



Full wwPDB EM Validation Report ⓘ

Jun 20, 2026 – 08:29 pm BST

PDB ID : 28UL / pdb_000028ul
EMDB ID : EMD-56831
Title : E. coli 70S ribosome, conformational ground state mutation in SSU-h41, with A/P- and P/E-site tRNA
Authors : Steinmetzger, C.; Riad, M.; Petzold, K.
Deposited on : 2026-02-20
Resolution : 2.50 Å(reported)
Based on initial model : 7K00

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

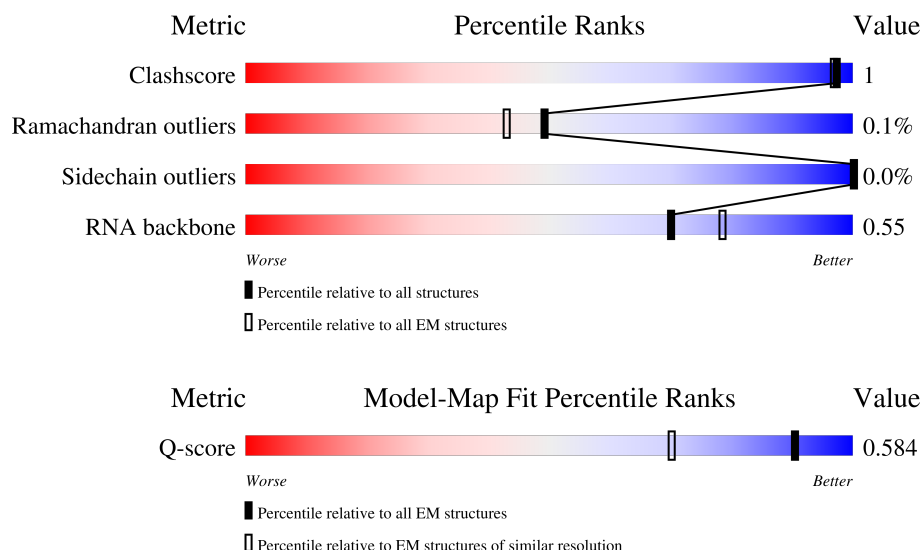
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	3	38	100%
2	4	70	24% 66% 33%
3	K	129	90% 9%

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Mol	Chain	Length	Quality of chain
4	L	124	
5	b	120	
6	c	273	
7	d	209	
8	k	144	
9	l	136	
10	m	127	
11	z	57	
12	A	1542	
13	Y	76	
14	Z	78	
15	a	2904	
16	0	55	
17	1	46	
18	2	65	
19	B	241	
20	C	233	
21	D	206	
22	E	167	
23	F	135	
24	G	179	
25	H	130	
26	I	130	
27	J	103	
28	M	118	

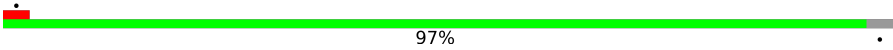
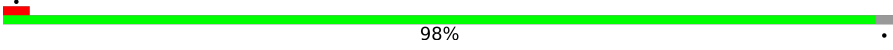
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Mol	Chain	Length	Quality of chain
29	N	101	
30	O	89	
31	P	82	
32	Q	84	
33	R	75	
34	S	92	
35	T	87	
36	U	71	
37	X	10	
38	e	201	
39	f	179	
40	g	177	
41	h	149	
42	i	142	
43	j	123	
44	n	117	
45	o	115	
46	p	118	
47	q	103	
48	r	110	
49	s	100	
50	t	104	
51	u	94	
52	v	85	
53	w	78	

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Mol	Chain	Length	Quality of chain
54	x	63	 97%
55	y	59	 98%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 146224 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 2 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 3 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 4 is a protein called Small ribosomal subunit protein uS12.

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

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

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 10 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 11 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 12 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	1519	Total	C	N	O	P	0	0
			32609	14551	5983	10556	1519		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1260	U	G	engineered mutation	GB 2971070070

- Molecule 13 is a RNA chain called A/P-site Val-tRNA^{Val}.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Y	72	Total	C	N	O	P	S	0	0
			1539	689	280	498	71	1		

- Molecule 14 is a RNA chain called P/E-site tRNA^{fMet}.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Z	72	Total	C	N	O	P	S	0	0
			1546	690	285	498	72	1		

- Molecule 15 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	a	2757	Total	C	N	O	P		0	0
			59216	26422	10911	19126	2757			

- Molecule 16 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 17 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 18 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 19 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 23 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 24 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 25 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 29 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 30 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 31 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 32 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 33 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 34 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 35 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 36 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	U	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	X	10	Total	C	N	O	P	0	0
			216	97	41	68	10		

- Molecule 38 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	46	Total	C	N	O	S	0	0
			348	224	61	62	1		

- Molecule 42 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 44 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 51 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 52 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 53 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 54 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 55 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	b	4	Total	Mg	0
			4	4	
57	c	1	Total	Mg	0
			1	1	
57	d	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	
57	A	38	Total	Mg	0
			38	38	
57	a	167	Total	Mg	0
			167	167	

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

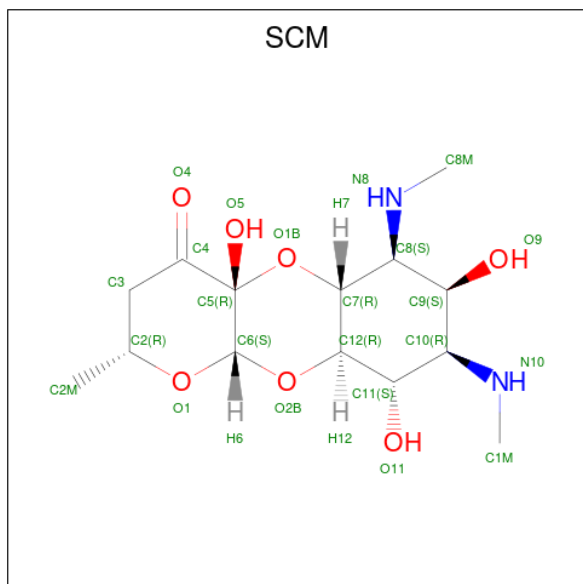
Mol	Chain	Residues	Atoms		AltConf
58	c	3	Total	K	0
			3	3	
58	A	9	Total	K	0
			9	9	
58	a	64	Total	K	0
			64	64	

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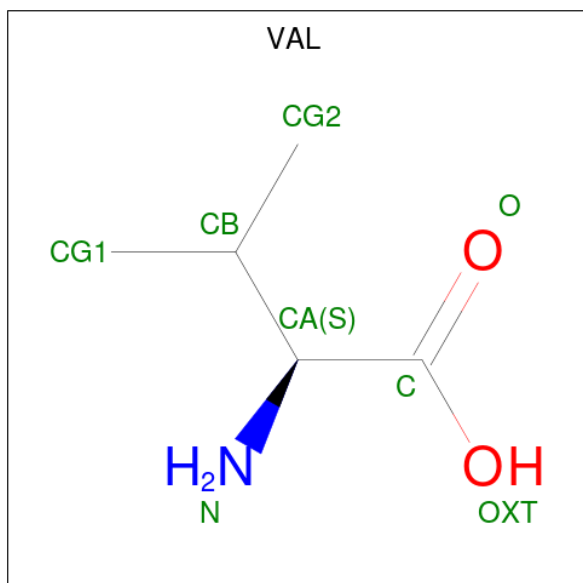
Mol	Chain	Residues	Atoms		AltConf
58	t	1	Total	K	0
			1	1	

- Molecule 59 is SPECTINOMYCIN (CCD ID: SCM) (formula: $C_{14}H_{24}N_2O_7$).



Mol	Chain	Residues	Atoms				AltConf
59	A	1	Total	C	N	O	0
			23	14	2	7	

- Molecule 60 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
60	Y	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms				AltConf
61	3	6	Total	O			0
			6	6			
61	4	1	Total	O			0
			1	1			
61	K	11	Total	O			0
			11	11			
61	L	6	Total	O			0
			6	6			
61	b	64	Total	O			0
			64	64			
61	c	65	Total	O			0
			65	65			
61	d	40	Total	O			0
			40	40			
61	k	39	Total	O			0
			39	39			
61	l	24	Total	O			0
			24	24			
61	m	18	Total	O			0
			18	18			
61	z	23	Total	O			0
			23	23			
61	A	780	Total	O			0
			780	780			
61	Y	11	Total	O			0
			11	11			
61	Z	13	Total	O			0
			13	13			
61	a	3115	Total	O			0
			3115	3115			
61	0	1	Total	O			0
			1	1			
61	1	12	Total	O			0
			12	12			
61	2	18	Total	O			0
			18	18			
61	B	6	Total	O			0
			6	6			

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Mol	Chain	Residues	Atoms		AltConf
61	C	4	Total 4	O 4	0
61	D	5	Total 5	O 5	0
61	E	9	Total 9	O 9	0
61	F	1	Total 1	O 1	0
61	G	6	Total 6	O 6	0
61	H	6	Total 6	O 6	0
61	I	3	Total 3	O 3	0
61	J	2	Total 2	O 2	0
61	N	2	Total 2	O 2	0
61	O	4	Total 4	O 4	0
61	P	2	Total 2	O 2	0
61	Q	1	Total 1	O 1	0
61	R	1	Total 1	O 1	0
61	S	2	Total 2	O 2	0
61	T	3	Total 3	O 3	0
61	U	10	Total 10	O 10	0
61	X	6	Total 6	O 6	0
61	e	37	Total 37	O 37	0
61	f	2	Total 2	O 2	0
61	g	5	Total 5	O 5	0
61	h	4	Total 4	O 4	0

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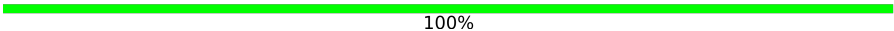
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Mol	Chain	Residues	Atoms		AltConf
61	i	18	Total 18	O 18	0
61	j	11	Total 11	O 11	0
61	n	5	Total 5	O 5	0
61	o	19	Total 19	O 19	0
61	p	31	Total 31	O 31	0
61	q	19	Total 19	O 19	0
61	r	23	Total 23	O 23	0
61	s	13	Total 13	O 13	0
61	t	10	Total 10	O 10	0
61	u	5	Total 5	O 5	0
61	v	9	Total 9	O 9	0
61	w	15	Total 15	O 15	0
61	x	3	Total 3	O 3	0
61	y	7	Total 7	O 7	0

3 Residue-property plots [i](#)

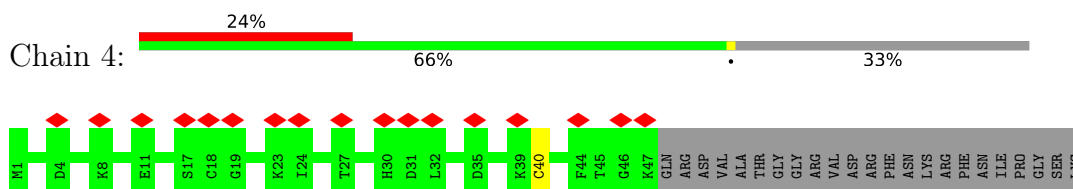
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Large ribosomal subunit protein bL36A

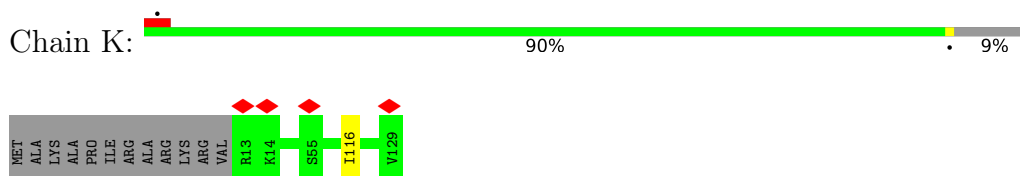
Chain 3:  100%

There are no outlier residues recorded for this chain.

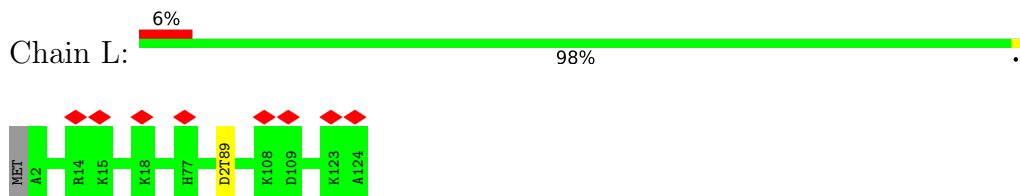
- Molecule 2: Large ribosomal subunit protein bL31



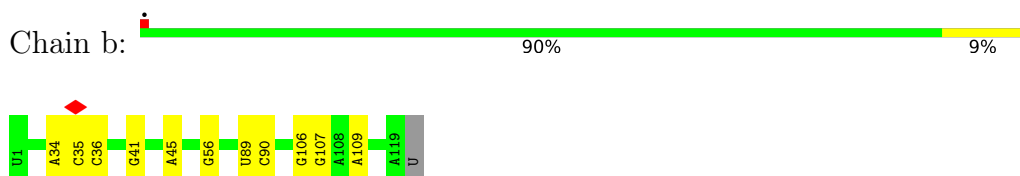
- Molecule 3: Small ribosomal subunit protein uS11



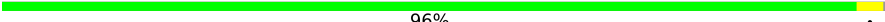
- Molecule 4: Small ribosomal subunit protein uS12



- Molecule 5: 5S rRNA



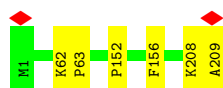
- Molecule 6: Large ribosomal subunit protein uL2

Chain c:  96% ..



- Molecule 7: Large ribosomal subunit protein uL3

Chain d:  97% .



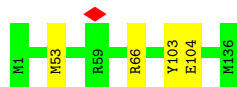
- Molecule 8: Large ribosomal subunit protein uL15

Chain k:  99% .



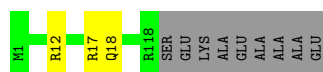
- Molecule 9: Large ribosomal subunit protein uL16

Chain l:  97% .



