	G	P-O3'-C3'	-5.56	113.03	119.70
49	a	2248	C	P-O3'-C3'	-5.50	113.10	119.70
49	a	2659	U	P-O3'-C3'	-5.48	113.13	119.70
49	a	451	G	P-O3'-C3'	-5.41	113.21	119.70
49	a	710	C	P-O3'-C3'	-5.38	113.24	119.70
49	a	932	U	N1-C2-O2	5.36	126.55	122.80
49	a	1914	C	N3-C2-O2	-5.27	118.21	121.90
49	a	2716	C	P-O3'-C3'	-5.23	113.42	119.70
49	a	271	G	C4'-C3'-C2'	-5.22	97.38	102.60
1	A	95	U	P-O3'-C3'	-5.22	113.44	119.70
49	a	2503	G	C4-N9-C1'	5.21	133.28	126.50
49	a	440	A	P-O3'-C3'	-5.16	113.50	119.70
49	a	2660	A	P-O3'-C3'	-5.13	113.55	119.70
1	A	194	U	P-O3'-C3'	-5.07	113.62	119.70
1	A	808	C	P-O3'-C3'	-5.02	113.68	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	L	44	LYS	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	198/201 (98%)	187 (94%)	10 (5%)	1 (0%)	25	52
3	E	177/215 (82%)	166 (94%)	10 (6%)	1 (1%)	22	48
4	F	94/96 (98%)	91 (97%)	2 (2%)	1 (1%)	12	33
5	H	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
6	K	115/135 (85%)	99 (86%)	15 (13%)	1 (1%)	14	38
7	L	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
8	O	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
9	Q	88/90 (98%)	79 (90%)	5 (6%)	4 (4%)	2	6
10	R	65/79 (82%)	58 (89%)	7 (11%)	0	100	100
11	T	85/88 (97%)	85 (100%)	0	0	100	100
12	P	126/147 (86%)	111 (88%)	9 (7%)	6 (5%)	2	5
13	X	30/33 (91%)	29 (97%)	0	1 (3%)	3	10
14	G	204/269 (76%)	196 (96%)	7 (3%)	1 (0%)	25	52
15	I	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
16	J	132/173 (76%)	114 (86%)	17 (13%)	1 (1%)	16	41
17	M	96/103 (93%)	91 (95%)	3 (3%)	2 (2%)	5	18
18	N	120/123 (98%)	110 (92%)	10 (8%)	0	100	100
19	S	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	23
20	U	82/93 (88%)	77 (94%)	4 (5%)	1 (1%)	11	31
21	B	231/283 (82%)	214 (93%)	16 (7%)	1 (0%)	30	58
22	c	272/278 (98%)	254 (93%)	16 (6%)	2 (1%)	19	45
23	d	212/223 (95%)	198 (93%)	13 (6%)	1 (0%)	25	52
24	e	208/301 (69%)	184 (88%)	19 (9%)	5 (2%)	5	15
25	f	182/210 (87%)	167 (92%)	15 (8%)	0	100	100
26	g	175/180 (97%)	162 (93%)	12 (7%)	1 (1%)	22	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	i	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
28	j	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
29	k	142/146 (97%)	120 (84%)	22 (16%)	0	100	100
30	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
31	m	118/187 (63%)	112 (95%)	5 (4%)	1 (1%)	16	41
32	n	124/127 (98%)	120 (97%)	3 (2%)	1 (1%)	16	41
33	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
34	p	117/123 (95%)	109 (93%)	7 (6%)	1 (1%)	14	38
35	q	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
36	r	130/153 (85%)	123 (95%)	6 (5%)	1 (1%)	16	41
37	s	93/102 (91%)	87 (94%)	5 (5%)	1 (1%)	12	33
38	t	103/122 (84%)	99 (96%)	3 (3%)	1 (1%)	13	36
39	u	177/205 (86%)	168 (95%)	7 (4%)	2 (1%)	12	33
40	v	76/89 (85%)	73 (96%)	3 (4%)	0	100	100
41	w	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	23
42	x	67/77 (87%)	62 (92%)	4 (6%)	1 (2%)	8	25
43	y	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
44	z	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	7	23
45	0	48/56 (86%)	42 (88%)	6 (12%)	0	100	100
46	1	42/44 (96%)	42 (100%)	0	0	100	100
47	2	65/68 (96%)	65 (100%)	0	0	100	100
48	4	64/69 (93%)	51 (80%)	10 (16%)	3 (5%)	2	5
51	V	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
54	3	35/37 (95%)	35 (100%)	0	0	100	100
All	All	5646/6322 (89%)	5277 (94%)	324 (6%)	45 (1%)	19	41

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	17	ARG
12	P	46	PRO
12	P	47	SER
13	X	4	VAL
14	G	27	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	J	46	ALA
22	c	26	ARG
24	e	151	ALA
24	e	159	VAL
24	e	186	ASN
34	p	93	LYS
48	4	30	SER
9	Q	10	THR
12	P	97	GLU
12	P	112	ALA
12	P	113	ASP
17	M	34	ALA
24	e	133	VAL
32	n	5	LEU
36	r	3	LYS
39	u	97	ARG
41	w	41	ASN
9	Q	5	THR
9	Q	9	THR
19	S	23	ARG
20	U	84	VAL
48	4	28	SER
37	s	93	ARG
48	4	49	GLN
3	E	207	ARG
17	M	6	ILE
22	c	262	LYS
24	e	138	PRO
31	m	37	THR
9	Q	8	ARG
21	B	100	MET
23	d	95	GLU
38	t	64	ILE
39	u	98	GLY
42	x	5	SER
12	P	115	ALA
44	z	55	GLY
2	D	170	PRO
6	K	23	VAL
26	g	161	GLY

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	
2	D	175/176 (99%)	170 (97%)	5 (3%)	37	68
3	E	130/155 (84%)	127 (98%)	3 (2%)	45	75
4	F	89/89 (100%)	88 (99%)	1 (1%)	70	88
5	H	108/109 (99%)	106 (98%)	2 (2%)	52	79
6	K	88/101 (87%)	86 (98%)	2 (2%)	45	75
7	L	103/104 (99%)	101 (98%)	2 (2%)	52	79
8	O	74/74 (100%)	73 (99%)	1 (1%)	62	85
9	Q	81/81 (100%)	77 (95%)	4 (5%)	21	49
10	R	55/65 (85%)	55 (100%)	0	100	100
11	T	68/69 (99%)	68 (100%)	0	100	100
12	P	103/115 (90%)	93 (90%)	10 (10%)	6	19
13	X	28/29 (97%)	27 (96%)	1 (4%)	30	61
14	G	160/200 (80%)	156 (98%)	4 (2%)	42	73
15	I	132/133 (99%)	132 (100%)	0	100	100
16	J	97/131 (74%)	95 (98%)	2 (2%)	48	77
17	M	89/93 (96%)	82 (92%)	7 (8%)	10	28
18	N	99/100 (99%)	98 (99%)	1 (1%)	73	89
19	S	48/49 (98%)	47 (98%)	1 (2%)	48	77
20	U	72/80 (90%)	72 (100%)	0	100	100
21	B	197/234 (84%)	196 (100%)	1 (0%)	86	95
22	c	216/220 (98%)	216 (100%)	0	100	100
23	d	166/172 (96%)	164 (99%)	2 (1%)	67	87
24	e	165/237 (70%)	163 (99%)	2 (1%)	67	87
25	f	154/175 (88%)	153 (99%)	1 (1%)	84	94
26	g	150/152 (99%)	142 (95%)	8 (5%)	19	46
27	i	118/120 (98%)	118 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	j	101/101 (100%)	99 (98%)	2 (2%)	50	78
29	k	111/113 (98%)	110 (99%)	1 (1%)	75	91
30	l	108/110 (98%)	107 (99%)	1 (1%)	75	91
31	m	100/142 (70%)	98 (98%)	2 (2%)	50	78
32	n	95/96 (99%)	95 (100%)	0	100	100
33	o	97/99 (98%)	97 (100%)	0	100	100
34	p	98/99 (99%)	98 (100%)	0	100	100
35	q	84/84 (100%)	84 (100%)	0	100	100
36	r	105/118 (89%)	102 (97%)	3 (3%)	37	68
37	s	84/89 (94%)	84 (100%)	0	100	100
38	t	91/103 (88%)	91 (100%)	0	100	100
39	u	149/168 (89%)	146 (98%)	3 (2%)	50	78
40	v	60/67 (90%)	60 (100%)	0	100	100
41	w	52/53 (98%)	52 (100%)	0	100	100
42	x	61/68 (90%)	61 (100%)	0	100	100
43	y	53/55 (96%)	53 (100%)	0	100	100
44	z	51/52 (98%)	51 (100%)	0	100	100
45	0	47/51 (92%)	46 (98%)	1 (2%)	48	77
46	1	36/36 (100%)	36 (100%)	0	100	100
47	2	54/55 (98%)	53 (98%)	1 (2%)	52	79
48	4	56/59 (95%)	54 (96%)	2 (4%)	30	61
51	V	16/17 (94%)	16 (100%)	0	100	100
54	3	35/35 (100%)	34 (97%)	1 (3%)	37	68
All	All	4709/5133 (92%)	4632 (98%)	77 (2%)	58	83

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	42	LYS
2	D	45	GLU
2	D	47	SER
2	D	171	ASN
2	D	172	LYS
3	E	201	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	207	ARG
3	E	209	GLU
4	F	17	ARG
5	H	55	LYS
5	H	120	GLN
6	K	87	ARG
6	K	100	GLU
7	L	43	LYS
7	L	44	LYS
8	O	86	ARG
9	Q	1	MET
9	Q	7	GLU
9	Q	8	ARG
9	Q	11	ARG
12	P	26	ARG
12	P	111	GLU
12	P	113	ASP
12	P	114	GLU
12	P	117	ARG
12	P	118	GLU
12	P	120	ILE
12	P	122	LYS
12	P	123	LYS
12	P	125	GLU
13	X	22	LYS
14	G	25	GLU
14	G	27	GLN
14	G	161	MET
14	G	189	ARG
16	J	44	MET
16	J	54	ARG
17	M	31	ARG
17	M	32	THR
17	M	35	LYS
17	M	66	GLU
17	M	67	MET
17	M	77	LEU
17	M	78	GLU
18	N	35	LYS
19	S	13	LYS
21	B	22	ARG
23	d	45	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	d	94	SER
24	e	114	ARG
24	e	144	LYS
25	f	32	ARG
26	g	54	GLU
26	g	155	LYS
26	g	157	GLU
26	g	160	LYS
26	g	173	ARG
26	g	174	LYS
26	g	175	VAL
26	g	177	LYS
28	j	23	ARG
28	j	122	ILE
29	k	27	SER
30	l	60	ARG
31	m	73	ARG
31	m	107	ASN
36	r	2	SER
36	r	3	LYS
36	r	95	GLU
39	u	95	VAL
39	u	100	LYS
39	u	180	GLU
45	0	20	LYS
47	2	68	ARG
48	4	48	LYS
48	4	49	GLN
54	3	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	178	HIS
3	E	161	HIS
6	K	124	HIS
14	G	27	GLN
15	I	40	GLN
18	N	52	GLN
20	U	23	ASN
21	B	24	ASN
21	B	94	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	B	103	ASN
21	B	105	GLN
23	d	55	GLN
24	e	142	GLN
29	k	75	GLN
36	r	56	GLN
39	u	58	ASN
45	0	29	ASN
45	0	32	ASN
48	4	20	ASN
48	4	29	GLN
48	4	49	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1500/1537 (97%)	203 (13%)	16 (1%)
49	a	2885/3086 (93%)	483 (16%)	0
50	b	118/120 (98%)	11 (9%)	0
52	Y	9/22 (40%)	7 (77%)	0
53	C	75/77 (97%)	10 (13%)	1 (1%)
All	All	4587/4842 (94%)	714 (15%)	17 (0%)