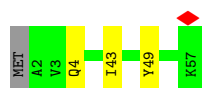
- Molecule 10: Large ribosomal subunit protein bL17

Chain m:  91% . 7%



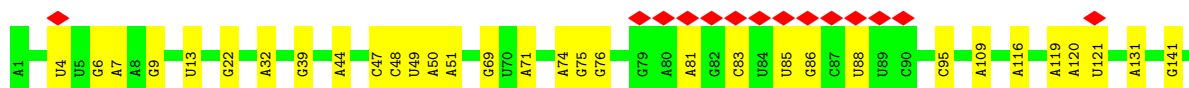
- Molecule 11: Large ribosomal subunit protein bL32

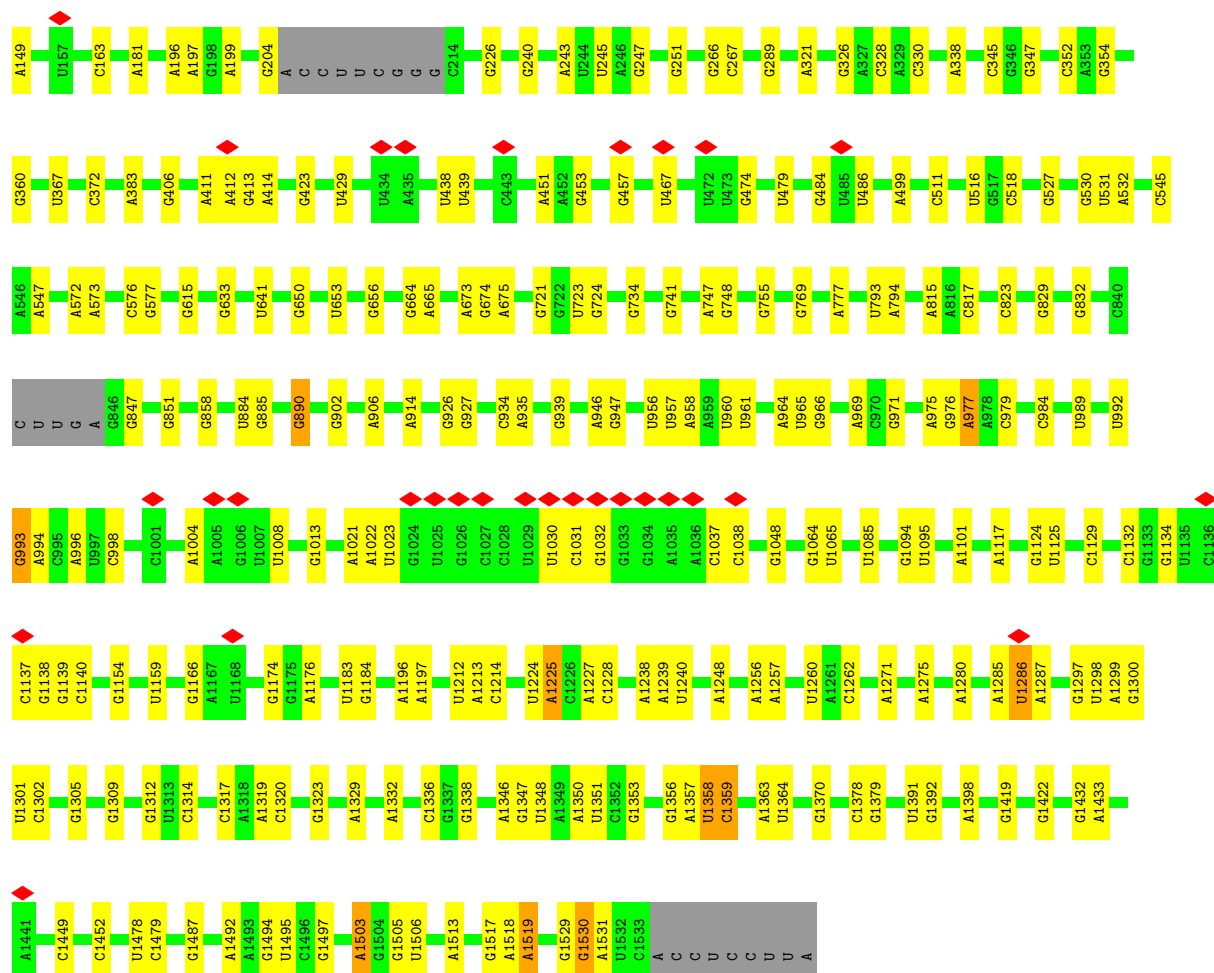
Chain z:  93% 5% .



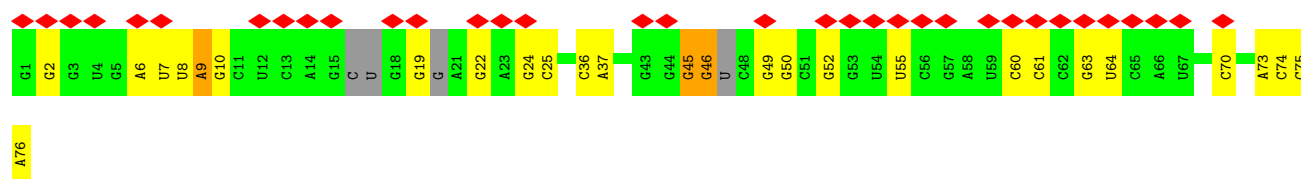
- Molecule 12: 16S rRNA

Chain A:  81% 17% ..

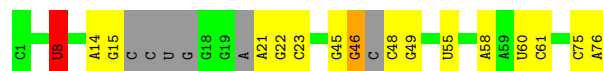




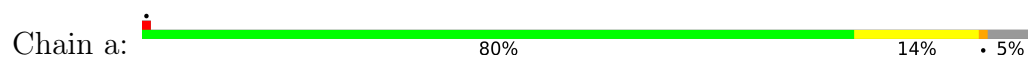
• Molecule 13: A/P-site Val-tRNA^{Val}



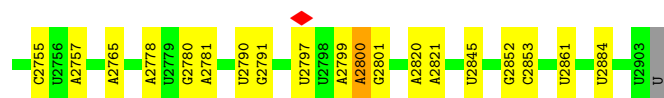
• Molecule 14: P/E-site tRNA^{fMet}



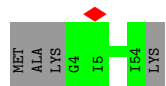
• Molecule 15: 23S rRNA



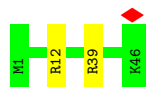




- Molecule 16: Large ribosomal subunit protein bL33



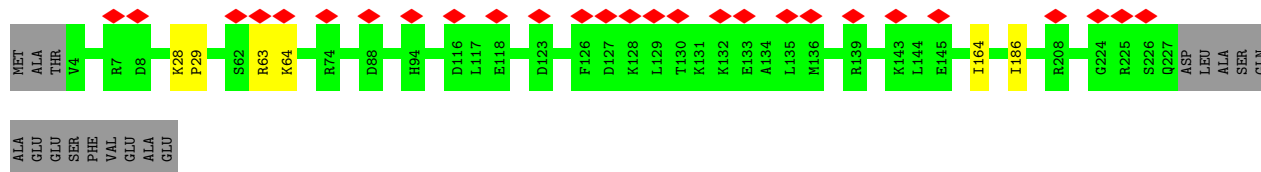
- Molecule 17: Large ribosomal subunit protein bL34



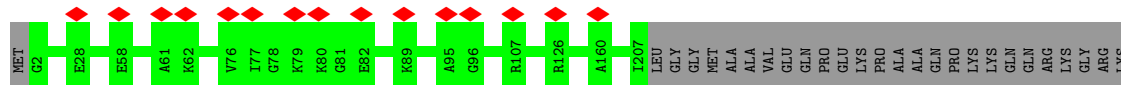
- Molecule 18: Large ribosomal subunit protein bL35



- Molecule 19: Small ribosomal subunit protein uS2

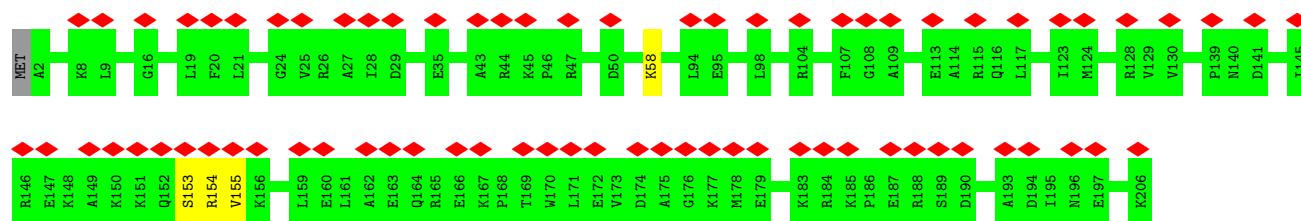


- Molecule 20: Small ribosomal subunit protein uS3

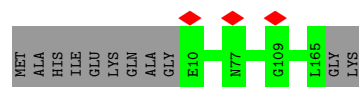


- Molecule 21: Small ribosomal subunit protein uS4

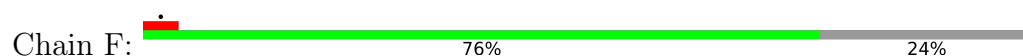




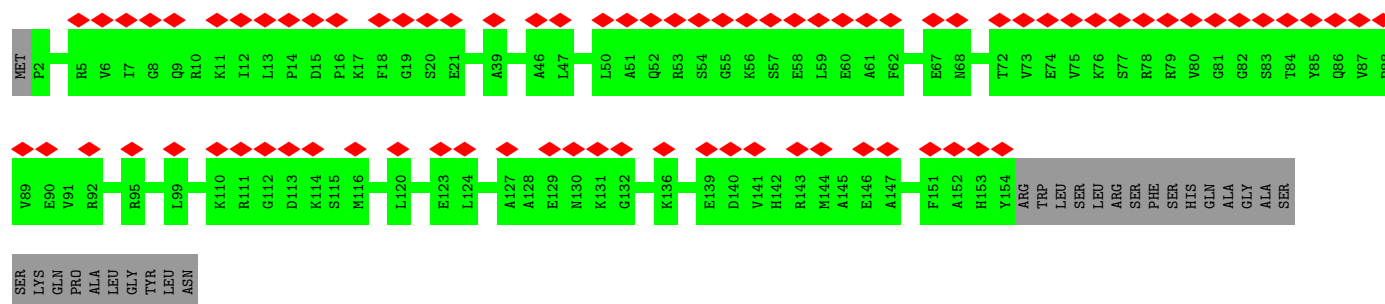
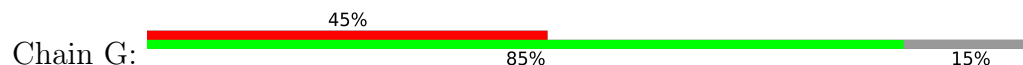
- Molecule 22: Small ribosomal subunit protein uS5



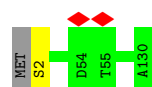
- Molecule 23: Small ribosomal subunit protein bS6, fully modified isoform



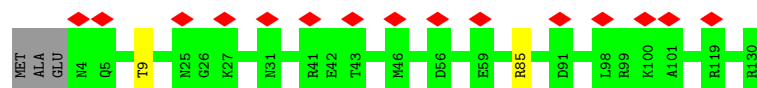
- Molecule 24: Small ribosomal subunit protein uS7



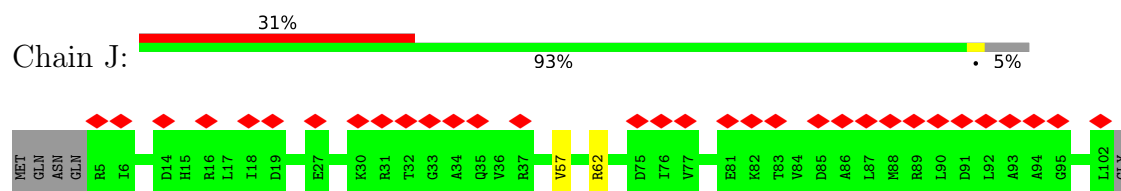
- Molecule 25: Small ribosomal subunit protein uS8



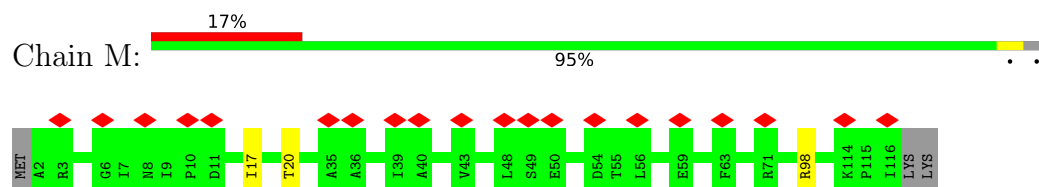
- Molecule 26: Small ribosomal subunit protein uS9



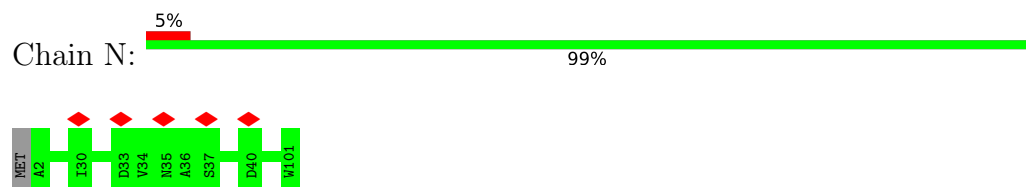
- Molecule 27: Small ribosomal subunit protein uS10



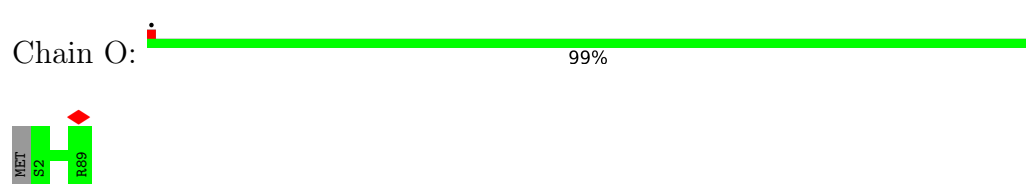
- Molecule 28: Small ribosomal subunit protein uS13



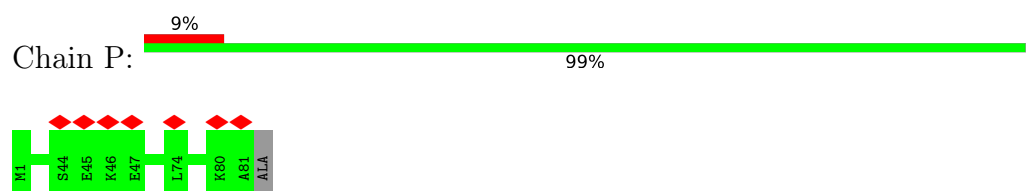
- Molecule 29: Small ribosomal subunit protein uS14



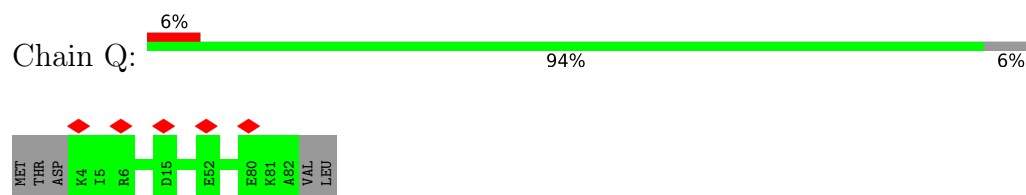
- Molecule 30: Small ribosomal subunit protein uS15



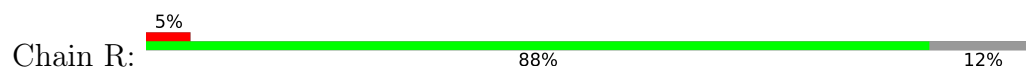
- Molecule 31: Small ribosomal subunit protein bS16

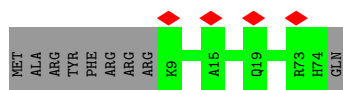


- Molecule 32: Small ribosomal subunit protein uS17

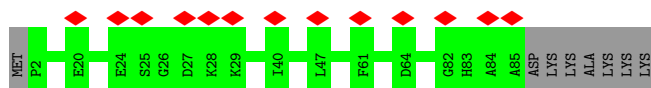
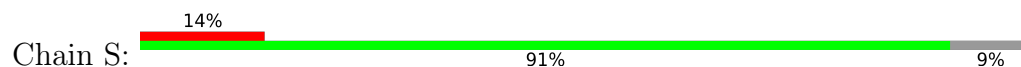


- Molecule 33: Small ribosomal subunit protein bS18

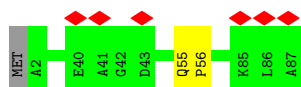




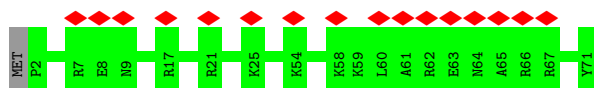
- Molecule 34: Small ribosomal subunit protein uS19



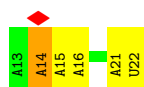
- Molecule 35: Small ribosomal subunit protein bS20



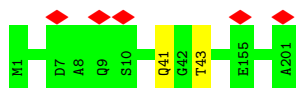
- Molecule 36: Small ribosomal subunit protein bS21



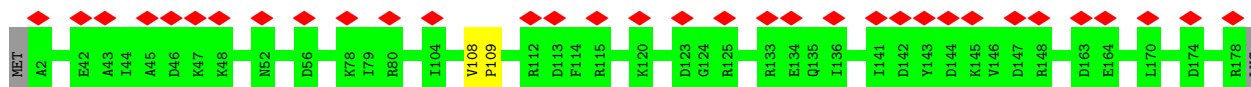
- Molecule 37: mRNA



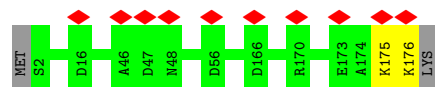
- Molecule 38: Large ribosomal subunit protein uL4



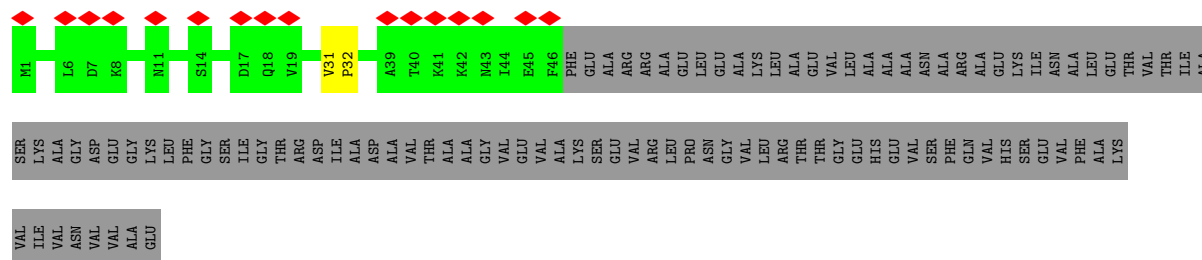
- Molecule 39: Large ribosomal subunit protein uL5



- Molecule 40: Large ribosomal subunit protein uL6



- Molecule 41: Large ribosomal subunit protein bL9



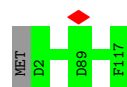
- Molecule 42: Large ribosomal subunit protein uL13



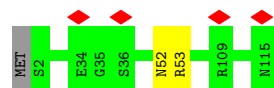
- Molecule 43: Large ribosomal subunit protein uL14



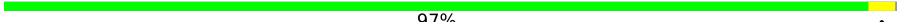
- Molecule 44: Large ribosomal subunit protein uL18



- Molecule 45: Large ribosomal subunit protein bL19



- Molecule 46: Large ribosomal subunit protein bL20

Chain p:  97%



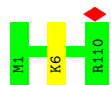
- Molecule 47: Large ribosomal subunit protein bL21

Chain q:  99%



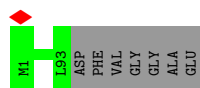
- Molecule 48: Large ribosomal subunit protein uL22

Chain r:  99%



- Molecule 49: Large ribosomal subunit protein uL23

Chain s:  93% 7%



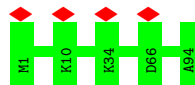
- Molecule 50: Large ribosomal subunit protein uL24

Chain t:  5% 93% 5%



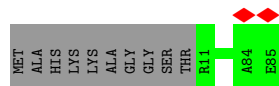
- Molecule 51: Large ribosomal subunit protein bL25

Chain u:  100%

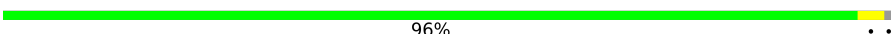


- Molecule 52: Large ribosomal subunit protein bL27

Chain v:  88% 12%

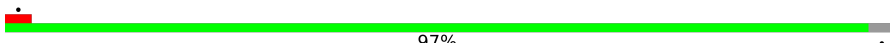


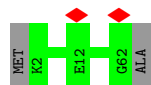
- Molecule 53: Large ribosomal subunit protein bL28

Chain w:  96% ..

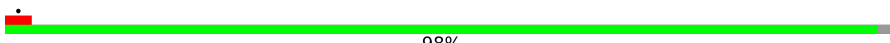


- Molecule 54: Large ribosomal subunit protein uL29

Chain x:  97% .



- Molecule 55: Large ribosomal subunit protein uL30

Chain y:  98% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.88	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.486	Depositor
Minimum map value	-0.171	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0507	Depositor
Map size (Å)	436.32, 436.32, 436.32	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7575, 0.7575, 0.7575	Depositor

5 Model quality

5.1 Standard geometry

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

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	3	0.50	0/303	0.80	0/397
2	4	0.47	0/371	0.82	0/496
3	K	0.51	0/884	0.86	0/1191
4	L	0.47	0/960	0.83	0/1286
5	b	0.53	0/2850	0.78	0/4444
6	c	0.48	0/2121	0.85	0/2852
7	d	0.46	0/1576	0.80	0/2119
8	k	0.47	0/1062	0.84	0/1413
9	l	0.46	0/1073	0.86	0/1433
10	m	0.44	0/958	0.89	0/1281
11	z	0.47	0/450	0.88	0/599
12	A	0.53	1/36232 (0.0%)	0.79	0/56513
13	Y	0.58	0/1596	0.81	0/2478
14	Z	0.56	0/1608	0.77	0/2500
15	a	0.51	1/65747 (0.0%)	0.81	4/102563 (0.0%)
16	0	0.46	0/424	0.79	0/565
17	1	0.47	0/380	0.94	0/498
18	2	0.49	0/513	0.90	0/676
19	B	0.45	0/1784	0.91	0/2403
20	C	0.46	0/1651	0.85	0/2225
21	D	0.44	0/1665	0.90	0/2227
22	E	0.47	0/1165	0.84	0/1568
23	F	0.46	0/858	0.85	0/1160
24	G	0.46	0/1219	0.94	0/1635
25	H	0.46	0/989	0.87	0/1326
26	I	0.45	0/1034	0.90	0/1375
27	J	0.46	0/796	0.86	0/1077
28	M	0.46	0/900	0.93	0/1204
29	N	0.46	0/817	0.92	0/1088
30	O	0.44	0/722	0.97	0/964
31	P	0.45	0/653	0.85	0/877