All (714) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	9	U
1	A	10	G
1	A	13	G
1	A	36	A
1	A	43	G
1	A	51	C
1	A	52	U
1	A	55	A
1	A	75	A
1	A	78	G
1	A	82	U
1	A	91	G
1	A	92	G
1	A	93	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	95	U
1	A	100	G
1	A	121	C
1	A	130	A
1	A	143	C
1	A	145	U
1	A	164	C
1	A	174	U
1	A	178	G
1	A	183	G
1	A	184	G
1	A	185	A
1	A	195	G
1	A	197	A
1	A	214	G
1	A	218	C
1	A	220	G
1	A	222	G
1	A	226	G
1	A	242	C
1	A	247	C
1	A	249	G
1	A	252	U
1	A	253	G
1	A	268	G
1	A	269	C
1	A	291	G
1	A	323	A
1	A	330	U
1	A	331	A
1	A	349	G
1	A	354	C
1	A	356	G
1	A	369	U
1	A	374	C
1	A	375	A
1	A	386	G
1	A	408	G
1	A	413	A
1	A	414	U
1	A	415	G
1	A	416	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	423	U
1	A	424	C
1	A	426	G
1	A	431	U
1	A	432	A
1	A	441	U
1	A	461	G
1	A	463	G
1	A	467	G
1	A	468	U
1	A	478	A
1	A	493	C
1	A	500	C
1	A	503	G
1	A	509	G7M
1	A	513	U
1	A	529	A
1	A	541	A
1	A	544	U
1	A	546	U
1	A	554	A
1	A	555	A
1	A	558	G
1	A	559	G
1	A	600	C
1	A	614	U
1	A	635	U
1	A	647	G
1	A	703	A
1	A	704	G
1	A	716	G
1	A	729	U
1	A	730	U
1	A	737	G
1	A	759	A
1	A	775	U
1	A	776	A
1	A	791	G
1	A	797	A
1	A	799	C
1	A	803	G
1	A	811	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	825	U
1	A	826	C
1	A	827	C
1	A	828	A
1	A	831	G
1	A	832	G
1	A	871	G
1	A	874	G
1	A	886	G
1	A	898	A
1	A	911	G
1	A	915	C
1	A	918	C
1	A	919	A
1	A	944	U
1	A	945	U
1	A	950	2MG
1	A	953	A
1	A	955	G
1	A	958	U
1	A	959	A
1	A	960	G
1	A	961	A
1	A	976	U
1	A	977	G
1	A	984	A
1	A	987	G
1	A	989	G
1	A	994	C
1	A	1009	G
1	A	1010	C
1	A	1012	U
1	A	1013	C
1	A	1025	G
1	A	1027	U
1	A	1029	A
1	A	1030	C
1	A	1038	G
1	A	1050	U
1	A	1051	C
1	A	1053	G
1	A	1066	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1070	U
1	A	1079	G
1	A	1080	U
1	A	1086	A
1	A	1121	U
1	A	1122	U
1	A	1124	U
1	A	1125	G
1	A	1126	G
1	A	1145	C
1	A	1146	G
1	A	1153	U
1	A	1155	A
1	A	1170	G
1	A	1182	A
1	A	1183	A
1	A	1188	U
1	A	1198	U
1	A	1199	A
1	A	1200	U
1	A	1210	U
1	A	1213	A
1	A	1224	A
1	A	1242	U
1	A	1244	G
1	A	1246	G
1	A	1256	G
1	A	1261	A
1	A	1266	A
1	A	1272	G
1	A	1273	A
1	A	1285	A
1	A	1286	G
1	A	1291	G
1	A	1306	C
1	A	1332	A
1	A	1333	G
1	A	1339	G
1	A	1351	C
1	A	1368	U
1	A	1382	C
1	A	1384	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1387	5MC
1	A	1388	G
1	A	1406	G
1	A	1409	G
1	A	1414	C
1	A	1416	C
1	A	1429	G
1	A	1433	A
1	A	1438	U
1	A	1440	G
1	A	1479	A
1	A	1480	A
1	A	1484	G
1	A	1486	A
1	A	1490	A
1	A	1493	U
1	A	1504	G
1	A	1516	G
1	A	1517	G
1	A	1521	A
49	a	11	G
49	a	12	U
49	a	31	C
49	a	33	U
49	a	34	G
49	a	42	G
49	a	50	G
49	a	62	G
49	a	70	A
49	a	73	A
49	a	74	G
49	a	82	G
49	a	91	A
49	a	94	G
49	a	98	U
49	a	99	G
49	a	100	U
49	a	101	G
49	a	117	A
49	a	118	A
49	a	119	U
49	a	124	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	132	A
49	a	133	A
49	a	135	G
49	a	137	C
49	a	147	G
49	a	166	A
49	a	180	U
49	a	188	A
49	a	203	A
49	a	206	A
49	a	222	G
49	a	223	A
49	a	229	A
49	a	230	A
49	a	236	U
49	a	255	G
49	a	272	A
49	a	273	G
49	a	279	A
49	a	283	U
49	a	284	G
49	a	285	U
49	a	286	G
49	a	287	U
49	a	288	G
49	a	289	U
49	a	290	G
49	a	304	G
49	a	305	U
49	a	307	U
49	a	309	G
49	a	310	C
49	a	311	A
49	a	312	U
49	a	313	G
49	a	314	U
49	a	316	C
49	a	318	G
49	a	321	U
49	a	322	U
49	a	324	U
49	a	325	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	332	U
49	a	335	U
49	a	336	G
49	a	337	G
49	a	338	U
49	a	339	U
49	a	340	C
49	a	341	U
49	a	342	G
49	a	345	G
49	a	346	C
49	a	347	C
49	a	348	G
49	a	353	A
49	a	354	U
49	a	355	U
49	a	356	G
49	a	358	C
49	a	359	C
49	a	360	A
49	a	366	A
49	a	367	A
49	a	369	U
49	a	370	G
49	a	373	G
49	a	379	A
49	a	380	G
49	a	385	A
49	a	386	G
49	a	387	C
49	a	393	G
49	a	396	A
49	a	402	A
49	a	408	G
49	a	415	A
49	a	419	U
49	a	423	G
49	a	431	A
49	a	432	A
49	a	433	G
49	a	434	C
49	a	435	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	447	U
49	a	453	U
49	a	454	G
49	a	460	A
49	a	475	G
49	a	476	U
49	a	477	G
49	a	480	A
49	a	494	U
49	a	500	G
49	a	501	A
49	a	532	A
49	a	533	C
49	a	544	U
49	a	545	G
49	a	546	A
49	a	570	G
49	a	592	G
49	a	593	A
49	a	596	U
49	a	618	G
49	a	619	C
49	a	620	C
49	a	621	G
49	a	632	U
49	a	633	G
49	a	635	G
49	a	639	A
49	a	646	G
49	a	656	G
49	a	658	A
49	a	674	G
49	a	675	U
49	a	676	G
49	a	687	A
49	a	699	G
49	a	700	G
49	a	701	U
49	a	707	A
49	a	713	A
49	a	720	G
49	a	723	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	731	A
49	a	733	G
49	a	739	G
49	a	740	A
49	a	741	G
49	a	770	A
49	a	771	U
49	a	802	G
49	a	815	U
49	a	832	U
49	a	842	G
49	a	849	A
49	a	860	G
49	a	861	G
49	a	867	A
49	a	869	G
49	a	870	G
49	a	874	A
49	a	875	U
49	a	877	A
49	a	890	G
49	a	897	C
49	a	912	U
49	a	931	G
49	a	944	G
49	a	968	G
49	a	969	C
49	a	970	U
49	a	972	A
49	a	973	U
49	a	974	C
49	a	975	G
49	a	978	U
49	a	979	U
49	a	980	A
49	a	981	C
49	a	991	C
49	a	994	A
49	a	1016	A
49	a	1028	A
49	a	1029	G
49	a	1042	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	1044	G
49	a	1057	G
49	a	1066	A
49	a	1073	A
49	a	1079	A
49	a	1096	G
49	a	1105	G
49	a	1109	G
49	a	1116	U
49	a	1119	G
49	a	1128	U
49	a	1129	A
49	a	1130	G
49	a	1141	G
49	a	1142	G
49	a	1144	U
49	a	1145	G
49	a	1149	U
49	a	1150	G
49	a	1151	G
49	a	1152	A
49	a	1153	A
49	a	1154	G
49	a	1156	A
49	a	1157	G
49	a	1161	U
49	a	1165	U
49	a	1172	G
49	a	1173	U
49	a	1177	U
49	a	1178	A
49	a	1179	A
49	a	1181	A
49	a	1189	G
49	a	1190	G
49	a	1193	A
49	a	1195	G
49	a	1196	U
49	a	1215	U
49	a	1216	A
49	a	1218	C
49	a	1225	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	1226	A
49	a	1227	A
49	a	1254	G
49	a	1255	U
49	a	1256	G
49	a	1257	U
49	a	1283	G
49	a	1297	G
49	a	1306	U
49	a	1307	G
49	a	1327	G
49	a	1330	A
49	a	1333	G
49	a	1348	G
49	a	1350	G
49	a	1351	U
49	a	1365	C
49	a	1376	A
49	a	1377	U
49	a	1390	C
49	a	1428	U
49	a	1441	A
49	a	1455	U
49	a	1460	A
49	a	1471	A
49	a	1472	U
49	a	1595	A
49	a	1601	G
49	a	1607	A
49	a	1608	C
49	a	1625	U
49	a	1626	C
49	a	1630	G
49	a	1633	G
49	a	1637	G
49	a	1639	U
49	a	1641	U
49	a	1642	C
49	a	1648	C
49	a	1663	G
49	a	1673	U
49	a	1674	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	1677	U
49	a	1689	G
49	a	1690	A
49	a	1691	A
49	a	1692	G
49	a	1697	A
49	a	1698	G
49	a	1706	G
49	a	1710	A
49	a	1712	C
49	a	1714	C
49	a	1717	G
49	a	1718	G
49	a	1719	U
49	a	1720	U
49	a	1721	G
49	a	1725	G
49	a	1726	U
49	a	1727	G
49	a	1743	A
49	a	1749	G
49	a	1752	A
49	a	1761	G
49	a	1768	A
49	a	1769	G
49	a	1774	C
49	a	1777	G
49	a	1792	A
49	a	1818	U
49	a	1830	A
49	a	1832	C
49	a	1837	G
49	a	1838	A
49	a	1858	G
49	a	1897	G
49	a	1898	C
49	a	1904	U
49	a	1911	G
49	a	1912	U
49	a	1913	G
49	a	1914	C
49	a	1915	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	1916	G
49	a	1921	G
49	a	1939	G
49	a	1947	G
49	a	1956	A
49	a	1965	C
49	a	1969	A
49	a	1974	A
49	a	1983	C
49	a	1984	G
49	a	1985	A
49	a	1999	U
49	a	2012	A
49	a	2031	A
49	a	2041	G
49	a	2052	G
49	a	2053	U
49	a	2054	A
49	a	2055	U
49	a	2056	G
49	a	2057	C
49	a	2068	A
49	a	2089	G
49	a	2096	A
49	a	2112	G
49	a	2113	G
49	a	2119	A
49	a	2120	A
49	a	2121	A
49	a	2138	U
49	a	2146	U
49	a	2150	C
49	a	2153	A
49	a	2154	U
49	a	2155	G
49	a	2174	U
49	a	2176	U
49	a	2186	G
49	a	2204	U
49	a	2206	A
49	a	2210	G
49	a	2214	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	2215	G
49	a	2216	A
49	a	2222	G
49	a	2226	C
49	a	2238	C
49	a	2239	G
49	a	2243	A
49	a	2275	G
49	a	2279	A
49	a	2283	G
49	a	2287	G
49	a	2289	U
49	a	2364	A
49	a	2365	U
49	a	2366	U
49	a	2367	G
49	a	2368	U
49	a	2369	U
49	a	2384	G
49	a	2385	U
49	a	2386	G
49	a	2393	G
49	a	2394	A
49	a	2407	A
49	a	2420	G
49	a	2421	G
49	a	2461	G
49	a	2464	G
49	a	2465	C
49	a	2469	A
49	a	2487	U
49	a	2490	G
49	a	2491	U
49	a	2501	G
49	a	2502	U
49	a	2503	G
49	a	2504	A
49	a	2507	G
49	a	2517	A
49	a	2518	A
49	a	2527	G
49	a	2529	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	2532	U
49	a	2536	A
49	a	2543	G
49	a	2565	G
49	a	2567	A
49	a	2588	U
49	a	2607	A
49	a	2611	G
49	a	2612	A
49	a	2613	U
49	a	2617	A
49	a	2623	C
49	a	2630	A
49	a	2652	G
49	a	2653	C
49	a	2654	G
49	a	2655	C
49	a	2656	U
49	a	2657	C
49	a	2658	A
49	a	2659	U
49	a	2660	A
49	a	2661	G
49	a	2663	G
49	a	2664	A
49	a	2673	U
49	a	2674	U
49	a	2679	A
49	a	2684	G
49	a	2687	G
49	a	2688	U
49	a	2700	A
49	a	2702	C
49	a	2711	G
49	a	2712	G
49	a	2713	A
49	a	2714	G
49	a	2716	C
49	a	2717	G
49	a	2720	C
49	a	2721	C
49	a	2722	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	a	2748	A
49	a	2749	G
49	a	2755	C
49	a	2767	U
49	a	2784	A
49	a	2795	U
49	a	2797	U
49	a	2811	A
49	a	2871	U
49	a	2872	G
49	a	2873	C
49	a	2900	G
49	a	2908	C
49	a	2911	C
49	a	2915	U
49	a	2917	G
49	a	2926	G
49	a	2930	A
49	a	2939	A
49	a	2944	G
49	a	2947	A
49	a	2948	G
49	a	2960	A
49	a	2962	A
49	a	2971	C
49	a	2972	A
49	a	2973	C
49	a	2979	U
49	a	2981	U
49	a	2982	U
49	a	2983	C
49	a	3000	G
49	a	3015	A
49	a	3041	G
49	a	3052	G
49	a	3063	A
49	a	3064	U
49	a	3066	G
49	a	3073	G
49	a	3074	A
49	a	3075	C
50	b	24	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	b	25	A
50	b	35	U
50	b	45	A
50	b	56	U
50	b	57	A
50	b	84	C
50	b	90	A
50	b	100	A
50	b	109	C
50	b	110	G
52	Y	14	A
52	Y	15	A
52	Y	16	A
52	Y	19	U
52	Y	20	U
52	Y	21	U
52	Y	22	U
53	C	9	G
53	C	16	C
53	C	17	C
53	C	17(A)	U
53	C	18	G
53	C	21	A
53	C	46	G
53	C	47	U
53	C	69	C
53	C	76	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	90	U
1	A	94	G
1	A	146	U
1	A	418	G
1	A	466	G
1	A	467	G
1	A	638	G
1	A	869	G
1	A	960	G
1	A	1050	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1052	A
1	A	1187	A
1	A	1271	G
1	A	1350	A
1	A	1387	5MC
53	C	17(A)	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	2MG	A	1503	1	18,26,27	1.19	3 (16%)	16,38,41	1.14	1 (6%)
49	PSU	a	2686	49	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
49	PSU	a	2787	49	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
1	G7M	A	509	1	20,26,27	2.73	7 (35%)	16,39,42	1.11	1 (6%)
1	4OC	A	1389	1	20,23,24	3.12	8 (40%)	25,32,35	0.92	1 (4%)
49	PSU	a	2100	49	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)
49	5MU	a	2122	49	19,22,23	0.47	0	27,32,35	0.47	0
53	5MC	C	32	53	19,22,23	0.49	0	26,32,35	0.61	0
49	PSU	a	2639	49	18,21,22	1.08	2 (11%)	21,30,33	2.02	5 (23%)
1	UR3	A	1485	1,56	19,22,23	2.76	8 (42%)	26,32,35	1.59	4 (15%)
1	5MC	A	951	1	19,22,23	0.56	0	26,32,35	0.64	0
53	5MU	C	54	53	19,22,23	0.38	0	27,32,35	0.62	0
1	5MC	A	1391	1	19,22,23	0.61	0	26,32,35	0.58	0
49	2MG	a	2018	49	18,26,27	1.20	2 (11%)	16,38,41	0.92	1 (6%)
1	MA6	A	1505	1	19,26,27	1.58	3 (15%)	18,38,41	4.92	4 (22%)
49	3TD	a	2098	49	19,22,23	4.27	6 (31%)	23,32,35	1.81	4 (17%)
49	2MA	a	2685	49,56	18,25,26	3.33	6 (33%)	20,37,40	1.77	3 (15%)
49	H2U	a	2631	49	18,21,22	0.48	0	19,30,33	1.08	1 (5%)
49	PSU	a	2786	49	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PSU	a	1038	49	18,21,22	1.03	1 (5%)	21,30,33	2.01	3 (14%)
1	PSU	A	498	1,56	18,21,22	1.10	2 (11%)	21,30,33	1.98	6 (28%)
49	5MC	a	2145	49	19,22,23	0.58	0	26,32,35	0.70	0
49	2MG	a	2627	49	18,26,27	1.24	3 (16%)	16,38,41	0.88	1 (6%)
49	OMC	a	2680	49,56	19,22,23	0.62	0	25,31,34	0.74	0
1	5MC	A	1387	1	19,22,23	0.53	0	26,32,35	0.66	0
49	PSU	a	2762	49	18,21,22	1.11	2 (11%)	21,30,33	1.96	5 (23%)
53	4SU	C	8	53	18,21,22	3.80	7 (38%)	25,30,33	2.30	5 (20%)
49	OMG	a	2433	53,49	19,26,27	1.10	3 (15%)	21,38,41	0.65	0
49	PSU	a	2094	49	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
1	2MG	A	950	1	18,26,27	1.17	2 (11%)	16,38,41	0.86	1 (6%)
1	5MC	A	1394	1	19,22,23	0.51	0	26,32,35	0.61	0
53	PSU	C	55	53	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
1	MA6	A	1506	1	19,26,27	1.55	3 (15%)	18,38,41	5.04	4 (22%)
49	OMU	a	2734	49	19,22,23	2.91	7 (36%)	25,31,34	1.85	5 (20%)

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	2MG	A	1503	1	-	0/5/27/28	0/3/3/3
49	PSU	a	2686	49	-	0/7/25/26	0/2/2/2
49	PSU	a	2787	49	-	0/7/25/26	0/2/2/2
1	G7M	A	509	1	-	2/3/25/26	0/3/3/3
1	4OC	A	1389	1	-	1/9/29/30	0/2/2/2
49	PSU	a	2100	49	-	0/7/25/26	0/2/2/2
49	5MU	a	2122	49	-	0/7/25/26	0/2/2/2
53	5MC	C	32	53	-	0/7/25/26	0/2/2/2
49	PSU	a	2639	49	-	0/7/25/26	0/2/2/2
1	UR3	A	1485	1,56	-	0/7/25/26	0/2/2/2
1	5MC	A	951	1	-	0/7/25/26	0/2/2/2
53	5MU	C	54	53	-	0/7/25/26	0/2/2/2
1	5MC	A	1391	1	-	0/7/25/26	0/2/2/2
49	2MG	a	2018	49	-	0/5/27/28	0/3/3/3
1	MA6	A	1505	1	-	0/7/29/30	0/3/3/3
49	3TD	a	2098	49	-	2/7/25/26	0/2/2/2
49	2MA	a	2685	49,56	-	2/3/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	H2U	a	2631	49	-	0/7/38/39	0/2/2/2
49	PSU	a	2786	49	-	0/7/25/26	0/2/2/2
49	PSU	a	1038	49	-	0/7/25/26	0/2/2/2
1	PSU	A	498	1,56	-	0/7/25/26	0/2/2/2
49	5MC	a	2145	49	-	1/7/25/26	0/2/2/2
49	2MG	a	2627	49	-	1/5/27/28	0/3/3/3
49	OMC	a	2680	49,56	-	0/9/27/28	0/2/2/2
1	5MC	A	1387	1	-	3/7/25/26	0/2/2/2
49	PSU	a	2762	49	-	0/7/25/26	0/2/2/2
53	4SU	C	8	53	-	0/7/25/26	0/2/2/2
49	OMG	a	2433	53,49	-	1/5/27/28	0/3/3/3
49	PSU	a	2094	49	-	0/7/25/26	0/2/2/2
1	2MG	A	950	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1394	1	-	0/7/25/26	0/2/2/2
53	PSU	C	55	53	-	0/7/25/26	0/2/2/2
1	MA6	A	1506	1	-	2/7/29/30	0/3/3/3
49	OMU	a	2734	49	-	0/9/27/28	0/2/2/2

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	a	2098	3TD	C6-C5	13.12	1.49	1.35
49	a	2098	3TD	C2-N1	9.47	1.48	1.37
49	a	2685	2MA	C4-N3	8.22	1.48	1.35
53	C	8	4SU	C2-N3	7.39	1.50	1.38
53	C	8	4SU	C2-N1	7.23	1.49	1.38
1	A	1485	UR3	C2-N1	7.19	1.48	1.38
1	A	1389	4OC	C4-N3	7.11	1.44	1.32
53	C	8	4SU	C4-N3	7.04	1.44	1.37
49	a	2734	OMU	C2-N1	6.90	1.49	1.38
49	a	2685	2MA	C2-N3	6.89	1.45	1.34
49	a	2685	2MA	C2-N1	6.86	1.45	1.34
49	a	2734	OMU	C2-N3	6.60	1.49	1.38
1	A	509	G7M	C2-N2	6.54	1.49	1.34
1	A	1389	4OC	C6-C5	6.24	1.49	1.35
53	C	8	4SU	C5-C4	6.15	1.49	1.42
1	A	1485	UR3	C6-C5	6.15	1.49	1.35
49	a	2098	3TD	C6-N1	6.14	1.46	1.36
1	A	1389	4OC	C2-N3	6.10	1.48	1.36
49	a	2734	OMU	C6-C5	5.79	1.48	1.35
1	A	509	G7M	C2-N3	5.61	1.46	1.33
53	C	8	4SU	C6-C5	5.61	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	509	G7M	C4-N3	5.11	1.49	1.37
1	A	1485	UR3	C2-N3	4.92	1.48	1.39
53	C	8	4SU	C4-S4	-4.83	1.60	1.68
1	A	1505	MA6	C6-C5	-4.81	1.37	1.44
49	a	2098	3TD	C2-N3	4.77	1.48	1.38
1	A	1506	MA6	C6-C5	-4.64	1.37	1.44
1	A	1389	4OC	C4-N4	4.44	1.45	1.36
1	A	509	G7M	C6-N1	4.11	1.44	1.37
1	A	1389	4OC	C2-N1	4.04	1.48	1.40
49	a	2685	2MA	C6-N1	3.97	1.41	1.33
53	C	55	PSU	C6-C5	3.79	1.39	1.35
49	a	2100	PSU	C6-C5	3.76	1.39	1.35
1	A	1389	4OC	C5-C4	3.69	1.49	1.41
49	a	2094	PSU	C6-C5	3.68	1.39	1.35
1	A	1506	MA6	C6-N6	3.66	1.45	1.37
1	A	1505	MA6	C6-N6	3.54	1.45	1.37
49	a	2734	OMU	C4-N3	3.47	1.44	1.38
49	a	2686	PSU	C6-C5	3.43	1.39	1.35
1	A	498	PSU	C6-C5	3.36	1.39	1.35
49	a	2762	PSU	C6-C5	3.33	1.39	1.35
49	a	2786	PSU	C6-C5	3.30	1.38	1.35
1	A	509	G7M	C5-C6	3.24	1.53	1.45
49	a	2787	PSU	C6-C5	3.24	1.38	1.35
49	a	2627	2MG	C8-N7	-3.24	1.29	1.34
49	a	1038	PSU	C6-C5	3.17	1.38	1.35
49	a	2639	PSU	C6-C5	3.11	1.38	1.35
49	a	2018	2MG	C8-N7	-3.11	1.30	1.34
1	A	1389	4OC	C6-N1	3.07	1.45	1.38
1	A	950	2MG	C8-N7	-2.98	1.30	1.34
49	a	2098	3TD	C4-N3	2.98	1.46	1.40
49	a	2433	OMG	C5-C6	-2.92	1.41	1.47
1	A	1485	UR3	C6-N1	2.91	1.45	1.38
1	A	509	G7M	C2-N1	2.91	1.44	1.37
1	A	1503	2MG	C8-N7	-2.86	1.30	1.34
49	a	2734	OMU	O2-C2	-2.84	1.18	1.23
49	a	2685	2MA	C6-C5	2.84	1.54	1.43
1	A	1389	4OC	O2-C2	-2.77	1.18	1.23
49	a	2734	OMU	O4-C4	-2.77	1.19	1.24
53	C	8	4SU	C6-N1	2.74	1.44	1.38
49	a	2627	2MG	C5-C6	-2.54	1.42	1.47
49	a	2018	2MG	C5-C6	-2.50	1.42	1.47
1	A	1485	UR3	C4-N3	2.46	1.45	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	a	2685	2MA	C6-N6	-2.41	1.25	1.34
1	A	950	2MG	C5-C6	-2.41	1.42	1.47
1	A	1503	2MG	C5-C6	-2.35	1.42	1.47
1	A	1485	UR3	O4-C4	-2.28	1.18	1.23
49	a	2433	OMG	C8-N7	-2.27	1.31	1.34
1	A	1505	MA6	C2-N3	2.25	1.35	1.32
1	A	1485	UR3	C5-C4	2.22	1.49	1.43
49	a	2098	3TD	O4-C4	-2.20	1.18	1.23
1	A	1485	UR3	O2-C2	-2.15	1.18	1.22
49	a	2627	2MG	C5-C4	-2.13	1.37	1.43
49	a	2433	OMG	C5-C4	-2.13	1.37	1.43
1	A	1503	2MG	C5-C4	-2.10	1.37	1.43
49	a	2762	PSU	C4-C5	-2.09	1.38	1.44
49	a	2734	OMU	C5-C4	2.06	1.48	1.43
1	A	1506	MA6	C2-N3	2.04	1.35	1.32
1	A	498	PSU	C4-C5	-2.04	1.38	1.44
1	A	509	G7M	O6-C6	-2.01	1.18	1.23
49	a	2639	PSU	C4-C5	-2.01	1.38	1.44