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Q	0.45	0/650	0.80	0/871
33	R	0.44	0/553	0.91	0/742
34	S	0.49	0/685	0.85	0/922
35	T	0.46	0/676	0.99	0/895
36	U	0.46	0/598	0.98	0/792
37	X	0.55	0/242	0.85	0/375
38	e	0.44	0/1571	0.87	0/2113
39	f	0.45	0/1434	0.89	0/1926
40	g	0.46	0/1333	0.84	0/1805
41	h	0.48	0/352	0.82	0/474
42	i	0.45	0/1152	0.85	0/1551
43	j	0.45	0/956	0.83	0/1279
44	n	0.46	0/902	0.90	0/1209
45	o	0.45	0/929	0.78	0/1242
46	p	0.44	0/960	0.93	0/1278
47	q	0.45	0/829	0.71	0/1107
48	r	0.47	0/864	0.86	0/1156
49	s	0.45	0/744	0.80	0/994
50	t	0.47	0/787	0.78	0/1051
51	u	0.45	0/766	0.81	0/1025
52	v	0.47	0/582	0.80	0/769
53	w	0.46	0/635	0.83	0/848
54	x	0.41	0/496	0.91	0/660
55	y	0.45	0/453	0.89	0/605
All	All	0.50	2/152510 (0.0%)	0.82	4/228122 (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
18	2	0	1
27	J	0	1
45	o	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	2069	G7M	O3'-P	5.06	1.61	1.56
12	A	527	G7M	O3'-P	5.00	1.61	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	781	A	O3'-P-O5'	-6.46	94.32	104.00
15	a	2519	U	O3'-P-O5'	-5.33	96.01	104.00
15	a	2501	C	O3'-P-O5'	-5.11	96.34	104.00
15	a	2601	C	C2'-C3'-O3'	5.09	121.34	113.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	2	13	ARG	Sidechain
27	J	62	ARG	Sidechain
45	o	53	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	302	0	340	0	0
2	4	364	0	362	0	0
3	K	877	0	884	1	0
4	L	957	0	1017	0	0
5	b	2549	0	1291	2	0
6	c	2082	0	2153	5	0
7	d	1566	0	1618	4	0
8	k	1053	0	1129	2	0
9	l	1075	0	1145	2	0
10	m	945	0	989	2	0
11	z	444	0	458	2	0
12	A	32609	0	16431	22	0
13	Y	1539	0	791	5	0
14	Z	1546	0	794	4	0
15	a	59216	0	29791	74	0
16	0	417	0	451	0	0
17	1	377	0	417	2	0
18	2	504	0	572	1	0
19	B	1753	0	1780	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	1624	0	1696	0	0
21	D	1643	0	1707	2	0
22	E	1152	0	1196	0	0
23	F	839	0	833	0	0
24	G	1203	0	1254	0	0
25	H	979	0	1031	1	0
26	I	1022	0	1070	1	0
27	J	786	0	828	0	0
28	M	891	0	952	2	0
29	N	805	0	844	0	0
30	O	714	0	734	0	0
31	P	643	0	661	0	0
32	Q	641	0	682	0	0
33	R	544	0	565	0	0
34	S	668	0	693	0	0
35	T	670	0	719	1	0
36	U	590	0	629	0	0
37	X	216	0	108	1	0
38	e	1552	0	1619	1	0
39	f	1410	0	1444	2	0
40	g	1313	0	1358	1	0
41	h	348	0	372	1	0
42	i	1129	0	1162	2	0
43	j	947	0	1023	1	0
44	n	892	0	923	0	0
45	o	917	0	962	1	0
46	p	947	0	1019	3	0
47	q	816	0	839	1	0
48	r	857	0	922	1	0
49	s	738	0	807	0	0
50	t	779	0	830	3	0
51	u	753	0	780	0	0
52	v	575	0	592	0	0
53	w	625	0	652	1	0
54	x	495	0	526	0	0
55	y	449	0	488	0	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	38	0	0	0	0
57	a	167	0	0	0	0
57	b	4	0	0	0	0
57	c	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	d	1	0	0	0	0
57	z	1	0	0	0	0
58	A	9	0	0	0	0
58	a	64	0	0	0	0
58	c	3	0	0	0	0
58	t	1	0	0	0	0
59	A	23	0	24	0	0
60	Y	7	0	8	0	0
61	0	1	0	0	0	0
61	1	12	0	0	0	0
61	2	18	0	0	0	0
61	3	6	0	0	0	0
61	4	1	0	0	0	0
61	A	780	0	0	0	0
61	B	6	0	0	0	0
61	C	4	0	0	0	0
61	D	5	0	0	0	0
61	E	9	0	0	0	0
61	F	1	0	0	0	0
61	G	6	0	0	0	0
61	H	6	0	0	0	0
61	I	3	0	0	0	0
61	J	2	0	0	0	0
61	K	11	0	0	0	0
61	L	6	0	0	0	0
61	N	2	0	0	0	0
61	O	4	0	0	0	0
61	P	2	0	0	0	0
61	Q	1	0	0	0	0
61	R	1	0	0	0	0
61	S	2	0	0	0	0
61	T	3	0	0	0	0
61	U	10	0	0	0	0
61	X	6	0	0	0	0
61	Y	11	0	0	0	0
61	Z	13	0	0	0	0
61	a	3115	0	0	0	0
61	b	64	0	0	0	0
61	c	65	0	0	0	0
61	d	40	0	0	0	0
61	e	37	0	0	0	0
61	f	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	g	5	0	0	0	0
61	h	4	0	0	0	0
61	i	18	0	0	0	0
61	j	11	0	0	0	0
61	k	39	0	0	0	0
61	l	24	0	0	0	0
61	m	18	0	0	0	0
61	n	5	0	0	0	0
61	o	19	0	0	0	0
61	p	31	0	0	0	0
61	q	19	0	0	0	0
61	r	23	0	0	0	0
61	s	13	0	0	0	0
61	t	10	0	0	0	0
61	u	5	0	0	0	0
61	v	9	0	0	0	0
61	w	15	0	0	0	0
61	x	3	0	0	0	0
61	y	7	0	0	0	0
61	z	23	0	0	0	0
All	All	146224	0	94965	133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:8:4SU:H6	14:Z:8:4SU:H5'	1.66	0.77
15:a:568:U:H1'	15:a:2030:6MZ:H9C1	1.69	0.74
15:a:2601:C:H1'	15:a:2602:A:N7	2.02	0.73
15:a:12:U:H2'	15:a:12:U:O2	1.90	0.70
12:A:1358:U:H3'	12:A:1359:C:H5''	1.80	0.63
6:c:271:ARG:O	6:c:272:SER:C	2.47	0.58
12:A:823:C:HO2'	25:H:2:SER:N	2.03	0.57
15:a:12:U:O2	15:a:12:U:C2'	2.54	0.55
12:A:1286:U:O2	12:A:1286:U:O4'	2.25	0.54
15:a:84:A:N1	15:a:98:G:O2'	2.36	0.54
15:a:1296:G:OP1	15:a:2709:G:O2'	2.20	0.53
15:a:1607:C:H4'	15:a:1608:A:O5'	2.08	0.53
50:t:54:GLN:N	50:t:55:PRO:CD	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:1508:A:O2'	15:a:1509:A:O4'	2.25	0.52
15:a:2845:U:H5''	45:o:52:ASN:O	2.10	0.52
7:d:62:LYS:N	7:d:63:PRO:HD2	2.26	0.51
15:a:2038:G:H2'	15:a:2039:U:O4'	2.11	0.51
15:a:2243:U:H2'	15:a:2244:U:C6	2.46	0.50
9:l:66:ARG:NH2	9:l:104:GLU:OE2	2.45	0.50
15:a:644:A:H2'	15:a:645:C:O4'	2.11	0.50
15:a:534:U:O2'	46:p:49:ASP:OD2	2.28	0.49
53:w:3:ARG:O	53:w:12:PRO:HD3	2.12	0.49
15:a:1115:G:O2'	15:a:1116:G:O5'	2.27	0.49
15:a:2522:U:O2'	15:a:2647:U:OP1	2.28	0.49
15:a:2747:G:O6	15:a:2755:C:H5''	2.13	0.49
15:a:1020:A:N1	15:a:1141:U:O2'	2.32	0.48
11:z:43:ILE:HG22	11:z:49:TYR:HB2	1.95	0.48
15:a:395:U:O2'	15:a:396:G:N7	2.45	0.48
26:I:9:THR:O	26:I:85:ARG:HD3	2.14	0.47
39:f:108:VAL:N	39:f:109:PRO:CD	2.77	0.47
12:A:673:A:H2'	12:A:674:G:C8	2.49	0.47
15:a:2780:G:OP2	42:i:120:ARG:HD3	2.13	0.47
15:a:639:U:H2'	15:a:640:C:C6	2.49	0.47
15:a:1182:G:H2'	15:a:1183:U:O4'	2.14	0.47
15:a:493:G:H2'	15:a:494:G:O4'	2.15	0.47
15:a:1508:A:HO2'	15:a:1509:A:C4'	2.27	0.47
12:A:664:G:H22	12:A:741:G:H1	1.63	0.46
13:Y:37:6MZ:O2'	15:a:1913:A:N1	2.46	0.46
15:a:580:U:O3'	46:p:31:VAL:HG13	2.16	0.46
15:a:1778:U:H2'	15:a:1784:A:N6	2.31	0.46
35:T:55:GLN:N	35:T:56:PRO:HD2	2.31	0.46
10:m:12:ARG:O	10:m:17:ARG:NH2	2.49	0.46
6:c:31:ALA:N	6:c:32:PRO:CD	2.79	0.46
21:D:153:SER:O	21:D:155:VAL:N	2.49	0.46
40:g:175:LYS:O	40:g:176:LYS:C	2.59	0.46
12:A:545:C:OP1	21:D:58:LYS:NZ	2.49	0.46
19:B:28:LYS:N	19:B:29:PRO:CD	2.79	0.45
12:A:769:G:H4'	12:A:1513:A:H4'	1.98	0.45
15:a:1141:U:H4'	15:a:1142:A:O4'	2.17	0.45
14:Z:8:4SU:H6	14:Z:8:4SU:C5'	2.40	0.45
15:a:2852:G:H2'	15:a:2853:C:O4'	2.16	0.45
12:A:1225:A:H2'	12:A:1225:A:N3	2.31	0.45
12:A:338:A:OP2	43:j:98:ARG:NH2	2.50	0.45
15:a:1024:G:C6	15:a:1025:G:C6	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:z:4:GLN:HA	15:a:2615:U:C2	2.52	0.45
15:a:221:A:N1	15:a:265:A:O2'	2.50	0.45
15:a:278:A:O2'	15:a:279:A:P	2.75	0.45
50:t:53:ASN:C	50:t:55:PRO:HD2	2.42	0.45
6:c:242:LYS:O	15:a:1902:C:H4'	2.16	0.44
15:a:468:G:N7	17:1:39:ARG:NH1	2.57	0.44
38:e:41:GLN:HG2	38:e:43:THR:HG23	1.98	0.44
15:a:494:G:H4'	48:r:6:LYS:HB2	2.00	0.44
19:B:164:ILE:O	19:B:186:ILE:HB	2.18	0.44
5:b:41:G:N2	15:a:2339:C:O3'	2.50	0.44
13:Y:24:G:H2'	13:Y:25:C:O4'	2.18	0.44
12:A:1391:U:H2'	12:A:1392:G:C8	2.52	0.44
12:A:50:A:O2'	12:A:360:G:N2	2.51	0.44
15:a:2273:A:H2'	15:a:2274:A:C8	2.53	0.44
15:a:2352:A:C4	15:a:2366:A:C2	3.06	0.44
15:a:2547:A:H2'	15:a:2548:U:C6	2.53	0.44
8:k:57:LEU:HD22	18:2:54:ASP:HB3	2.00	0.43
12:A:1356:G:H2'	12:A:1357:A:C8	2.53	0.43
15:a:1394:U:H4'	15:a:1603:A:H4'	1.99	0.43
15:a:565:C:H2'	15:a:566:U:O4'	2.19	0.43
15:a:687:C:H2'	15:a:688:U:O4'	2.18	0.43
15:a:747:5MU:O2	15:a:2014:A:H1'	2.19	0.43
15:a:1405:U:H2'	15:a:1406:U:C6	2.53	0.43
15:a:819:A:C4	15:a:1189:A:C2	3.06	0.43
14:Z:75:C:O4'	15:a:2432:A:H1'	2.18	0.43
15:a:723:C:H2'	15:a:724:U:O4'	2.18	0.43
37:X:14:A:H2'	37:X:14:A:N3	2.34	0.43
3:K:116:ILE:O	12:A:675:A:O2'	2.33	0.43
5:b:106:G:H2'	5:b:107:G:O4'	2.19	0.43
7:d:208:LYS:O	7:d:209:ALA:C	2.61	0.43
15:a:58:G:O2'	15:a:73:A:N1	2.50	0.43
12:A:993:G:H2'	12:A:993:G:N3	2.33	0.43
15:a:1668:A:O2'	15:a:1674:G:N7	2.49	0.43
15:a:2627:G:O2'	15:a:2781:A:N1	2.37	0.43
28:M:17:ILE:O	28:M:20:THR:OG1	2.34	0.43
6:c:50:THR:HB	15:a:1805:A:N3	2.34	0.42
8:k:21:ARG:HA	15:a:811:U:H2'	2.00	0.42
50:t:54:GLN:N	50:t:55:PRO:HD2	2.34	0.42
7:d:156:PHE:CE1	42:i:81:ILE:HD13	2.54	0.42
15:a:247:G:H4'	15:a:386:G:C5	2.55	0.42
10:m:18:GLN:NE2	15:a:2709:G:OP1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1530:G:H2'	12:A:1531:A:C8	2.54	0.42
15:a:2327:A:H2'	15:a:2328:A:C8	2.55	0.42
15:a:2601:C:O2'	15:a:2602:A:OP2	2.37	0.42
12:A:927:G:O2'	12:A:1503:A:N7	2.43	0.42
15:a:465:G:OP1	17:1:12:ARG:NH1	2.51	0.42
15:a:1939:5MU:OP1	15:a:2604:PSU:O2'	2.35	0.42
19:B:63:ARG:O	19:B:64:LYS:C	2.63	0.42
15:a:1932:A:H2'	15:a:1933:G:O4'	2.20	0.42
15:a:118:A:N3	15:a:178:G:H1'	2.34	0.42
39:f:108:VAL:HG12	39:f:109:PRO:HD3	2.02	0.42
15:a:710:U:H2'	15:a:711:G:H5''	2.02	0.42
15:a:2799:A:O2'	15:a:2800:A:O5'	2.34	0.42
15:a:1020:A:C2	15:a:1141:U:C2	3.08	0.42
12:A:977:A:O2'	12:A:979:C:OP2	2.34	0.41
15:a:714:U:O2'	15:a:716:A:N7	2.45	0.41
15:a:993:G:OP2	46:p:51:ARG:NH1	2.52	0.41
15:a:2202:U:O2'	15:a:2204:G:OP1	2.28	0.41
9:l:53:MET:HE1	9:l:103:TYR:CD1	2.55	0.41
12:A:1309:G:N7	28:M:98:ARG:NH1	2.68	0.41
14:Z:8:4SU:O2'	14:Z:21:A:N1	2.46	0.41
15:a:1730:C:O2	15:a:1730:C:O4'	2.38	0.41
15:a:2328:A:H2'	15:a:2329:U:C6	2.55	0.41
12:A:1359:C:H5''	12:A:1359:C:H6	1.85	0.41
7:d:152:PRO:HG3	7:d:156:PHE:CZ	2.56	0.41
15:a:1009:A:N3	15:a:1153:C:O2'	2.51	0.41
41:h:31:VAL:N	41:h:32:PRO:HD2	2.35	0.41
12:A:1495:U:O2'	15:a:1919:A:N1	2.42	0.41
15:a:340:A:H2'	15:a:341:C:O4'	2.21	0.41
15:a:2291:U:H2'	15:a:2292:U:C6	2.56	0.41
12:A:109:A:C6	12:A:326:G:C6	3.09	0.41
13:Y:63:G:H2'	13:Y:64:U:O4'	2.20	0.41
6:c:72:ASP:OD2	6:c:189:ARG:NH1	2.54	0.40
13:Y:52:G:C2	13:Y:63:G:C2	3.09	0.40
15:a:2245:U:O2'	15:a:2436:G:OP2	2.37	0.40
47:q:74:ILE:N	47:q:74:ILE:HD12	2.37	0.40
12:A:890:G:O2'	12:A:906:A:N6	2.55	0.40
13:Y:9:A:O2'	13:Y:45:G:N2	2.54	0.40
15:a:1548:A:H2'	15:a:1549:A:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	36/38 (95%)	36 (100%)	0	0	100	100
2	4	45/70 (64%)	39 (87%)	5 (11%)	1 (2%)	5	9
3	K	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
4	L	120/124 (97%)	110 (92%)	10 (8%)	0	100	100
6	c	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
7	d	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
8	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
9	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
10	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
11	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
16	0	49/55 (89%)	49 (100%)	0	0	100	100
17	1	44/46 (96%)	44 (100%)	0	0	100	100
18	2	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
19	B	222/241 (92%)	215 (97%)	7 (3%)	0	100	100
20	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
21	D	203/206 (98%)	189 (93%)	13 (6%)	1 (0%)	24	43
22	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
23	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
24	G	151/179 (84%)	144 (95%)	7 (5%)	0	100	100
25	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
26	I	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
27	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	24
28	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
29	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
30	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
32	Q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
33	R	64/75 (85%)	64 (100%)	0	0	100	100
34	S	82/92 (89%)	77 (94%)	5 (6%)	0	100	100
35	T	84/87 (97%)	84 (100%)	0	0	100	100
36	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
38	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
39	f	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
40	g	173/177 (98%)	166 (96%)	7 (4%)	0	100	100
41	h	44/149 (30%)	40 (91%)	4 (9%)	0	100	100
42	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
43	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
44	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
45	o	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
46	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
47	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
48	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
49	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
50	t	100/104 (96%)	97 (97%)	2 (2%)	1 (1%)	12	24
51	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
52	v	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
53	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
54	x	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
55	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
All	All	5470/5913 (92%)	5263 (96%)	203 (4%)	4 (0%)	49	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	40	CYS
27	J	57	VAL
50	t	51	ALA
21	D	154	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	34/34 (100%)	34 (100%)	0	100	100
2	4	43/62 (69%)	43 (100%)	0	100	100
3	K	89/98 (91%)	89 (100%)	0	100	100
4	L	102/103 (99%)	102 (100%)	0	100	100
6	c	216/218 (99%)	216 (100%)	0	100	100
7	d	163/163 (100%)	163 (100%)	0	100	100
8	k	103/103 (100%)	103 (100%)	0	100	100
9	l	107/107 (100%)	107 (100%)	0	100	100
10	m	98/103 (95%)	98 (100%)	0	100	100
11	z	47/48 (98%)	47 (100%)	0	100	100
16	0	46/49 (94%)	46 (100%)	0	100	100
17	1	38/38 (100%)	38 (100%)	0	100	100
18	2	51/52 (98%)	51 (100%)	0	100	100
19	B	186/199 (94%)	186 (100%)	0	100	100
20	C	170/190 (90%)	170 (100%)	0	100	100
21	D	172/173 (99%)	172 (100%)	0	100	100
22	E	119/126 (94%)	119 (100%)	0	100	100
23	F	90/116 (78%)	90 (100%)	0	100	100
24	G	126/147 (86%)	126 (100%)	0	100	100
25	H	104/105 (99%)	104 (100%)	0	100	100
26	I	105/107 (98%)	105 (100%)	0	100	100
27	J	86/90 (96%)	86 (100%)	0	100	100
28	M	93/96 (97%)	93 (100%)	0	100	100
29	N	83/84 (99%)	83 (100%)	0	100	100
30	O	76/77 (99%)	76 (100%)	0	100	100
31	P	65/65 (100%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Q	73/78 (94%)	73 (100%)	0	100	100
33	R	57/65 (88%)	57 (100%)	0	100	100
34	S	72/79 (91%)	72 (100%)	0	100	100
35	T	65/66 (98%)	65 (100%)	0	100	100
36	U	60/61 (98%)	60 (100%)	0	100	100
38	e	165/165 (100%)	165 (100%)	0	100	100
39	f	148/150 (99%)	148 (100%)	0	100	100
40	g	136/138 (99%)	136 (100%)	0	100	100
41	h	37/114 (32%)	37 (100%)	0	100	100
42	i	116/116 (100%)	116 (100%)	0	100	100
43	j	104/104 (100%)	104 (100%)	0	100	100
44	n	86/87 (99%)	86 (100%)	0	100	100
45	o	99/100 (99%)	99 (100%)	0	100	100
46	p	89/90 (99%)	89 (100%)	0	100	100
47	q	84/84 (100%)	84 (100%)	0	100	100
48	r	93/93 (100%)	93 (100%)	0	100	100
49	s	80/84 (95%)	80 (100%)	0	100	100
50	t	83/85 (98%)	82 (99%)	1 (1%)	63	83
51	u	78/78 (100%)	78 (100%)	0	100	100
52	v	57/63 (90%)	57 (100%)	0	100	100
53	w	67/68 (98%)	67 (100%)	0	100	100
54	x	54/55 (98%)	54 (100%)	0	100	100
55	y	48/49 (98%)	48 (100%)	0	100	100
All	All	4563/4825 (95%)	4562 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	t	52	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	118	HIS
4	L	75	GLN
6	c	60	GLN
6	c	134	ASN
7	d	173	GLN
8	k	35	HIS
9	l	60	GLN
10	m	9	GLN
10	m	31	HIS
17	l	6	GLN
19	B	58	ASN
19	B	120	GLN
20	C	139	GLN
21	D	54	GLN
21	D	89	ASN
22	E	82	GLN
22	E	121	HIS
22	E	132	ASN
22	E	148	ASN
23	F	3	HIS
23	F	17	GLN
23	F	46	GLN
24	G	68	ASN
24	G	130	ASN
24	G	142	HIS
25	H	21	ASN
26	I	4	ASN
28	M	8	ASN
29	N	4	GLN
29	N	60	GLN
30	O	50	HIS
31	P	29	ASN
31	P	59	HIS
33	R	54	GLN
34	S	57	HIS
38	e	92	HIS
38	e	94	GLN
40	g	73	ASN
42	i	47	HIS
42	i	128	ASN
44	n	29	HIS
45	o	66	ASN
46	p	52	GLN

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Mol	Chain	Res	Type
48	r	40	ASN
52	v	12	ASN
52	v	57	HIS
53	w	17	ASN
53	w	36	HIS
54	x	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	A	1516/1542 (98%)	235 (15%)	30 (1%)
13	Y	68/76 (89%)	18 (26%)	4 (5%)
14	Z	69/78 (88%)	12 (17%)	3 (4%)
15	a	2753/2904 (94%)	315 (11%)	0
37	X	9/10 (90%)	5 (55%)	0
5	b	118/120 (98%)	8 (6%)	0
All	All	4533/4730 (95%)	593 (13%)	37 (0%)

All (593) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	b	34	A
5	b	35	C
5	b	36	C
5	b	45	A
5	b	56	G
5	b	89	U
5	b	90	C
5	b	109	A
12	A	4	U
12	A	6	G
12	A	9	G
12	A	22	G
12	A	32	A
12	A	39	G
12	A	44	A
12	A	47	C
12	A	48	C
12	A	49	U
12	A	51	A
12	A	69	G

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Mol	Chain	Res	Type
12	A	71	A
12	A	74	A
12	A	75	G
12	A	76	G
12	A	81	A
12	A	83	C
12	A	85	U
12	A	86	G
12	A	88	U
12	A	95	C
12	A	116	A
12	A	119	A
12	A	120	A
12	A	121	U
12	A	131	A
12	A	141	G
12	A	149	A
12	A	163	C
12	A	197	A
12	A	204	G
12	A	226	G
12	A	240	G
12	A	245	U
12	A	247	G
12	A	251	G
12	A	266	G
12	A	267	C
12	A	289	G
12	A	321	A
12	A	328	C
12	A	330	C
12	A	345	C
12	A	347	G
12	A	352	C
12	A	354	G
12	A	367	U
12	A	372	C
12	A	383	A
12	A	406	G
12	A	411	A
12	A	412	A
12	A	413	G

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Mol	Chain	Res	Type
12	A	414	A
12	A	423	G
12	A	429	U
12	A	438	U
12	A	439	U
12	A	451	A
12	A	453	G
12	A	457	G
12	A	467	U
12	A	474	G
12	A	479	U
12	A	484	G
12	A	486	U
12	A	499	A
12	A	511	C
12	A	518	C
12	A	530	G
12	A	531	U
12	A	532	A
12	A	547	A
12	A	572	A
12	A	573	A
12	A	576	C
12	A	577	G
12	A	615	G
12	A	633	G
12	A	650	G
12	A	653	U
12	A	656	G
12	A	665	A
12	A	721	G
12	A	723	U
12	A	724	G
12	A	734	G
12	A	747	A
12	A	748	G
12	A	755	G
12	A	777	A
12	A	793	U
12	A	794	A
12	A	815	A
12	A	817	C

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Mol	Chain	Res	Type
12	A	829	G
12	A	832	G
12	A	847	G
12	A	851	G
12	A	884	U
12	A	885	G
12	A	890	G
12	A	902	G
12	A	914	A
12	A	926	G
12	A	934	C
12	A	935	A
12	A	939	G
12	A	946	A
12	A	947	G
12	A	956	U
12	A	957	U
12	A	958	A
12	A	960	U
12	A	961	U
12	A	964	A
12	A	965	U
12	A	966	2MG
12	A	969	A
12	A	971	G
12	A	975	A
12	A	976	G
12	A	977	A
12	A	984	C
12	A	989	U
12	A	992	U
12	A	993	G
12	A	994	A
12	A	996	A
12	A	998	C
12	A	1004	A
12	A	1008	U
12	A	1013	G
12	A	1021	A
12	A	1022	A
12	A	1023	U
12	A	1030	U

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Mol	Chain	Res	Type
12	A	1031	C
12	A	1032	G
12	A	1037	C
12	A	1038	C
12	A	1048	G
12	A	1064	G
12	A	1065	U
12	A	1085	U
12	A	1094	G
12	A	1095	U
12	A	1101	A
12	A	1117	A
12	A	1124	G
12	A	1125	U
12	A	1132	C
12	A	1134	G
12	A	1137	C
12	A	1138	G
12	A	1139	G
12	A	1140	C
12	A	1154	G
12	A	1159	U
12	A	1166	G
12	A	1174	G
12	A	1176	A
12	A	1184	G
12	A	1196	A
12	A	1197	A
12	A	1212	U
12	A	1213	A
12	A	1214	C
12	A	1224	U
12	A	1225	A
12	A	1227	A
12	A	1228	C
12	A	1238	A
12	A	1239	A
12	A	1240	U
12	A	1248	A
12	A	1256	A
12	A	1257	A
12	A	1260	U

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Mol	Chain	Res	Type
12	A	1262	C
12	A	1271	A
12	A	1275	A
12	A	1280	A
12	A	1285	A
12	A	1286	U
12	A	1287	A
12	A	1297	G
12	A	1298	U
12	A	1299	A
12	A	1300	G
12	A	1301	U
12	A	1302	C
12	A	1305	G
12	A	1312	G
12	A	1314	C
12	A	1317	C
12	A	1320	C
12	A	1323	G
12	A	1329	A
12	A	1332	A
12	A	1336	C
12	A	1338	G
12	A	1346	A
12	A	1347	G
12	A	1348	U
12	A	1350	A
12	A	1351	U
12	A	1353	G
12	A	1358	U
12	A	1359	C
12	A	1363	A
12	A	1364	U
12	A	1370	G
12	A	1378	C
12	A	1379	G
12	A	1398	A
12	A	1419	G
12	A	1422	G
12	A	1432	G
12	A	1433	A
12	A	1449	C

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Mol	Chain	Res	Type
12	A	1452	C
12	A	1479	C
12	A	1487	G
12	A	1492	A
12	A	1494	G
12	A	1497	G
12	A	1503	A
12	A	1505	G
12	A	1506	U
12	A	1517	G
12	A	1519	MA6
12	A	1529	G
12	A	1530	G
13	Y	2	G
13	Y	6	A
13	Y	7	U
13	Y	9	A
13	Y	10	G
13	Y	19	G
13	Y	22	G
13	Y	36	C
13	Y	45	G
13	Y	46	G7M
13	Y	49	G
13	Y	50	G
13	Y	61	C
13	Y	70	C
13	Y	73	A
13	Y	74	C
13	Y	75	C
13	Y	76	A
14	Z	8	4SU
14	Z	14	A
14	Z	15	G
14	Z	22	G
14	Z	23	C
14	Z	45	G
14	Z	46	G7M
14	Z	49	G
14	Z	58	A
14	Z	60	U
14	Z	61	C

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Mol	Chain	Res	Type
14	Z	76	A
15	a	10	A
15	a	12	U
15	a	34	U
15	a	45	G
15	a	63	A
15	a	71	A
15	a	74	A
15	a	75	G
15	a	101	A
15	a	102	U
15	a	110	G
15	a	118	A
15	a	119	A
15	a	120	U
15	a	131	A
15	a	139	U
15	a	140	C
15	a	142	A
15	a	165	A
15	a	181	A
15	a	196	A
15	a	199	A
15	a	200	U
15	a	215	G
15	a	216	A
15	a	221	A
15	a	222	A
15	a	248	G
15	a	272	A
15	a	276	U
15	a	278	A
15	a	279	A
15	a	282	A
15	a	285	G
15	a	287	G
15	a	289	G
15	a	310	A
15	a	311	A
15	a	330	A
15	a	361	G
15	a	386	G

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Mol	Chain	Res	Type
15	a	396	G
15	a	404	A
15	a	405	U
15	a	411	G
15	a	412	A
15	a	451	U
15	a	481	G
15	a	491	G
15	a	503	A
15	a	504	A
15	a	505	A
15	a	509	C
15	a	530	G
15	a	531	C
15	a	532	A
15	a	533	G
15	a	545	U
15	a	547	A
15	a	548	G
15	a	549	G
15	a	563	A
15	a	573	U
15	a	574	A
15	a	575	A
15	a	586	A
15	a	603	A
15	a	615	U
15	a	627	A
15	a	637	A
15	a	645	C
15	a	646	U
15	a	647	G
15	a	654	A
15	a	655	A
15	a	686	U
15	a	711	G
15	a	717	C
15	a	730	A
15	a	738	G
15	a	747	5MU
15	a	764	A
15	a	765	C

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Mol	Chain	Res	Type
15	a	775	G
15	a	776	G
15	a	782	A
15	a	784	G
15	a	785	G
15	a	792	A
15	a	805	G
15	a	812	C
15	a	827	U
15	a	828	U
15	a	846	U
15	a	847	U
15	a	858	G
15	a	859	G
15	a	869	G
15	a	877	A
15	a	883	G
15	a	884	U
15	a	888	C
15	a	890	C
15	a	891	G
15	a	895	U
15	a	896	A
15	a	897	C
15	a	899	A
15	a	910	A
15	a	914	G
15	a	915	C
15	a	927	A
15	a	931	U
15	a	934	U
15	a	946	C
15	a	961	C
15	a	974	G
15	a	983	A
15	a	984	A
15	a	985	C
15	a	996	A
15	a	1005	C
15	a	1012	U
15	a	1013	C
15	a	1022	G

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Mol	Chain	Res	Type
15	a	1033	U
15	a	1040	A
15	a	1047	G
15	a	1108	U
15	a	1110	G
15	a	1111	A
15	a	1112	G
15	a	1116	G
15	a	1128	G
15	a	1129	A
15	a	1130	U
15	a	1132	U
15	a	1133	A
15	a	1135	C
15	a	1141	U
15	a	1142	A
15	a	1171	G
15	a	1253	A
15	a	1256	G
15	a	1271	G
15	a	1272	A
15	a	1273	U
15	a	1300	G
15	a	1301	A
15	a	1321	A
15	a	1345	C
15	a	1352	U
15	a	1365	A
15	a	1379	U
15	a	1380	G
15	a	1383	A
15	a	1416	G
15	a	1428	C
15	a	1452	G
15	a	1453	A
15	a	1482	G
15	a	1490	A
15	a	1493	C
15	a	1508	A
15	a	1515	A
15	a	1529	G
15	a	1535	A

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Mol	Chain	Res	Type
15	a	1536	C
15	a	1537	G
15	a	1569	A
15	a	1578	U
15	a	1584	U
15	a	1585	C
15	a	1608	A
15	a	1609	A
15	a	1644	C
15	a	1647	U
15	a	1648	U
15	a	1649	G
15	a	1674	G
15	a	1715	G
15	a	1729	U
15	a	1730	C
15	a	1732	C
15	a	1738	G
15	a	1764	C
15	a	1773	A
15	a	1782	U
15	a	1800	C
15	a	1801	A
15	a	1807	G
15	a	1808	A
15	a	1816	C
15	a	1829	A
15	a	1842	G
15	a	1847	A
15	a	1848	A
15	a	1858	A
15	a	1862	G
15	a	1869	G
15	a	1872	A
15	a	1873	G
15	a	1907	G
15	a	1910	G
15	a	1911	PSU
15	a	1918	A
15	a	1919	A
15	a	1925	C
15	a	1930	G

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Mol	Chain	Res	Type
15	a	1931	U
15	a	1937	A
15	a	1938	A
15	a	1955	U
15	a	1967	C
15	a	1970	A
15	a	1971	U
15	a	1972	G
15	a	1991	U
15	a	1993	U
15	a	2020	A
15	a	2023	C
15	a	2027	G
15	a	2031	A
15	a	2033	A
15	a	2043	C
15	a	2049	G
15	a	2055	C
15	a	2056	G
15	a	2060	A
15	a	2061	G
15	a	2062	A
15	a	2069	G7M
15	a	2099	U
15	a	2198	A
15	a	2204	G
15	a	2211	A
15	a	2225	A
15	a	2238	G
15	a	2239	G
15	a	2268	A
15	a	2278	A
15	a	2279	G
15	a	2282	G
15	a	2283	C
15	a	2286	G
15	a	2287	A
15	a	2288	A
15	a	2305	U
15	a	2307	G
15	a	2309	A
15	a	2310	C

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Mol	Chain	Res	Type
15	a	2311	A
15	a	2312	U
15	a	2317	A
15	a	2322	A
15	a	2324	U
15	a	2325	G
15	a	2333	A
15	a	2335	A
15	a	2347	C
15	a	2350	C
15	a	2361	G
15	a	2383	G
15	a	2385	C
15	a	2396	G
15	a	2402	U
15	a	2406	A
15	a	2425	A
15	a	2429	G
15	a	2430	A
15	a	2431	U
15	a	2435	A
15	a	2441	U
15	a	2448	A
15	a	2470	G
15	a	2474	U
15	a	2476	A
15	a	2491	U
15	a	2502	G
15	a	2505	G
15	a	2518	A
15	a	2525	G
15	a	2529	G
15	a	2535	G
15	a	2547	A
15	a	2566	A
15	a	2567	G
15	a	2573	C
15	a	2602	A
15	a	2609	U
15	a	2613	U
15	a	2615	U
15	a	2629	U

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Mol	Chain	Res	Type
15	a	2661	G
15	a	2663	G
15	a	2689	U
15	a	2690	U
15	a	2714	G
15	a	2716	C
15	a	2718	G
15	a	2726	A
15	a	2744	G
15	a	2748	A
15	a	2757	A
15	a	2765	A
15	a	2778	A
15	a	2790	U
15	a	2791	G
15	a	2797	U
15	a	2800	A
15	a	2801	G
15	a	2820	A
15	a	2821	A
15	a	2861	U
15	a	2884	U
37	X	14	A
37	X	15	A
37	X	16	A
37	X	21	A
37	X	22	U

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	A	7	A
12	A	13	U
12	A	119	A
12	A	181	A
12	A	196	A
12	A	199	A
12	A	243	A
12	A	438	U
12	A	530	G
12	A	532	A
12	A	641	U

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Mol	Chain	Res	Type
12	A	793	U
12	A	858	G
12	A	884	U
12	A	964	A
12	A	971	G
12	A	993	G
12	A	1124	G
12	A	1129	C
12	A	1183	U
12	A	1224	U
12	A	1225	A
12	A	1239	A
12	A	1240	U
12	A	1297	G
12	A	1319	A
12	A	1320	C
12	A	1363	A
12	A	1432	G
12	A	1478	U
13	Y	6	A
13	Y	49	G
13	Y	60	C
13	Y	74	C
14	Z	48	C
14	Z	58	A
14	Z	60	U