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1506	MA6	N1-C6-N6	-17.44	96.68	116.83
1	A	1505	MA6	N1-C6-N6	-16.64	97.60	116.83
1	A	1505	MA6	C1'-N9-C4	-10.22	108.69	126.64
1	A	1506	MA6	C1'-N9-C4	-9.82	109.40	126.64
53	C	8	4SU	C4-N3-C2	-7.91	119.73	127.31
1	A	1506	MA6	N3-C2-N1	-6.32	120.10	128.67
1	A	1505	MA6	N3-C2-N1	-6.17	120.30	128.67
49	a	2734	OMU	C4-N3-C2	-5.81	119.40	126.61
49	a	2098	3TD	N1-C2-N3	5.73	120.30	116.13
49	a	2685	2MA	C2-N3-C4	5.70	120.06	115.46
1	A	1485	UR3	C4-N3-C2	-5.51	120.14	124.58
49	a	1038	PSU	C4-N3-C2	-5.51	118.78	126.37
53	C	8	4SU	C5-C4-N3	5.39	119.76	114.75
49	a	2639	PSU	N1-C2-N3	5.09	120.53	115.17
1	A	498	PSU	C4-N3-C2	-5.06	119.41	126.37
49	a	2786	PSU	C4-N3-C2	-5.05	119.41	126.37
49	a	2787	PSU	C4-N3-C2	-5.02	119.46	126.37
49	a	1038	PSU	N1-C2-N3	4.98	120.42	115.17
49	a	2762	PSU	C4-N3-C2	-4.96	119.53	126.37
49	a	2639	PSU	C4-N3-C2	-4.89	119.64	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	a	2786	PSU	N1-C2-N3	4.88	120.31	115.17
49	a	2686	PSU	C4-N3-C2	-4.87	119.66	126.37
49	a	2686	PSU	N1-C2-N3	4.85	120.28	115.17
1	A	498	PSU	N1-C2-N3	4.84	120.27	115.17
49	a	2094	PSU	C4-N3-C2	-4.83	119.72	126.37
49	a	2762	PSU	N1-C2-N3	4.82	120.25	115.17
53	C	55	PSU	C4-N3-C2	-4.82	119.73	126.37
49	a	2094	PSU	N1-C2-N3	4.79	120.22	115.17
49	a	2100	PSU	C4-N3-C2	-4.78	119.78	126.37
49	a	2787	PSU	N1-C2-N3	4.77	120.20	115.17
53	C	55	PSU	N1-C2-N3	4.74	120.17	115.17
49	a	2100	PSU	N1-C2-N3	4.70	120.12	115.17
49	a	2098	3TD	C4-N3-C2	-4.15	120.22	124.61
49	a	2734	OMU	N3-C2-N1	3.87	119.93	114.89
53	C	8	4SU	C5-C4-S4	-3.86	119.90	124.31
53	C	8	4SU	N3-C2-N1	3.81	119.85	114.89
49	a	2734	OMU	C5-C4-N3	3.77	120.08	114.80
1	A	1485	UR3	C5-C4-N3	3.59	119.76	115.04
49	a	2631	H2U	C5-C4-N3	-3.41	113.06	116.69
1	A	1506	MA6	C2-N1-C6	3.40	120.18	116.84
49	a	2685	2MA	N3-C2-N1	-3.34	119.92	125.77
1	A	1505	MA6	C2-N1-C6	3.30	120.08	116.84
1	A	509	G7M	C2-N1-C6	-3.11	119.42	125.11
49	a	2734	OMU	O4-C4-C5	-2.98	120.02	125.16
49	a	2639	PSU	O2-C2-N1	-2.91	119.78	122.79
49	a	2686	PSU	O2-C2-N1	-2.84	119.86	122.79
49	a	2094	PSU	O2-C2-N1	-2.79	119.91	122.79
53	C	55	PSU	O2-C2-N1	-2.77	119.93	122.79
1	A	498	PSU	O2-C2-N1	-2.75	119.95	122.79
49	a	2639	PSU	C6-N1-C2	-2.67	120.21	122.69
49	a	2762	PSU	O2-C2-N1	-2.67	120.04	122.79
49	a	2786	PSU	O2-C2-N1	-2.61	120.10	122.79
49	a	2100	PSU	O2-C2-N1	-2.60	120.10	122.79
49	a	2639	PSU	C6-C5-C4	2.57	119.91	118.17
49	a	2787	PSU	O2-C2-N1	-2.46	120.25	122.79
49	a	2686	PSU	C6-N1-C2	-2.43	120.43	122.69
49	a	2094	PSU	C6-N1-C2	-2.42	120.45	122.69
49	a	2098	3TD	C6-C5-C4	2.41	119.81	118.19
49	a	1038	PSU	O2-C2-N1	-2.36	120.35	122.79
49	a	2762	PSU	C6-N1-C2	-2.35	120.51	122.69
1	A	498	PSU	C6-N1-C2	-2.34	120.52	122.69
49	a	2786	PSU	C6-C5-C4	2.33	119.75	118.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	C	55	PSU	C6-N1-C2	-2.33	120.53	122.69
49	a	2762	PSU	C6-C5-C4	2.31	119.73	118.17
1	A	1503	2MG	O6-C6-C5	2.28	128.85	124.32
49	a	2627	2MG	O6-C6-C5	2.28	128.84	124.32
1	A	950	2MG	O6-C6-C5	2.24	128.77	124.32
49	a	2786	PSU	C6-N1-C2	-2.24	120.61	122.69
49	a	2100	PSU	C6-N1-C2	-2.22	120.63	122.69
1	A	1389	4OC	C6-C5-C4	2.22	119.67	117.00
49	a	2734	OMU	O2-C2-N1	-2.20	119.93	122.80
49	a	2787	PSU	C6-N1-C2	-2.16	120.69	122.69
49	a	2094	PSU	C6-C5-C4	2.15	119.62	118.17
1	A	1485	UR3	C6-N1-C2	-2.14	120.05	121.80
53	C	8	4SU	O2-C2-N1	-2.11	120.05	122.80
53	C	55	PSU	C6-C5-C4	2.10	119.59	118.17
49	a	2018	2MG	O6-C6-C5	2.10	128.48	124.32
1	A	498	PSU	C6-C5-C4	2.10	119.59	118.17
1	A	498	PSU	O4'-C1'-C2'	2.09	108.04	105.15
49	a	2098	3TD	C1'-C5-C4	2.08	120.77	117.61
49	a	2685	2MA	CM2-C2-N1	2.08	120.23	117.13
1	A	1485	UR3	C1'-N1-C2	2.02	120.34	117.04

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1387	5MC	O4'-C4'-C5'-O5'
1	A	1506	MA6	O4'-C4'-C5'-O5'
49	a	2098	3TD	O4'-C4'-C5'-O5'
49	a	2433	OMG	C1'-C2'-O2'-CM2
49	a	2098	3TD	C3'-C4'-C5'-O5'
1	A	1387	5MC	C3'-C4'-C5'-O5'
1	A	1506	MA6	C3'-C4'-C5'-O5'
49	a	2685	2MA	O4'-C4'-C5'-O5'
49	a	2685	2MA	C3'-C4'-C5'-O5'
1	A	509	G7M	C3'-C4'-C5'-O5'
49	a	2627	2MG	C3'-C4'-C5'-O5'
1	A	1389	4OC	O4'-C4'-C5'-O5'
1	A	1387	5MC	C4'-C5'-O5'-P
1	A	509	G7M	C4'-C5'-O5'-P
49	a	2145	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 393 ligands modelled in this entry, 391 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	V7A	a	3101	-	37,38,38	1.05	2 (5%)	43,60,60	0.89	2 (4%)
55	V7A	A	1601	56	37,38,38	1.25	2 (5%)	43,60,60	2.22	6 (13%)

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	V7A	a	3101	-	-	8/13/72/72	0/4/4/4
55	V7A	A	1601	56	-	5/13/72/72	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	1601	V7A	CBC-NBD	6.21	1.51	1.33
55	a	3101	V7A	CBC-NBD	4.99	1.47	1.33
55	A	1601	V7A	OAY-CAH	2.37	1.28	1.23
55	a	3101	V7A	OAY-CAH	2.24	1.27	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A	1601	V7A	CAH-CAI-CAL	9.09	125.99	118.80
55	A	1601	V7A	CAP-CAM-CAL	7.95	119.19	109.88
55	A	1601	V7A	CBC-CAQ-CAP	3.29	124.86	120.97
55	A	1601	V7A	OBA-CAM-CAL	-2.63	105.94	110.14
55	A	1601	V7A	CAQ-CBC-NBD	2.53	123.80	118.64
55	a	3101	V7A	CAM-CAP-CAQ	2.46	119.65	115.75
55	A	1601	V7A	OBE-CBC-NBD	-2.36	117.59	122.89
55	a	3101	V7A	CAP-CAM-CAL	2.09	112.33	109.88

There are no chirality outliers.

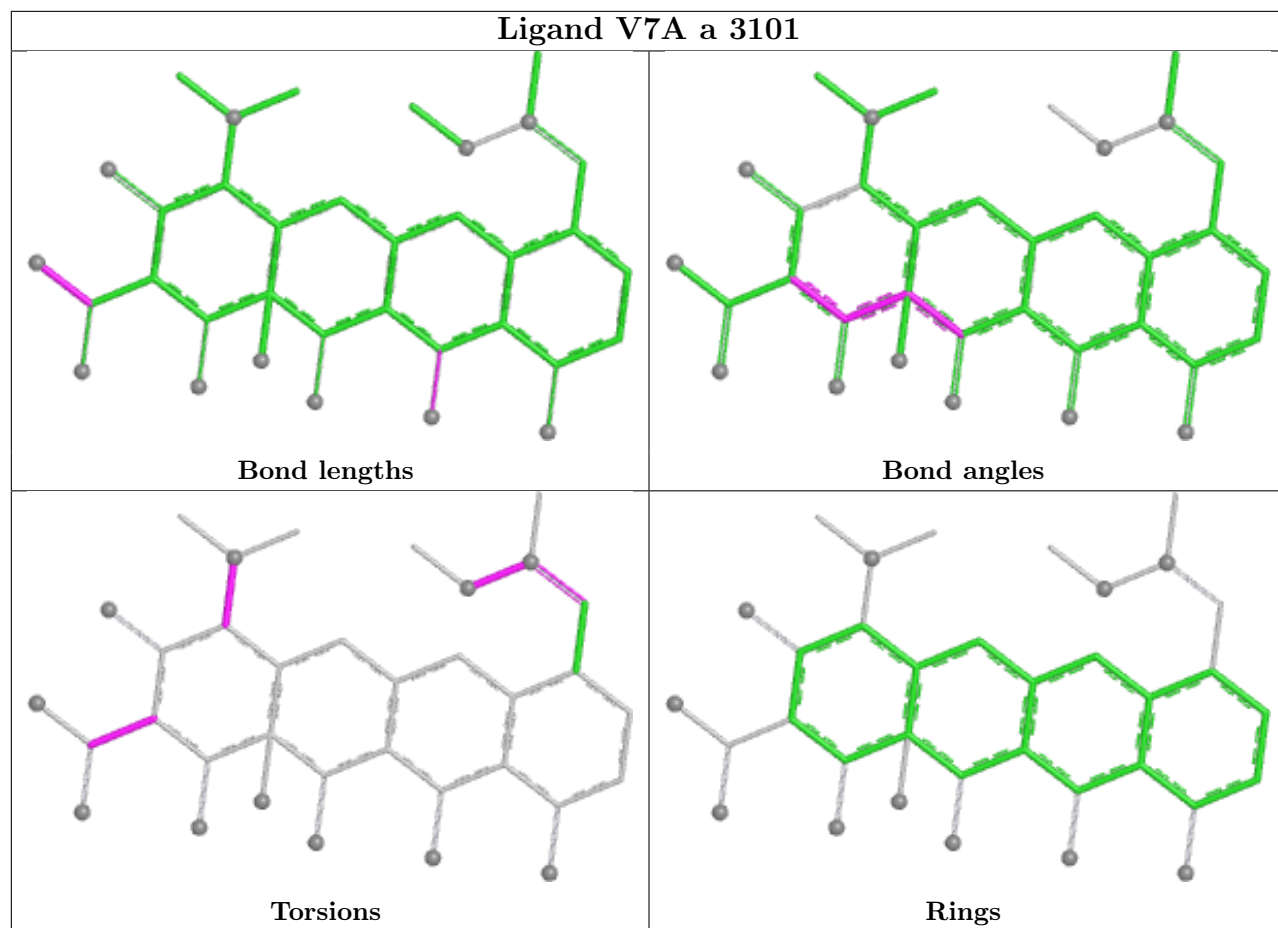
All (13) torsion outliers are listed below:

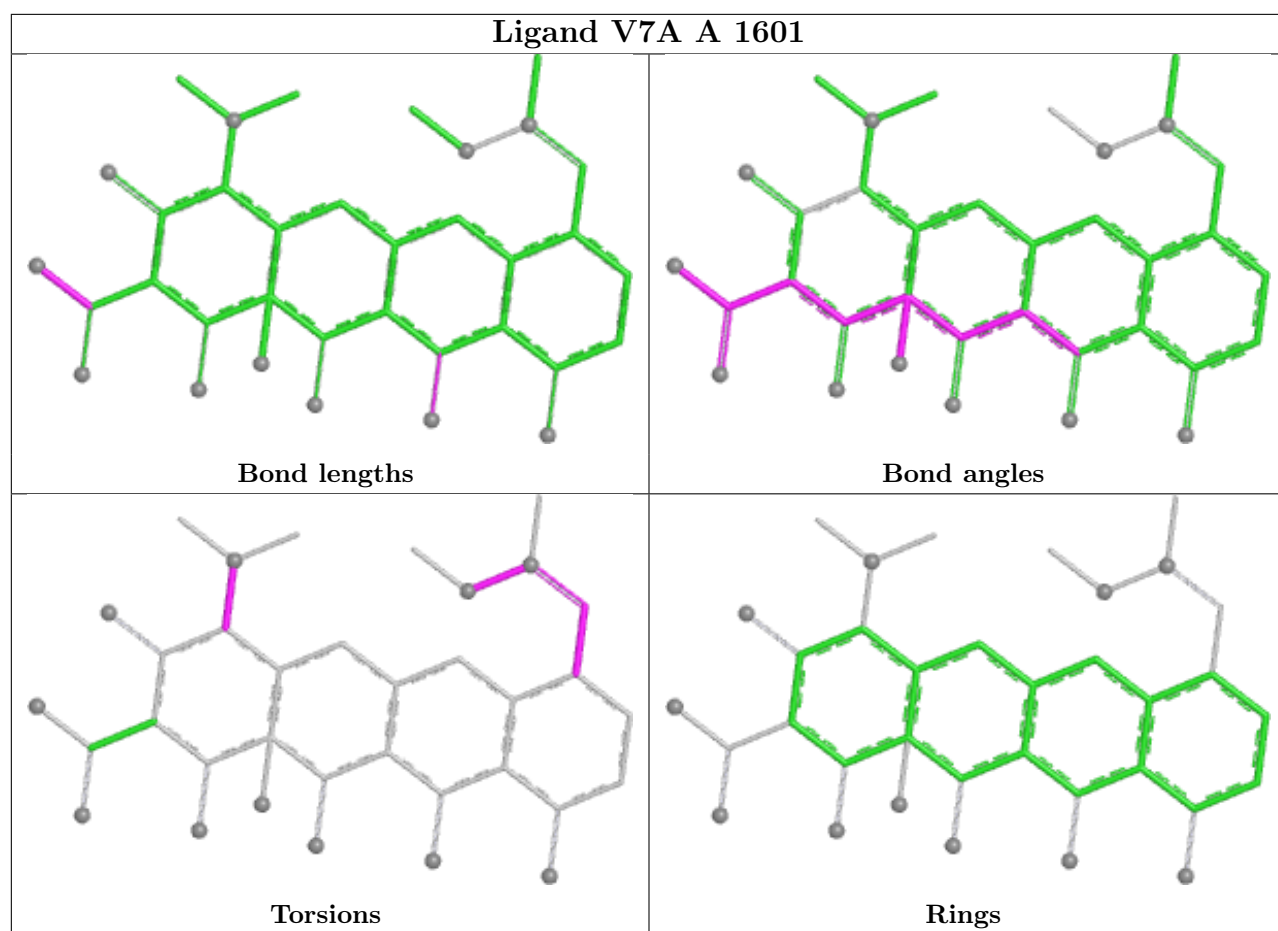
Mol	Chain	Res	Type	Atoms
55	A	1601	V7A	CAA-CAS-NAT-OAU
55	A	1601	V7A	CAW-NAT-OAU-CAV
55	a	3101	V7A	CAN-CAO-NBF-CBH
55	a	3101	V7A	CAP-CAQ-CBC-OBE
55	a	3101	V7A	CAR-CAQ-CBC-NBD
55	a	3101	V7A	CAR-CAQ-CBC-OBE
55	a	3101	V7A	CAA-CAS-NAT-CAW
55	a	3101	V7A	CAA-CAS-NAT-OAU
55	a	3101	V7A	CAW-NAT-OAU-CAV
55	a	3101	V7A	CAP-CAQ-CBC-NBD
55	A	1601	V7A	CAF-CAA-CAS-NAT
55	A	1601	V7A	CAA-CAS-NAT-CAW
55	A	1601	V7A	CAN-CAO-NBF-CBG

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.

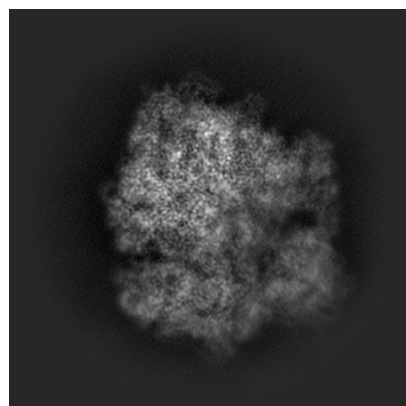
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26959. These allow visual inspection of the internal detail of the map and identification of artifacts.

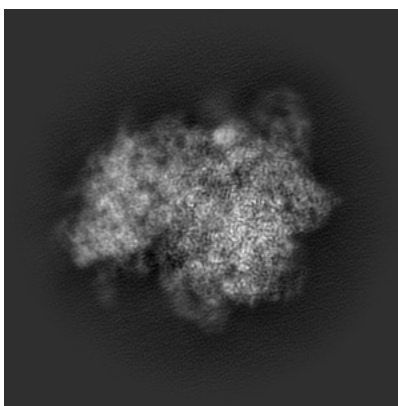
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

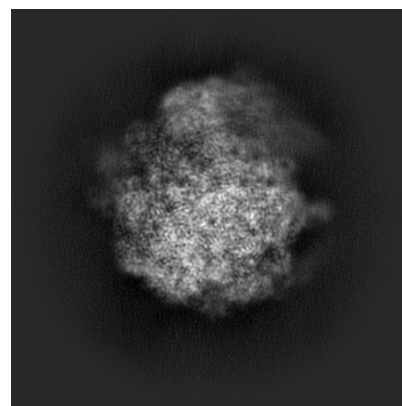
6.1.1 Primary map



X

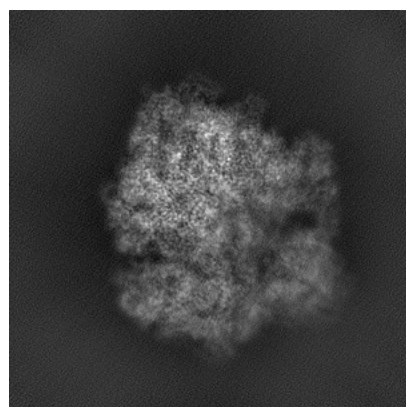


Y

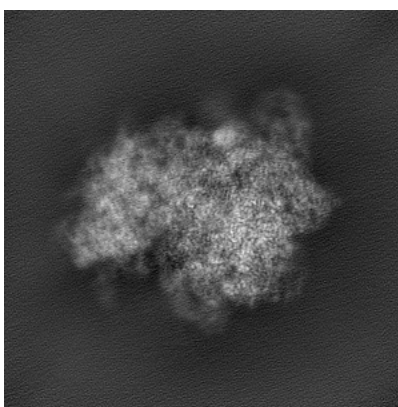


Z

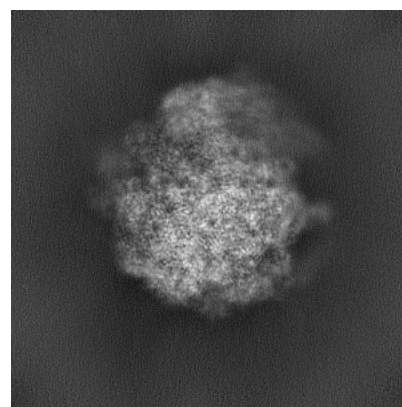
6.1.2 Raw map



X



Y

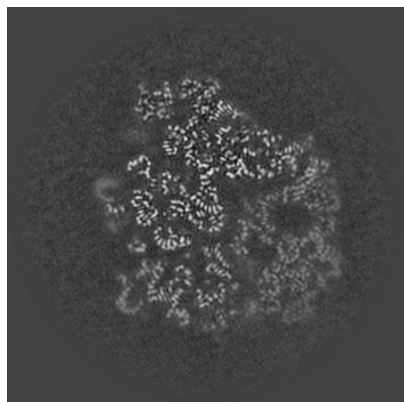


Z

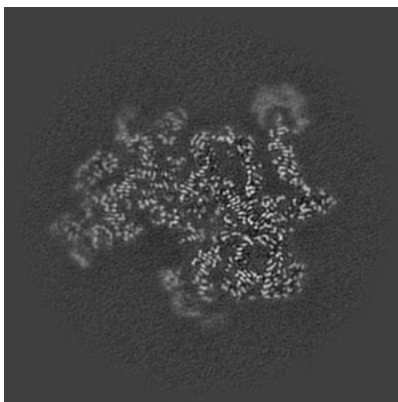
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

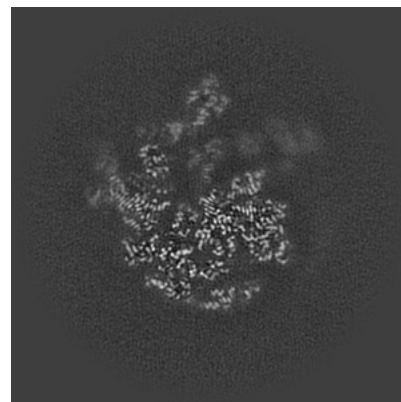
6.2.1 Primary map



X Index: 170

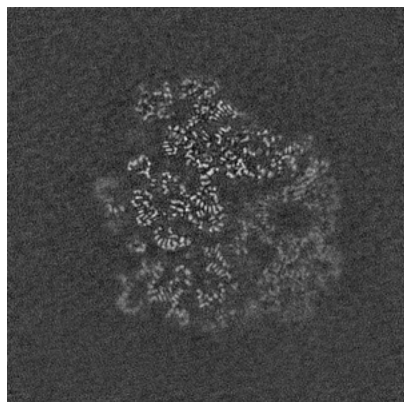


Y Index: 170

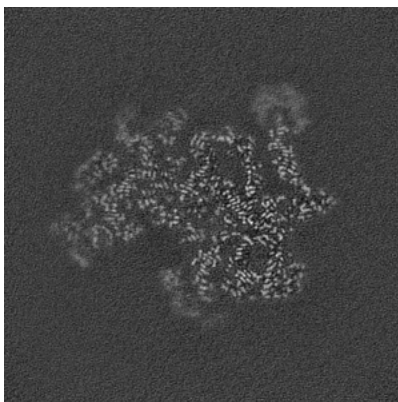


Z Index: 170

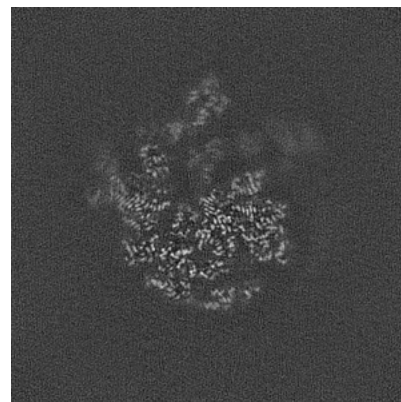
6.2.2 Raw map



X Index: 170



Y Index: 170

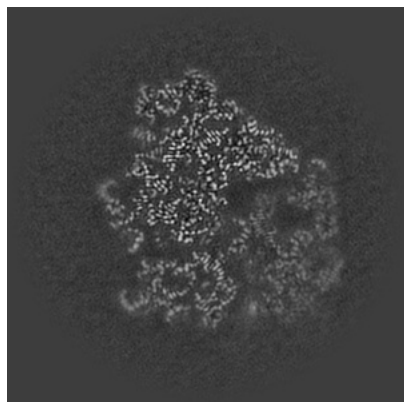


Z Index: 170

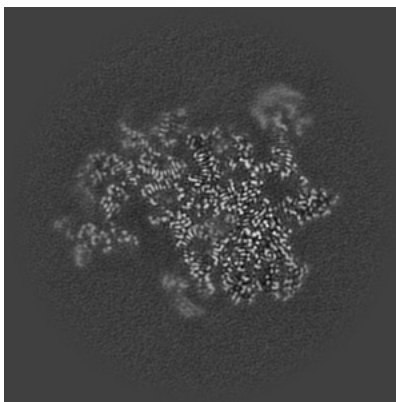
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