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

50 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	$\# Z > 2$
15	PSU	a	955	58,15	18,21,22	0.91	1 (5%)	22,30,33	0.57	0
12	2MG	A	966	12	23,26,27	0.42	0	32,38,41	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	UR3	A	1498	12	19,22,23	0.28	0	26,32,35	0.64	0
13	6MZ	Y	37	13	22,25,26	0.34	0	30,36,39	0.53	0
3	IAS	K	119	3	6,7,8	0.87	0	6,8,10	0.95	0
15	PSU	a	746	57,15	18,21,22	0.93	1 (5%)	22,30,33	0.57	0
15	5MC	a	1962	58,15	18,22,23	0.34	0	26,32,35	0.47	0
15	OMC	a	2498	57,15	19,22,23	0.25	0	26,31,34	0.51	0
12	MA6	A	1518	12	23,26,27	0.26	0	34,38,41	0.65	1 (2%)
15	6MZ	a	2030	15	22,25,26	0.33	0	30,36,39	0.57	0
9	MS6	l	82	9	5,7,8	0.20	0	2,7,9	0.12	0
14	4SU	Z	8	14	18,21,22	0.39	0	26,30,33	1.16	3 (11%)
15	3TD	a	1915	15	18,22,23	0.96	1 (5%)	22,32,35	0.66	0
14	OMC	Z	32	14	19,22,23	0.26	0	26,31,34	0.35	0
15	OMG	a	2251	58,15,13	23,26,27	0.33	0	33,38,41	0.41	0
12	G7M	A	527	12	23,26,27	0.72	1 (4%)	35,39,42	0.66	0
12	4OC	A	1402	12	20,23,24	0.36	0	26,32,35	0.49	0
15	PSU	a	1911	15	18,21,22	0.89	1 (5%)	22,30,33	0.53	0
15	2MA	a	2503	57,58,15	22,25,26	0.25	0	33,37,40	0.63	1 (3%)
15	OMU	a	2552	15	19,22,23	0.20	0	26,31,34	0.42	0
15	PSU	a	2580	58,15	18,21,22	0.93	1 (5%)	22,30,33	0.70	1 (4%)
12	MA6	A	1519	12	23,26,27	0.25	0	34,38,41	0.74	1 (2%)
15	H2U	a	2449	15	18,21,22	0.58	0	21,30,33	0.74	1 (4%)
15	1MG	a	745	15	22,26,27	0.52	0	33,39,42	0.49	0
15	PSU	a	2605	15	18,21,22	0.90	1 (5%)	22,30,33	0.80	0
15	PSU	a	2457	15	18,21,22	0.90	1 (5%)	22,30,33	0.60	0
14	G7M	Z	46	14	23,26,27	0.73	1 (4%)	35,39,42	0.58	0
13	4SU	Y	8	13	18,21,22	0.37	0	26,30,33	1.20	3 (11%)
15	PSU	a	2604	15	18,21,22	0.89	1 (5%)	22,30,33	0.79	1 (4%)
15	2MG	a	2445	15	23,26,27	0.40	0	32,38,41	0.38	0
15	5MU	a	747	15	19,22,23	0.25	0	28,32,35	0.33	0
15	PSU	a	1917	15	18,21,22	0.91	1 (5%)	22,30,33	0.55	0
15	PSU	a	2504	58,15	18,21,22	0.90	1 (5%)	22,30,33	0.71	0
12	5MC	A	967	12	18,22,23	0.32	0	26,32,35	0.52	0
9	4D4	l	81	9	9,11,12	0.51	0	8,13,15	0.75	0
14	PSU	Z	55	14	18,21,22	0.91	1 (5%)	22,30,33	0.63	0
15	2MG	a	1835	15	23,26,27	0.39	0	32,38,41	0.37	0
13	5MU	Y	54	13	19,22,23	0.27	0	28,32,35	0.29	0
13	G7M	Y	46	13	23,26,27	0.71	1 (4%)	35,39,42	0.57	0
15	5MU	a	1939	15	19,22,23	0.29	0	28,32,35	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	2MG	A	1207	12	23,26,27	0.38	0	32,38,41	0.38	0
14	5MU	Z	54	14	19,22,23	0.27	0	28,32,35	0.26	0
12	PSU	A	516	12	18,21,22	0.90	1 (5%)	22,30,33	0.70	1 (4%)
12	2MG	A	1516	12	23,26,27	0.38	0	32,38,41	0.50	0
7	MEQ	d	150	7	8,9,10	0.42	0	5,10,12	0.71	0
15	6MZ	a	1618	15	22,25,26	0.34	0	30,36,39	0.52	0
15	G7M	a	2069	15	23,26,27	0.71	1 (4%)	35,39,42	0.63	1 (2%)
4	D2T	L	89	4	7,9,10	0.95	0	6,11,13	1.60	2 (33%)
13	PSU	Y	55	13	18,21,22	0.93	1 (5%)	22,30,33	0.65	0
12	5MC	A	1407	12	18,22,23	0.32	0	26,32,35	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PSU	a	955	58,15	-	0/7/25/26	0/2/2/2
12	2MG	A	966	12	-	3/9/27/28	0/3/3/3
12	UR3	A	1498	12	-	0/7/25/26	0/2/2/2
13	6MZ	Y	37	13	-	0/9/27/28	0/3/3/3
3	IAS	K	119	3	-	0/7/7/8	-
15	PSU	a	746	57,15	-	2/7/25/26	0/2/2/2
15	5MC	a	1962	58,15	-	0/7/25/26	0/2/2/2
15	OMC	a	2498	57,15	-	0/9/27/28	0/2/2/2
12	MA6	A	1518	12	-	0/11/29/30	0/3/3/3
15	6MZ	a	2030	15	-	2/9/27/28	0/3/3/3
9	MS6	l	82	9	-	1/4/6/8	-
14	4SU	Z	8	14	-	2/7/25/26	0/2/2/2
15	3TD	a	1915	15	-	0/7/25/26	0/2/2/2
14	OMC	Z	32	14	-	0/9/27/28	0/2/2/2
15	OMG	a	2251	58,15,13	-	0/9/27/28	0/3/3/3
12	G7M	A	527	12	-	1/7/25/26	0/3/3/3
12	4OC	A	1402	12	-	0/9/29/30	0/2/2/2
15	PSU	a	1911	15	-	3/7/25/26	0/2/2/2
15	2MA	a	2503	57,58,15	-	1/7/25/26	0/3/3/3
15	OMU	a	2552	15	-	0/9/27/28	0/2/2/2
15	PSU	a	2580	58,15	-	0/7/25/26	0/2/2/2
12	MA6	A	1519	12	-	3/11/29/30	0/3/3/3
15	H2U	a	2449	15	-	0/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	1MG	a	745	15	-	0/7/25/26	0/3/3/3
15	PSU	a	2605	15	-	0/7/25/26	0/2/2/2
15	PSU	a	2457	15	-	0/7/25/26	0/2/2/2
14	G7M	Z	46	14	-	1/7/25/26	0/3/3/3
13	4SU	Y	8	13	-	1/7/25/26	0/2/2/2
15	PSU	a	2604	15	-	0/7/25/26	0/2/2/2
15	2MG	a	2445	15	-	0/9/27/28	0/3/3/3
15	5MU	a	747	15	-	1/7/25/26	0/2/2/2
15	PSU	a	1917	15	-	0/7/25/26	0/2/2/2
15	PSU	a	2504	58,15	-	0/7/25/26	0/2/2/2
12	5MC	A	967	12	-	0/7/25/26	0/2/2/2
9	4D4	l	81	9	-	3/11/12/14	-
14	PSU	Z	55	14	-	2/7/25/26	0/2/2/2
15	2MG	a	1835	15	-	0/9/27/28	0/3/3/3
13	5MU	Y	54	13	-	0/7/25/26	0/2/2/2
13	G7M	Y	46	13	-	3/7/25/26	0/3/3/3
15	5MU	a	1939	15	-	0/7/25/26	0/2/2/2
12	2MG	A	1207	12	-	0/9/27/28	0/3/3/3
14	5MU	Z	54	14	-	0/7/25/26	0/2/2/2
12	PSU	A	516	12	-	0/7/25/26	0/2/2/2
12	2MG	A	1516	12	-	0/9/27/28	0/3/3/3
7	MEQ	d	150	7	-	2/8/9/11	-
15	6MZ	a	1618	15	-	0/9/27/28	0/3/3/3
15	G7M	a	2069	15	-	2/7/25/26	0/3/3/3
4	D2T	L	89	4	-	2/7/12/14	-
13	PSU	Y	55	13	-	0/7/25/26	0/2/2/2
12	5MC	A	1407	12	-	0/7/25/26	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	746	PSU	C6-C5	3.66	1.39	1.35
13	Y	55	PSU	C6-C5	3.64	1.39	1.35
15	a	1915	3TD	C6-C5	3.63	1.39	1.35
14	Z	55	PSU	C6-C5	3.59	1.39	1.35
15	a	1917	PSU	C6-C5	3.58	1.39	1.35
15	a	2580	PSU	C6-C5	3.55	1.39	1.35
12	A	516	PSU	C6-C5	3.54	1.39	1.35
15	a	2457	PSU	C6-C5	3.53	1.39	1.35
15	a	1911	PSU	C6-C5	3.52	1.39	1.35
15	a	2605	PSU	C6-C5	3.50	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	2504	PSU	C6-C5	3.50	1.39	1.35
15	a	2604	PSU	C6-C5	3.48	1.39	1.35
15	a	955	PSU	C6-C5	3.45	1.39	1.35
15	a	2069	G7M	C8-N7	2.63	1.37	1.33
12	A	527	G7M	C8-N7	2.60	1.37	1.33
13	Y	46	G7M	C8-N7	2.57	1.37	1.33
14	Z	46	G7M	C8-N7	2.51	1.37	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Y	8	4SU	C4-N3-C2	-4.36	123.11	127.34
14	Z	8	4SU	C4-N3-C2	-4.32	123.15	127.34
12	A	1519	MA6	C2-N1-C6	2.93	118.67	111.75
12	A	1518	MA6	C2-N1-C6	2.89	118.59	111.75
13	Y	8	4SU	C5-C4-N3	2.79	117.28	114.69
14	Z	8	4SU	C5-C4-N3	2.68	117.18	114.69
4	L	89	D2T	OD1-CG-CB	-2.47	117.27	122.44
15	a	2503	2MA	C5-C4-N3	-2.35	124.55	127.19
15	a	2604	PSU	C2'-C3'-C4'	-2.31	98.16	102.64
13	Y	8	4SU	N3-C2-N1	2.18	117.78	114.89
15	a	2580	PSU	C3'-C2'-C1'	2.12	104.11	101.64
15	a	2449	H2U	O2-C2-N1	-2.12	120.44	123.11
14	Z	8	4SU	N3-C2-N1	2.11	117.69	114.89
12	A	516	PSU	C3'-C2'-C1'	2.08	104.06	101.64
4	L	89	D2T	OD2-CG-CB	2.02	117.51	113.15
15	a	2069	G7M	N9-C8-N7	-2.01	107.23	112.21

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	89	D2T	CA-CB-SB-CB1
12	A	1519	MA6	O4'-C4'-C5'-O5'
15	a	746	PSU	C2'-C1'-C5-C4
12	A	966	2MG	O4'-C4'-C5'-O5'
12	A	966	2MG	C3'-C4'-C5'-O5'
12	A	1519	MA6	C3'-C4'-C5'-O5'
13	Y	46	G7M	O4'-C4'-C5'-O5'
13	Y	46	G7M	C3'-C4'-C5'-O5'
14	Z	8	4SU	C3'-C4'-C5'-O5'
15	a	2030	6MZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
15	a	1911	PSU	C3'-C4'-C5'-O5'
15	a	1911	PSU	O4'-C4'-C5'-O5'
7	d	150	MEQ	NE2-CD-CG-CB
7	d	150	MEQ	OE1-CD-CG-CB
13	Y	46	G7M	C4'-C5'-O5'-P
15	a	2030	6MZ	C3'-C4'-C5'-O5'
14	Z	8	4SU	O4'-C4'-C5'-O5'
15	a	1911	PSU	C4'-C5'-O5'-P
13	Y	8	4SU	C4'-C5'-O5'-P
15	a	2069	G7M	C4'-C5'-O5'-P
15	a	747	5MU	C3'-C4'-C5'-O5'
9	l	81	4D4	OB-CB-CG-CD
9	l	81	4D4	CA-CB-CG-CD
12	A	966	2MG	C4'-C5'-O5'-P
9	l	82	MS6	CB-CG-SD-CE
12	A	527	G7M	C4'-C5'-O5'-P
14	Z	46	G7M	C4'-C5'-O5'-P
9	l	81	4D4	CG-CD-NE-CZ
14	Z	55	PSU	O4'-C1'-C5-C4
4	L	89	D2T	CG-CB-SB-CB1
14	Z	55	PSU	O4'-C1'-C5-C6
15	a	746	PSU	O4'-C1'-C5-C6
15	a	2069	G7M	O4'-C4'-C5'-O5'
15	a	2503	2MA	O4'-C4'-C5'-O5'
12	A	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Y	37	6MZ	1	0
15	a	2030	6MZ	1	0
14	Z	8	4SU	3	0
15	a	2604	PSU	1	0
15	a	747	5MU	1	0
15	a	1939	5MU	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 293 ligands modelled in this entry, 291 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
60	VAL	Y	101	13	4,6,7	0.58	0	6,7,9	0.84	0
59	SCM	A	1601	-	23,25,25	0.26	0	26,39,39	0.69	1 (3%)

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
60	VAL	Y	101	13	-	1/5/6/8	-
59	SCM	A	1601	-	-	2/4/57/57	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	A	1601	SCM	C11-C10-C9	2.07	114.94	110.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