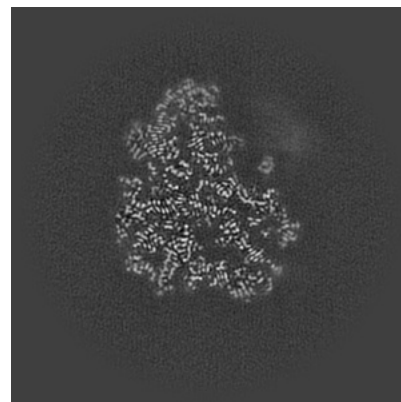
6.3.1 Primary map



X Index: 175

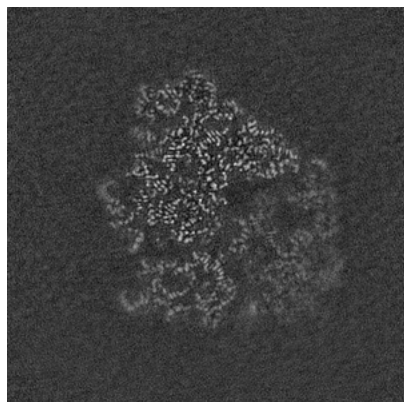


Y Index: 165

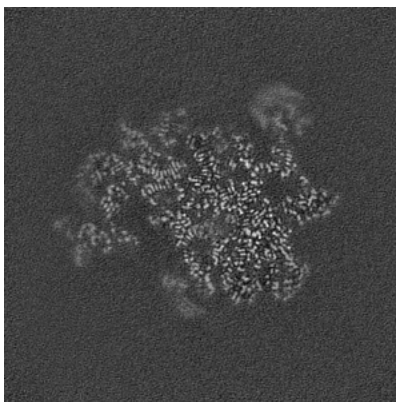


Z Index: 203

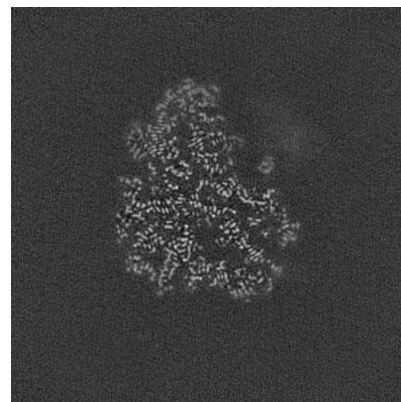
6.3.2 Raw map



X Index: 175



Y Index: 165

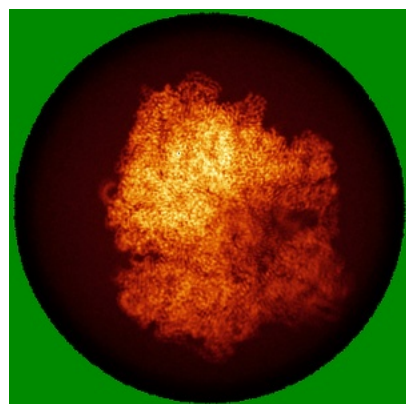


Z Index: 203

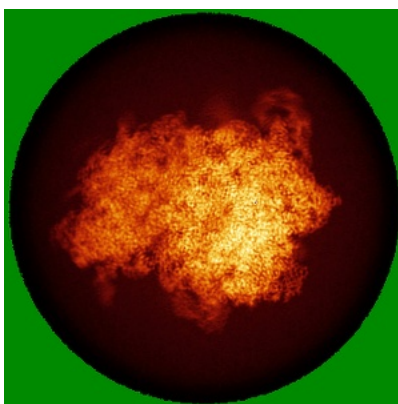
The images above show the largest variance slices of the map in three orthogonal directions.

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

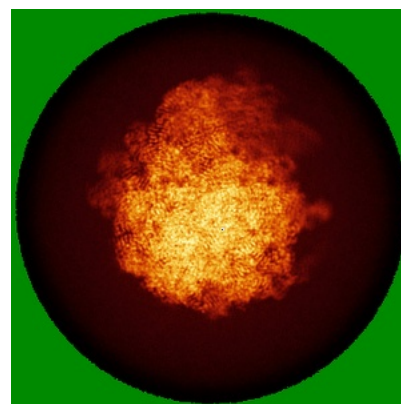
6.4.1 Primary map



X

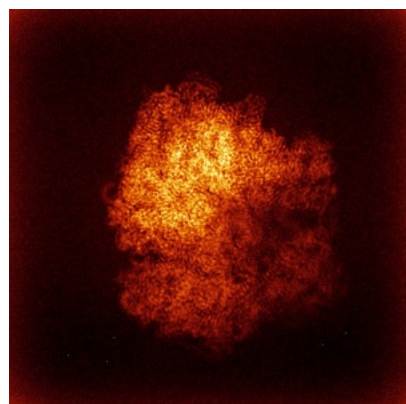


Y

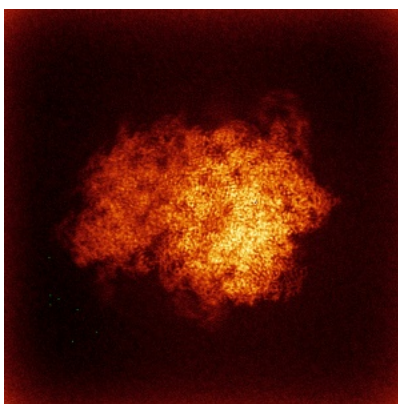


Z

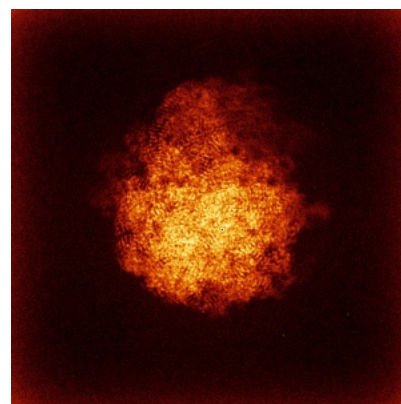
6.4.2 Raw map



X



Y

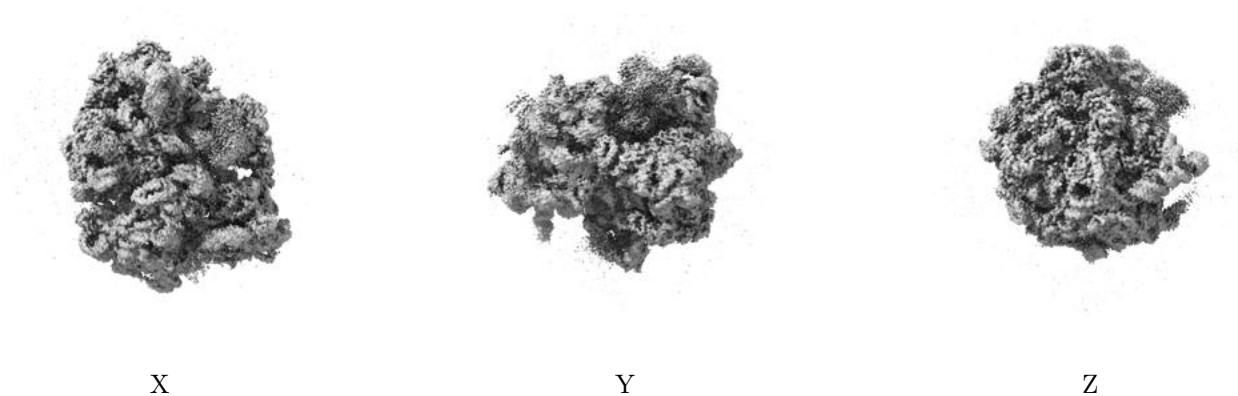


Z

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.

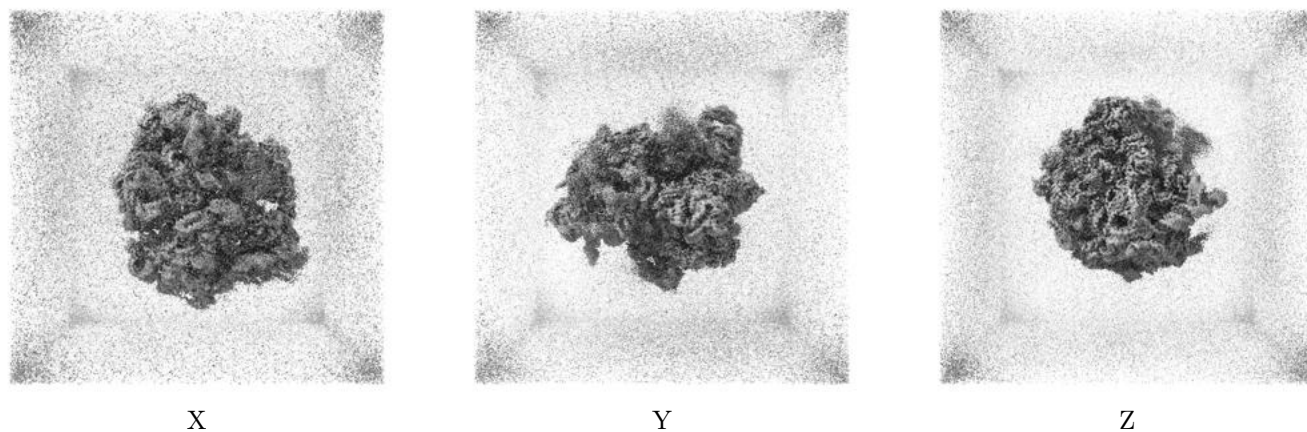
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

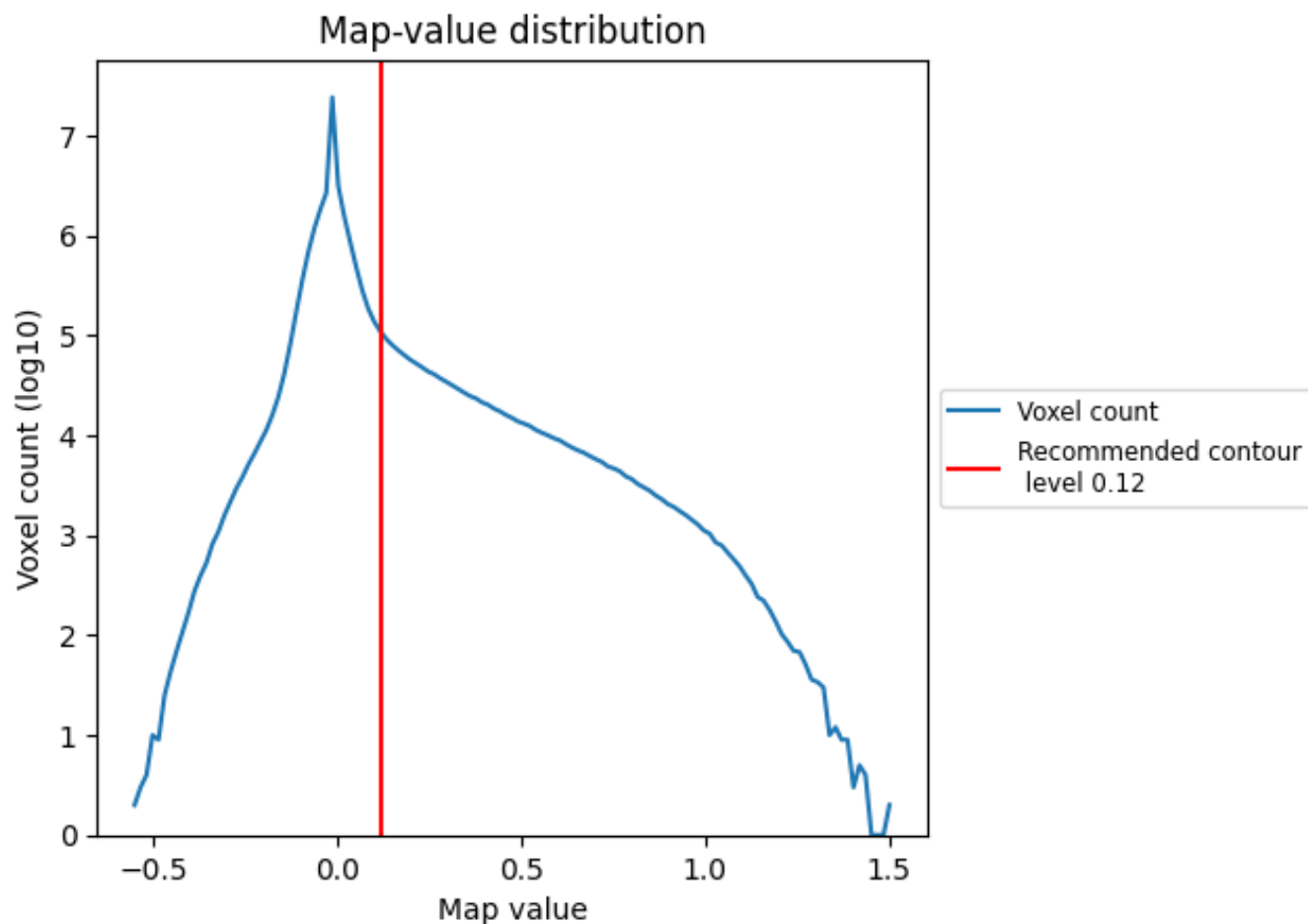
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

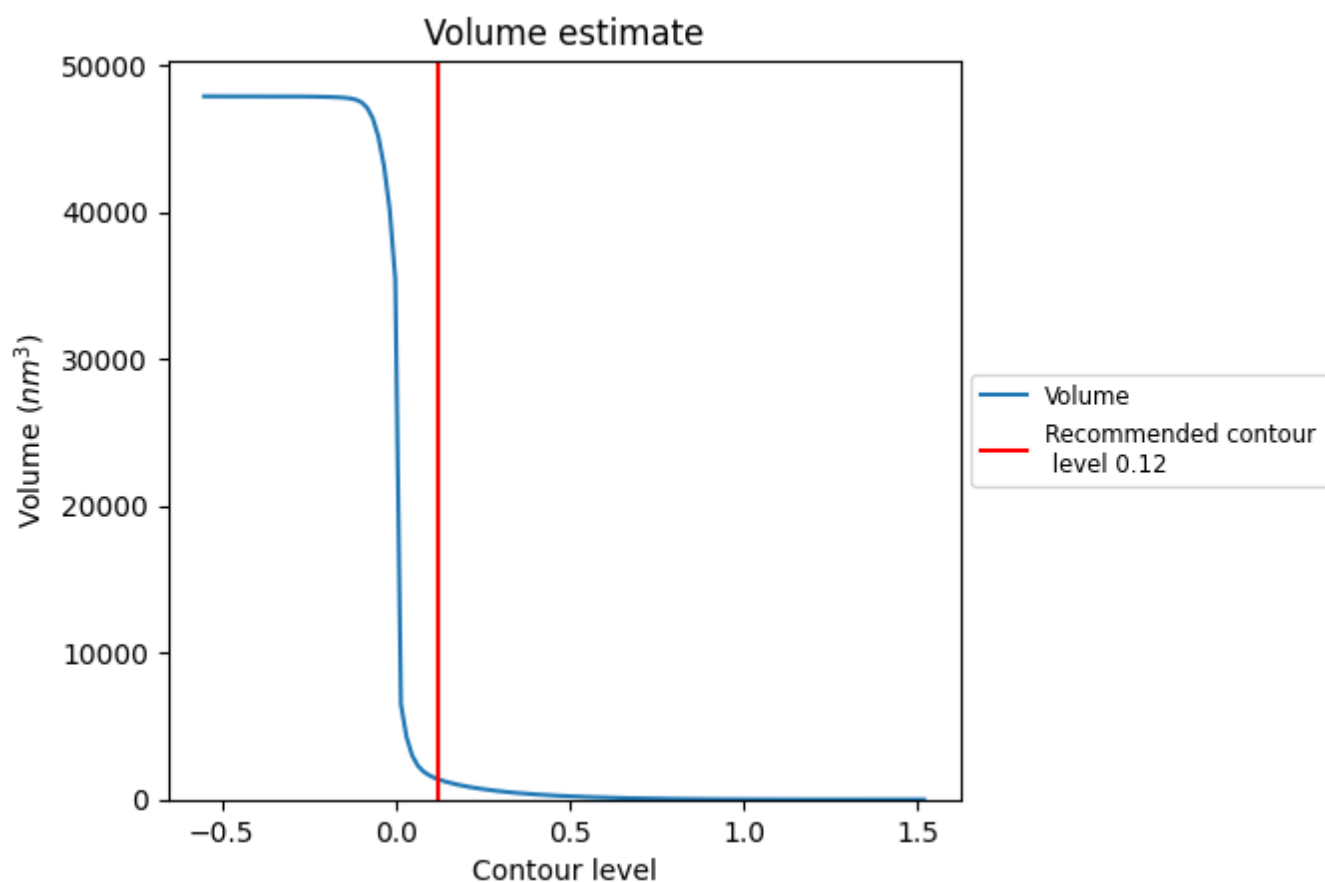
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

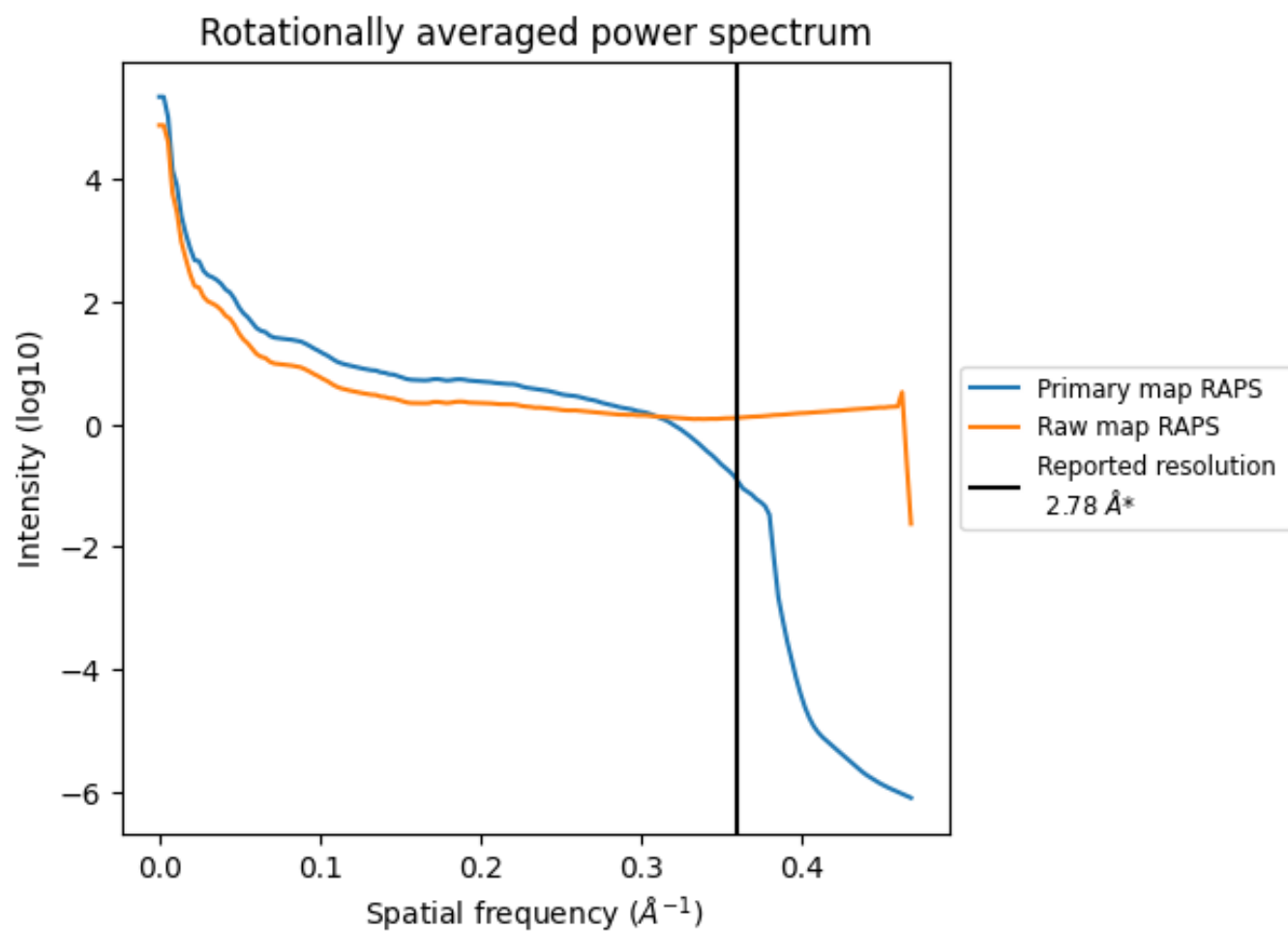
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1399 nm³; this corresponds to an approximate mass of 1263 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 ⓘ