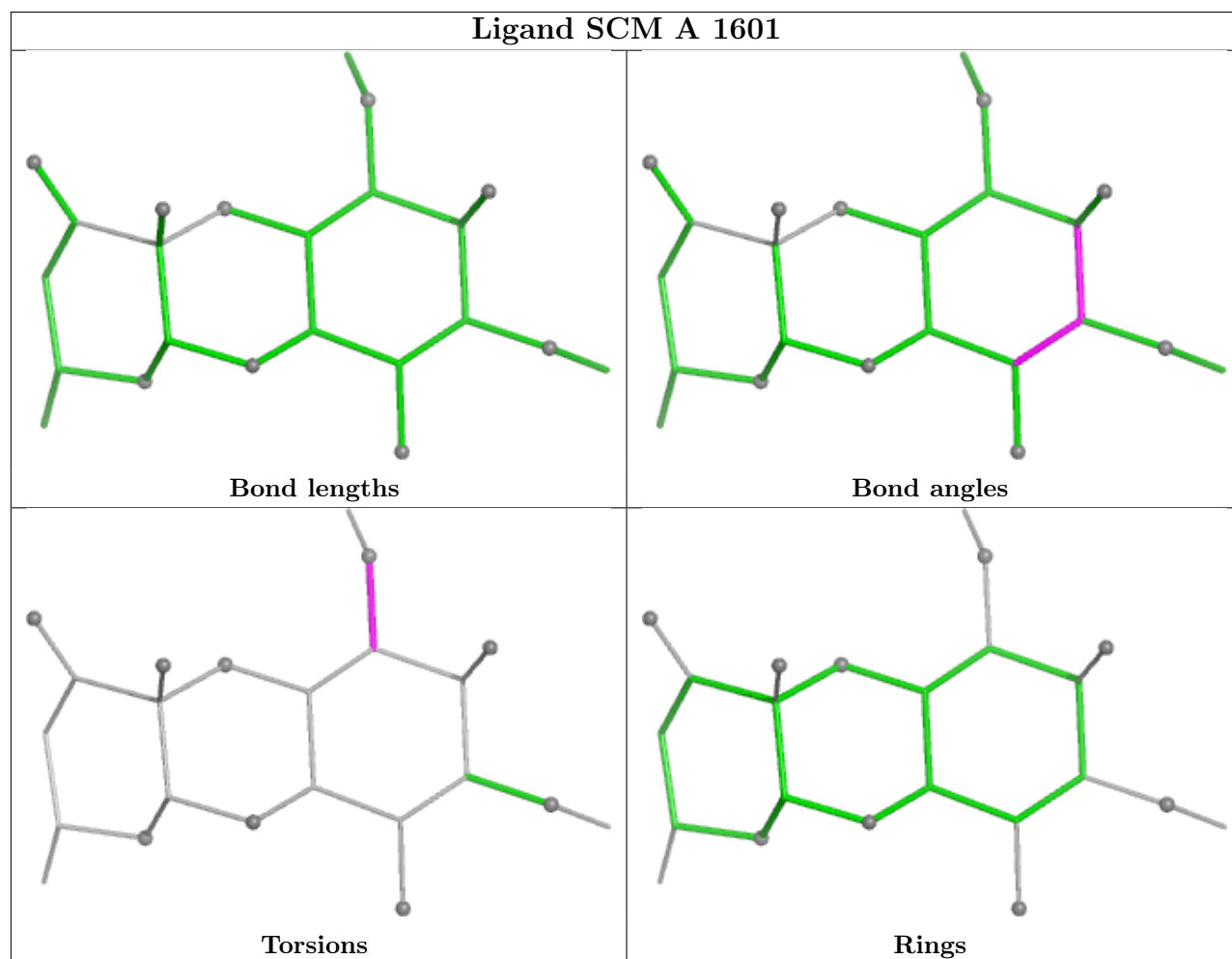
Mol	Chain	Res	Type	Atoms
59	A	1601	SCM	C7-C8-N8-C8M
59	A	1601	SCM	C9-C8-N8-C8M
60	Y	101	VAL	O-C-CA-CB

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

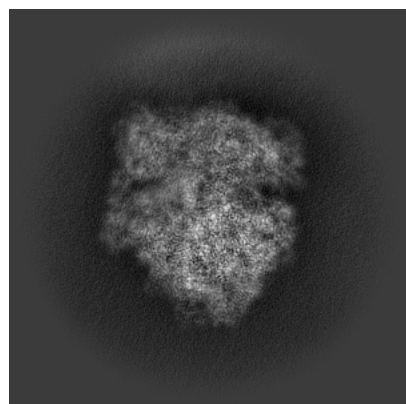
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56831. These allow visual inspection of the internal detail of the map and identification of artifacts.

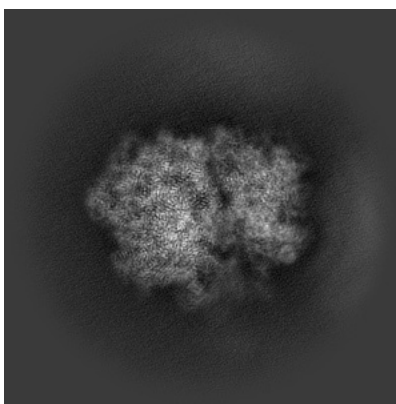
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

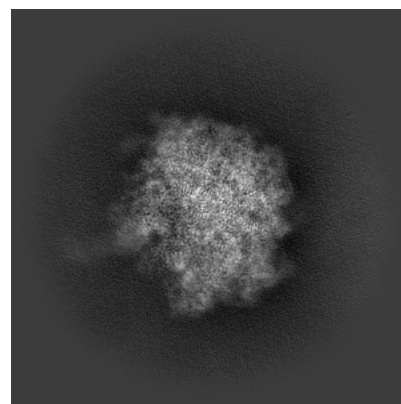
6.1.1 Primary map



X

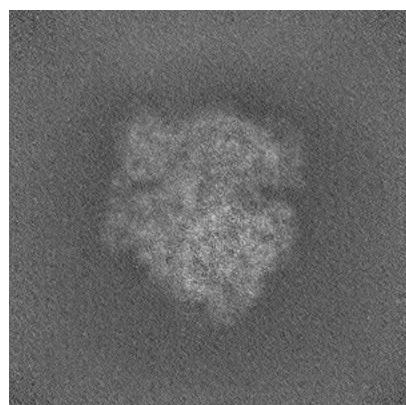


Y

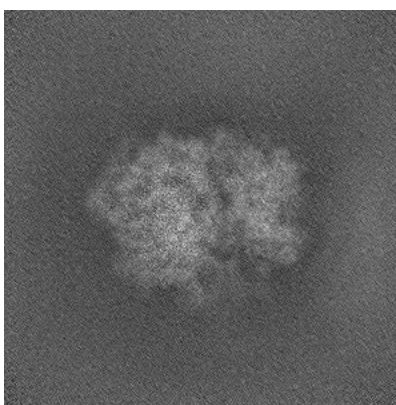


Z

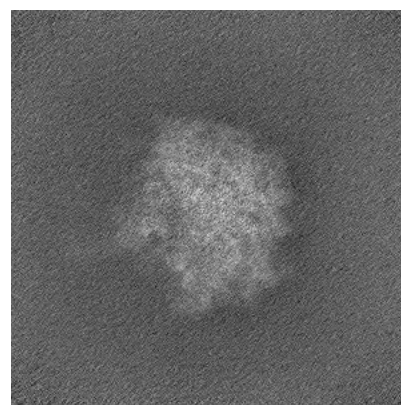
6.1.2 Raw map



X



Y

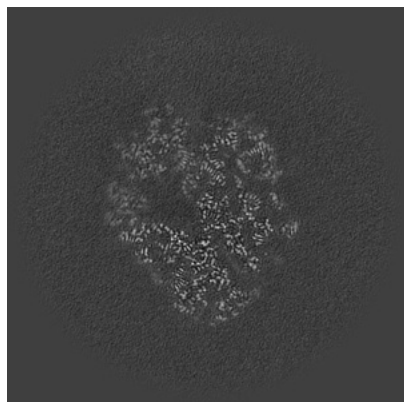


Z

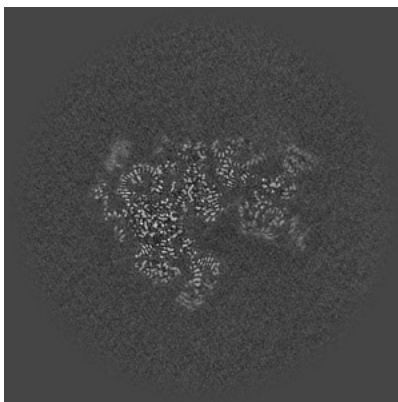
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

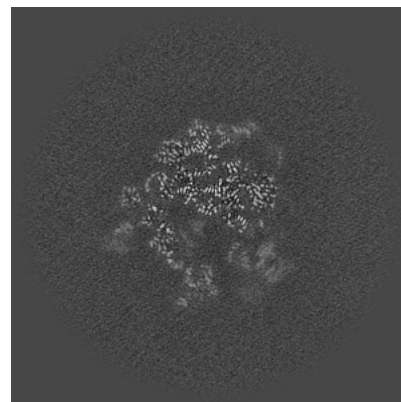
6.2.1 Primary map



X Index: 288

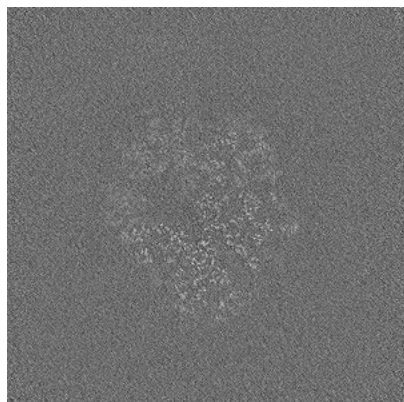


Y Index: 288

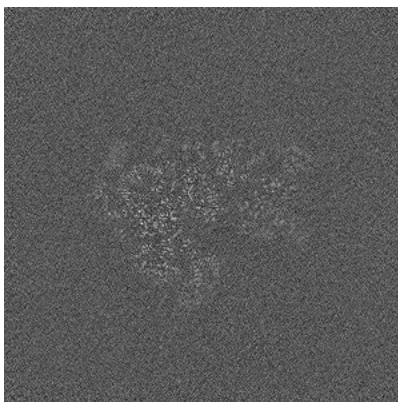


Z Index: 288

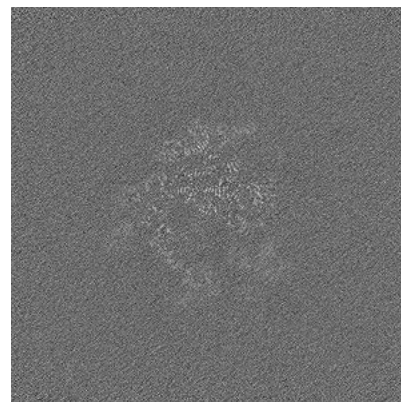
6.2.2 Raw map



X Index: 288



Y Index: 288

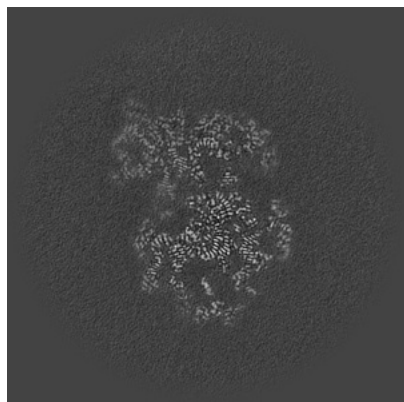


Z Index: 288

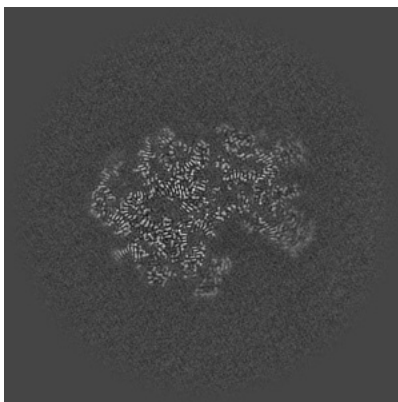
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

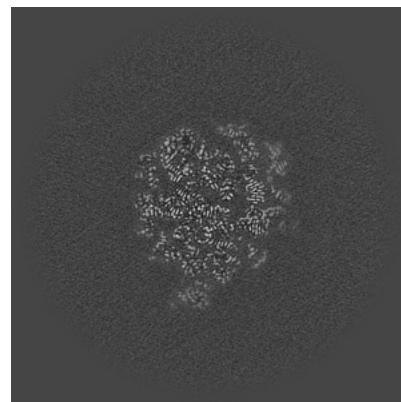
6.3.1 Primary map



X Index: 312

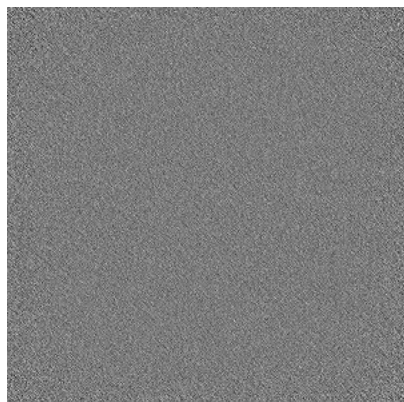


Y Index: 304

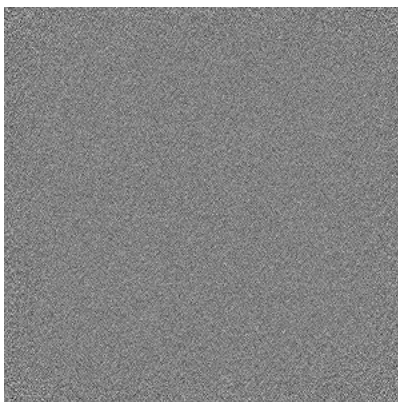


Z Index: 234

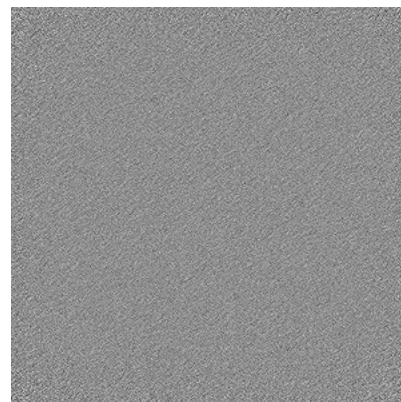
6.3.2 Raw map



X Index: 0



Y Index: 0

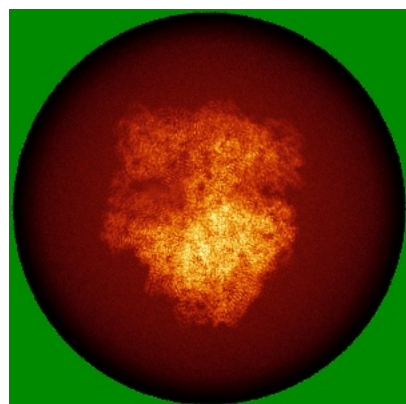


Z Index: 0

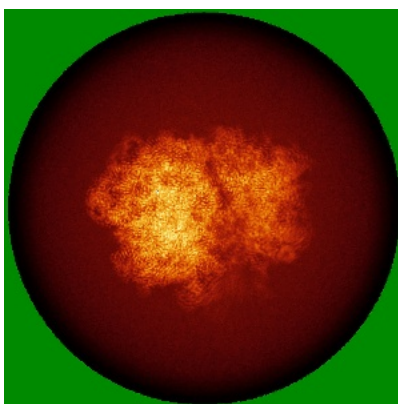
The images above show the largest variance slices of the map in three orthogonal directions.