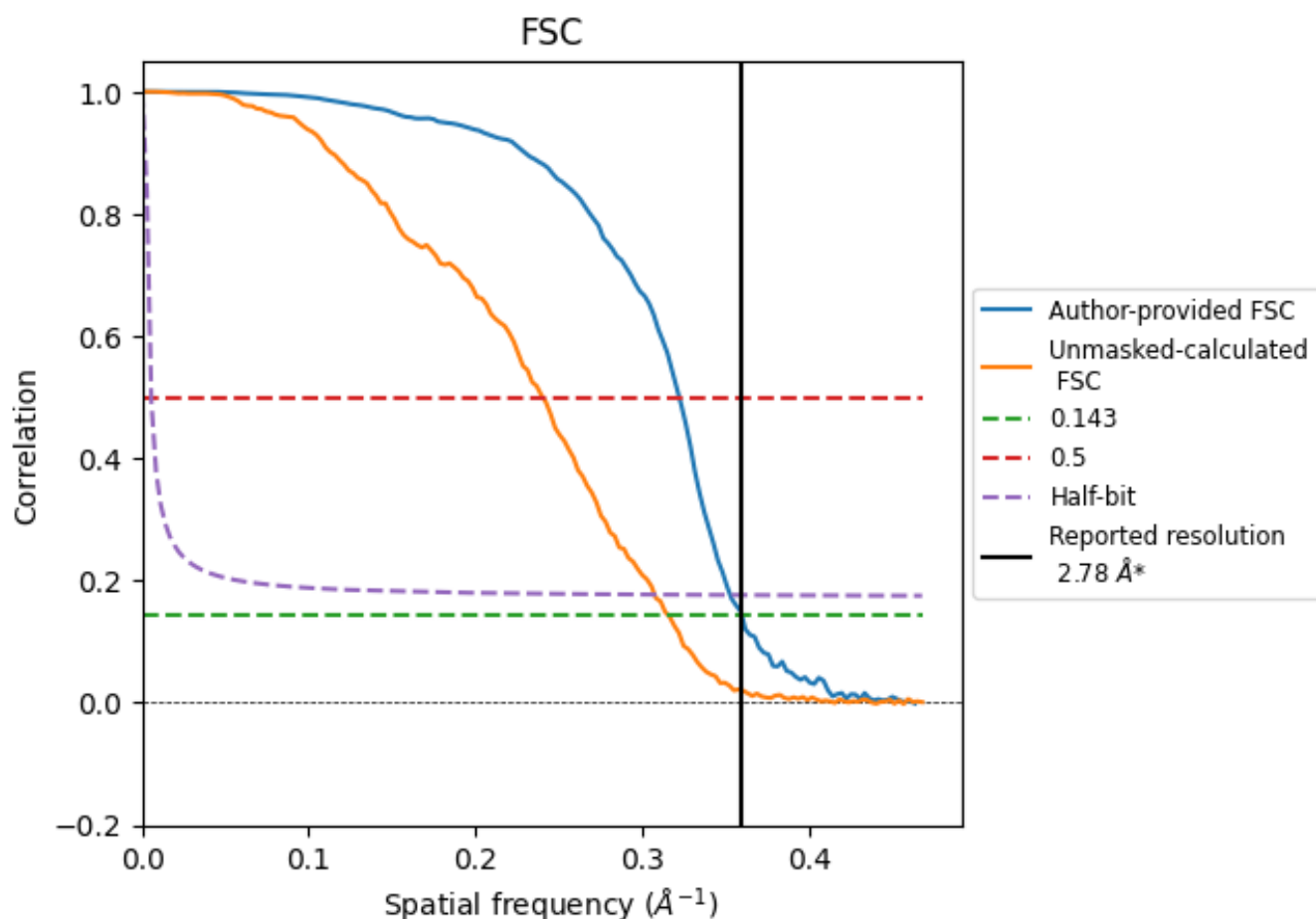


*Reported resolution corresponds to spatial frequency of 0.360 \AA^{-1}

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 0.360 \AA^{-1}

8.2 Resolution estimates [i](#)

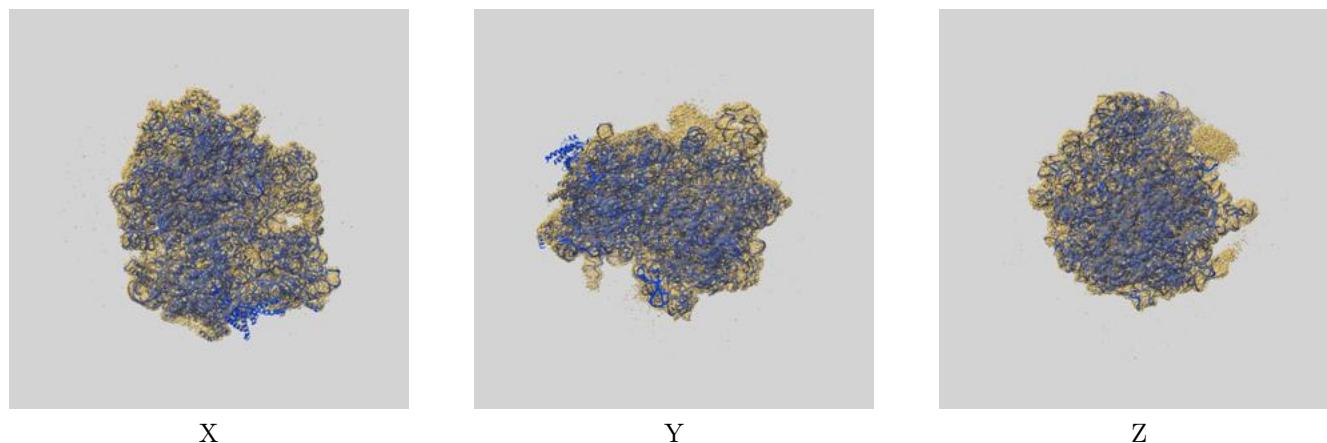
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.10	2.83
Unmasked-calculated*	3.17	4.16	3.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.17 differs from the reported value 2.78 by more than 10 %

9 Map-model fit [i](#)

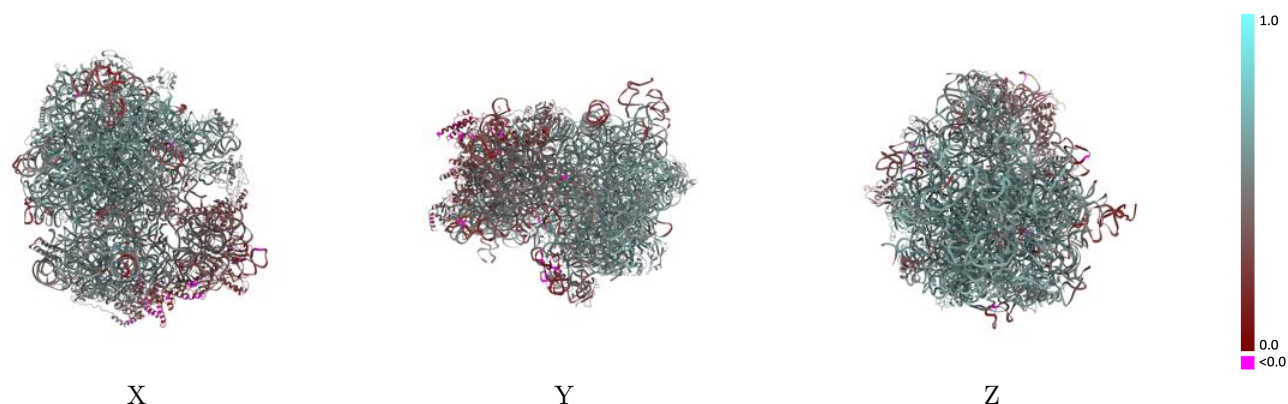
This section contains information regarding the fit between EMDB map EMD-26959 and PDB model 8CRX. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



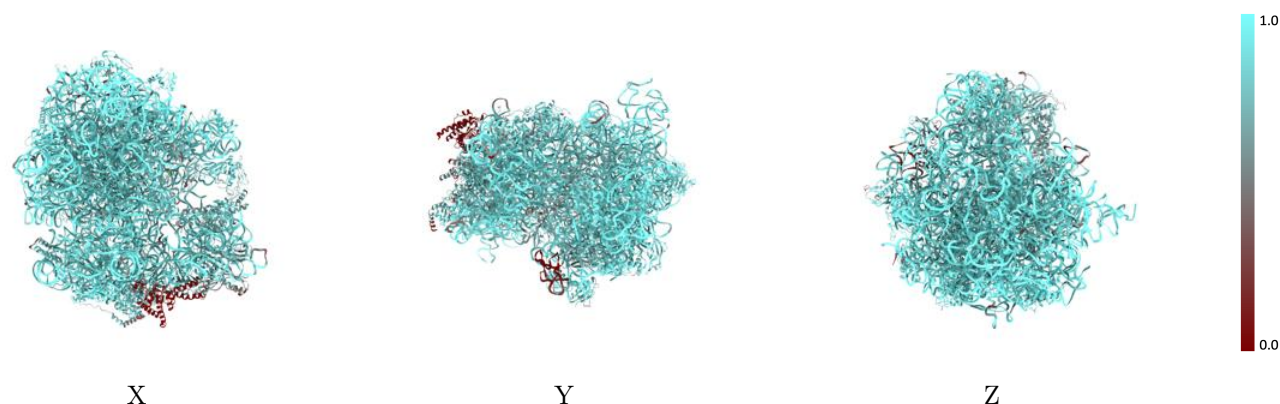
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



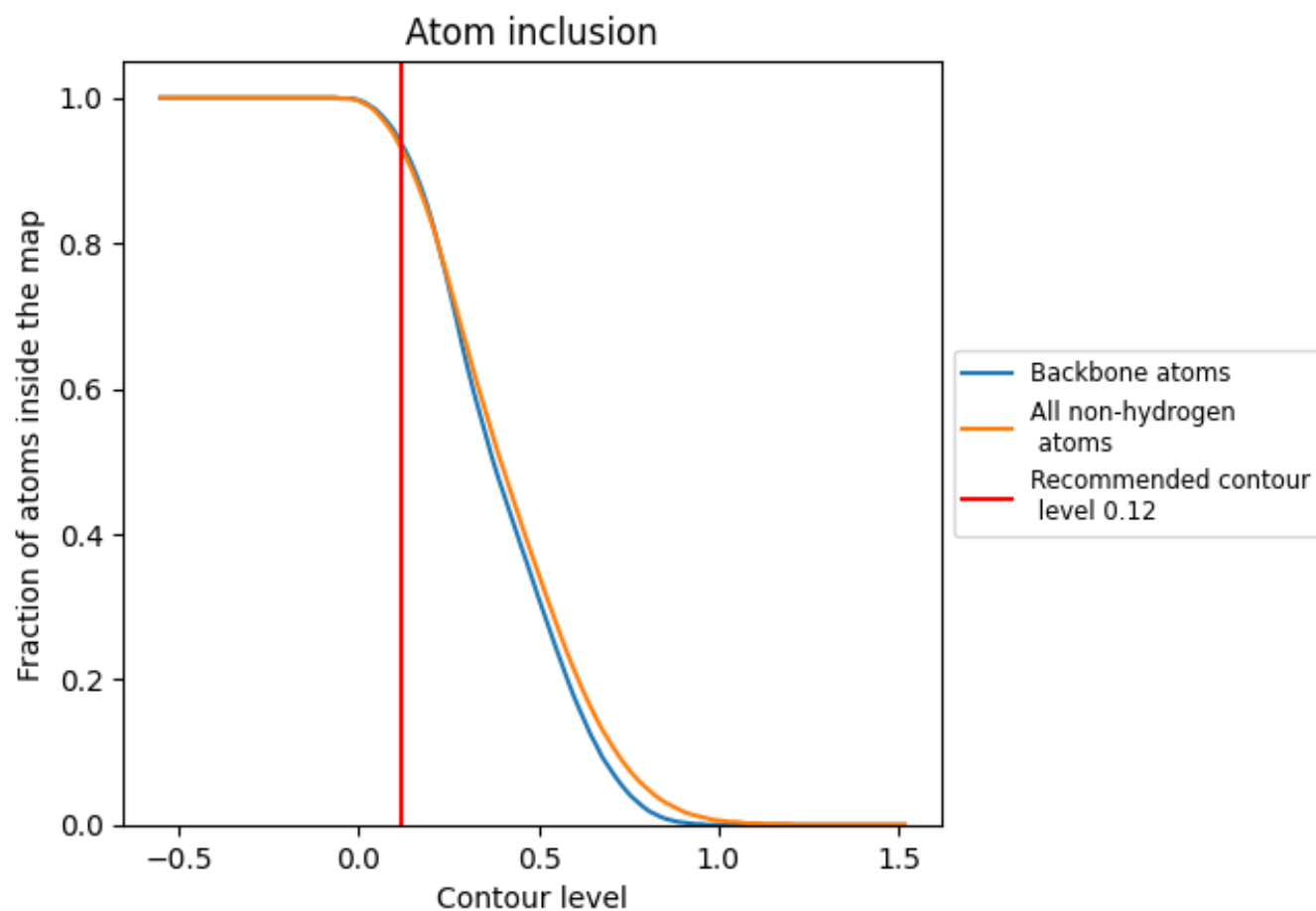
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.5190
0	 0.9260	 0.5600
1	 0.9790	 0.6190
2	 0.9760	 0.6050
3	 0.5750	 0.4940
4	 0.6410	 0.3670
A	 0.9670	 0.4880
B	 0.0710	 0.1600
C	 0.8760	 0.4990
D	 0.8780	 0.4550
E	 0.8540	 0.4620
F	 0.8530	 0.3820
G	 0.7280	 0.3440
H	 0.9270	 0.5190
I	 0.7330	 0.3060
J	 0.7540	 0.2820
K	 0.8900	 0.4290
L	 0.9110	 0.5300
M	 0.6180	 0.2970
N	 0.7460	 0.3380
O	 0.8990	 0.4870
P	 0.8130	 0.4330
Q	 0.8760	 0.4990
R	 0.8030	 0.4040
S	 0.7980	 0.3910
T	 0.9020	 0.4950
U	 0.7700	 0.3380
V	 0.9650	 0.6190
X	 0.8530	 0.5450
Y	 0.7110	 0.3600
a	 0.9670	 0.5610
b	 0.9970	 0.5580
c	 0.9700	 0.5940
d	 0.9730	 0.5900
e	 0.9430	 0.5450



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.9140	 0.4730
g	 0.8580	 0.4050
i	 0.9790	 0.5990
j	 0.9480	 0.5740
k	 0.9510	 0.5700
l	 0.9640	 0.5890
m	 0.9640	 0.5870
n	 0.9410	 0.5310
o	 0.9410	 0.5680
p	 0.9690	 0.5990
q	 0.9420	 0.5720
r	 0.9600	 0.5900
s	 0.9560	 0.5700
t	 0.9630	 0.5560
u	 0.7710	 0.4720
v	 0.9610	 0.5980
w	 0.9850	 0.6060
x	 0.9340	 0.5420
y	 0.9670	 0.5880
z	 0.9630	 0.5980