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

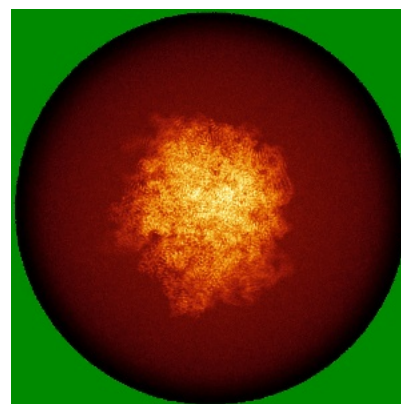
6.4.1 Primary map



X

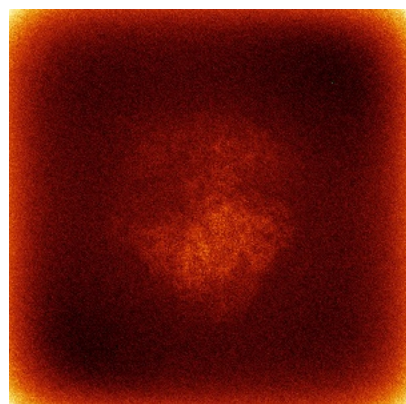


Y

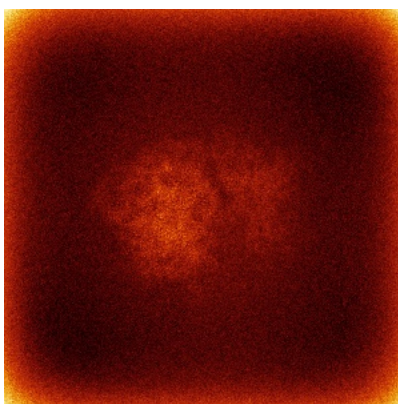


Z

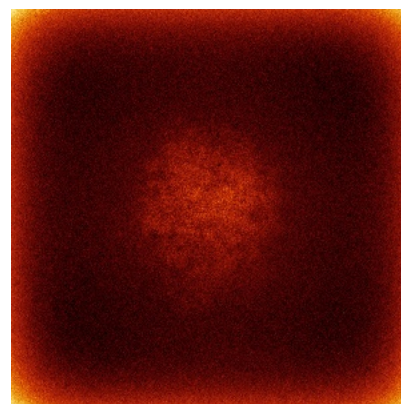
6.4.2 Raw map



X



Y

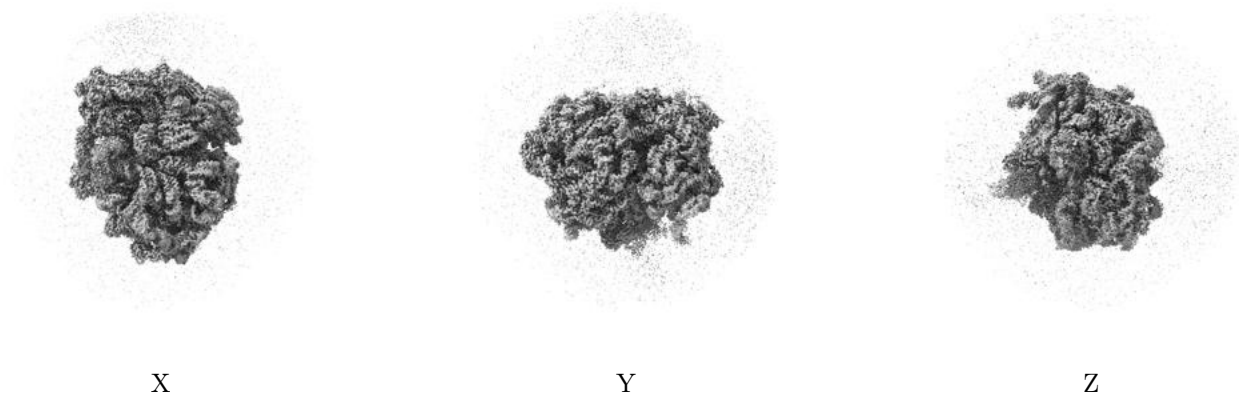


Z

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.

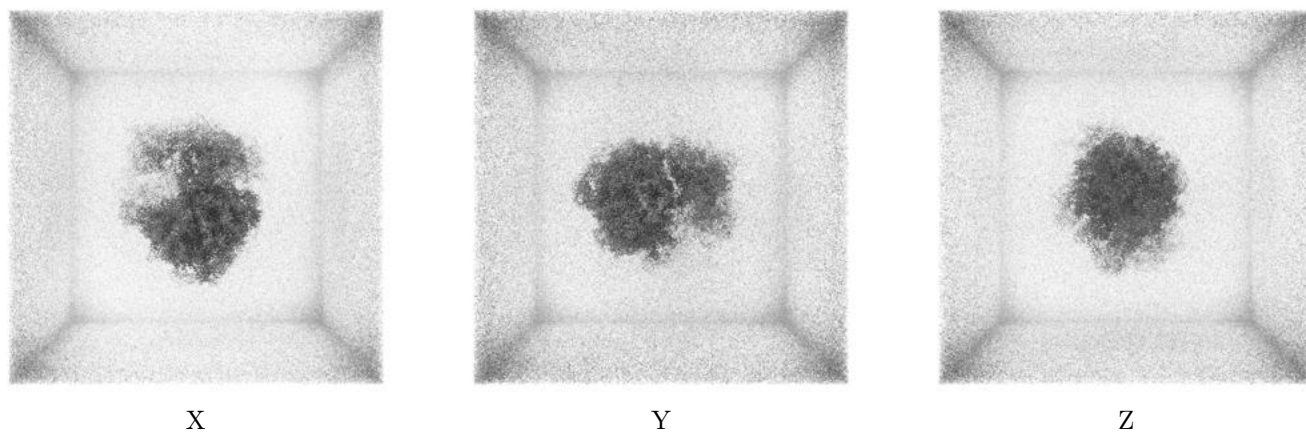
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0507. 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.

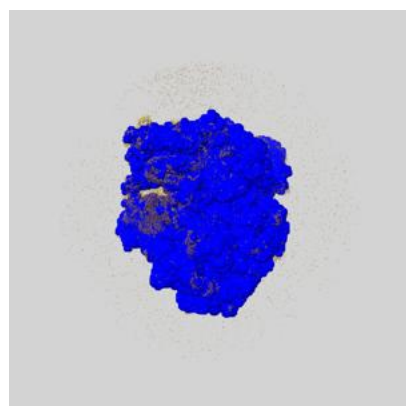
6.6 Mask visualisation [i](#)

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

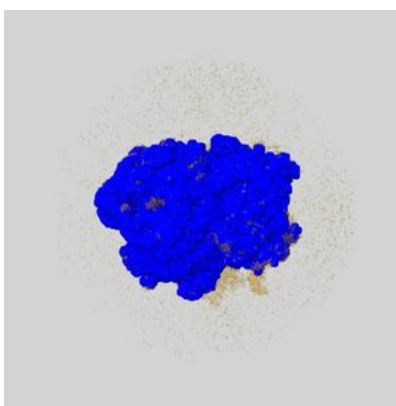
A mask typically either:

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

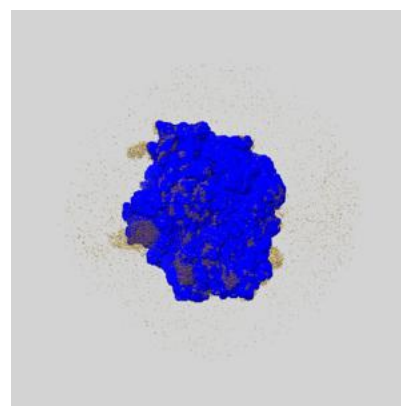
6.6.1 emd_56831_msk_1.map [i](#)



X



Y

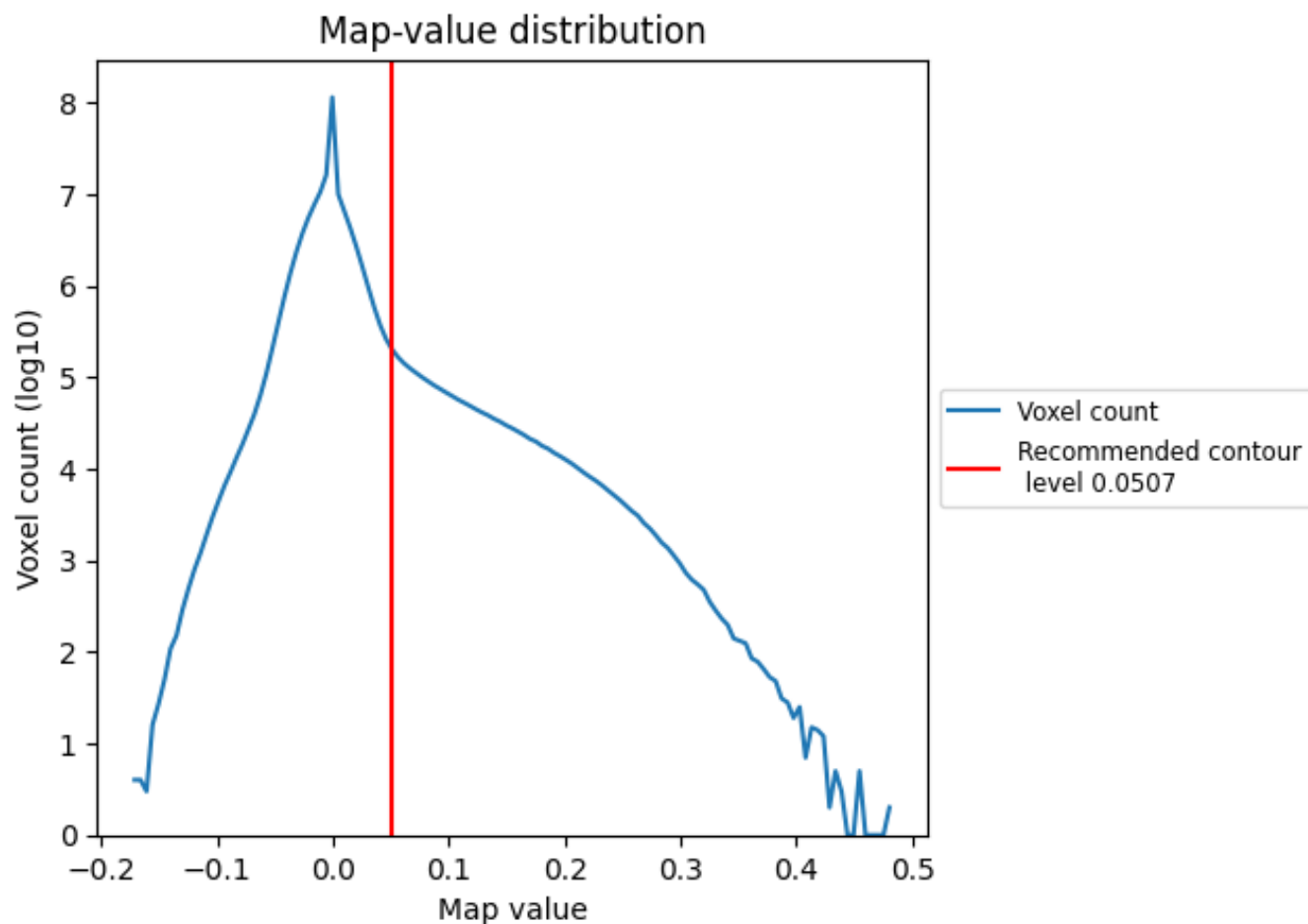


Z

7 Map analysis [i](#)

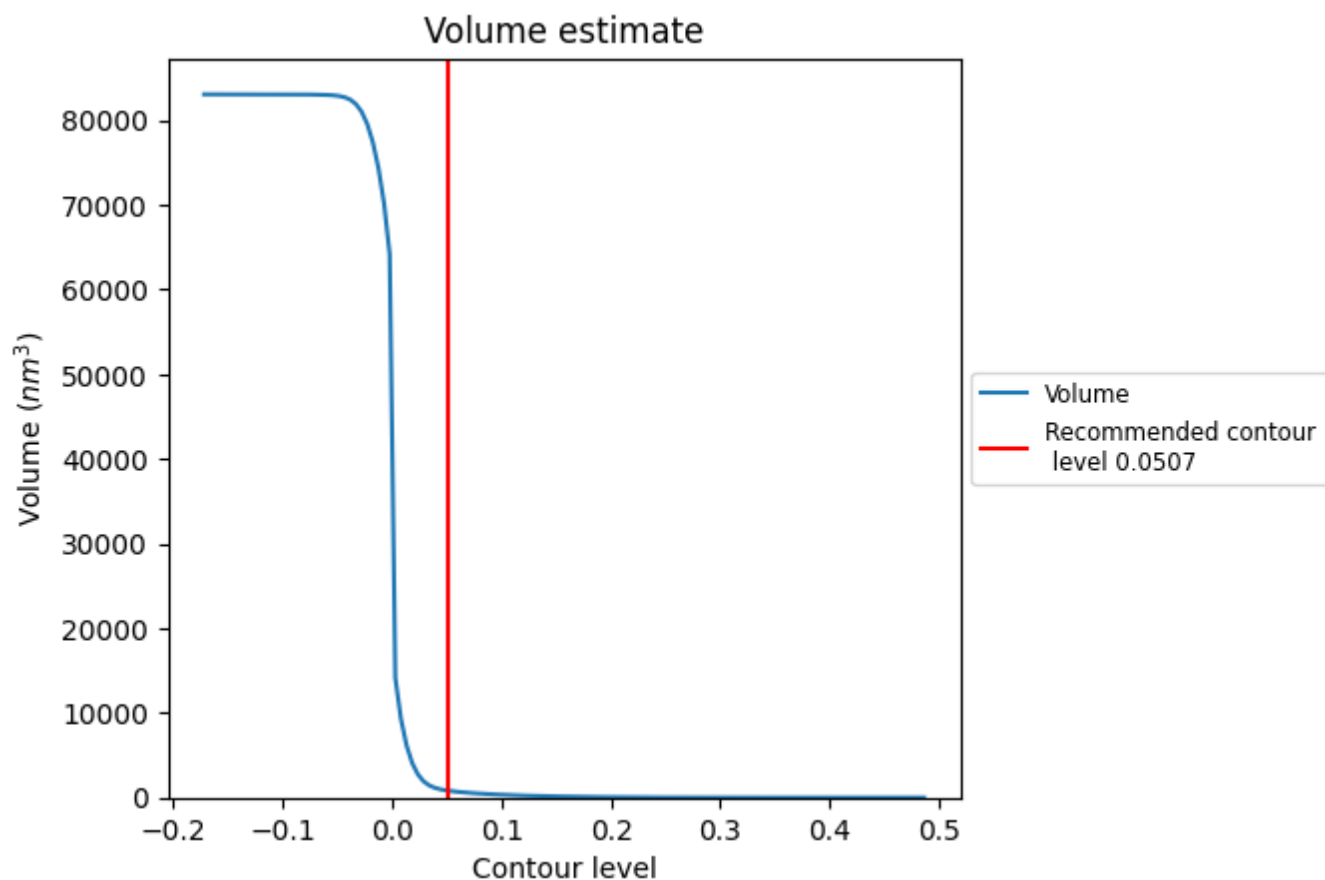
This section contains the results of statistical analysis of the map.

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.

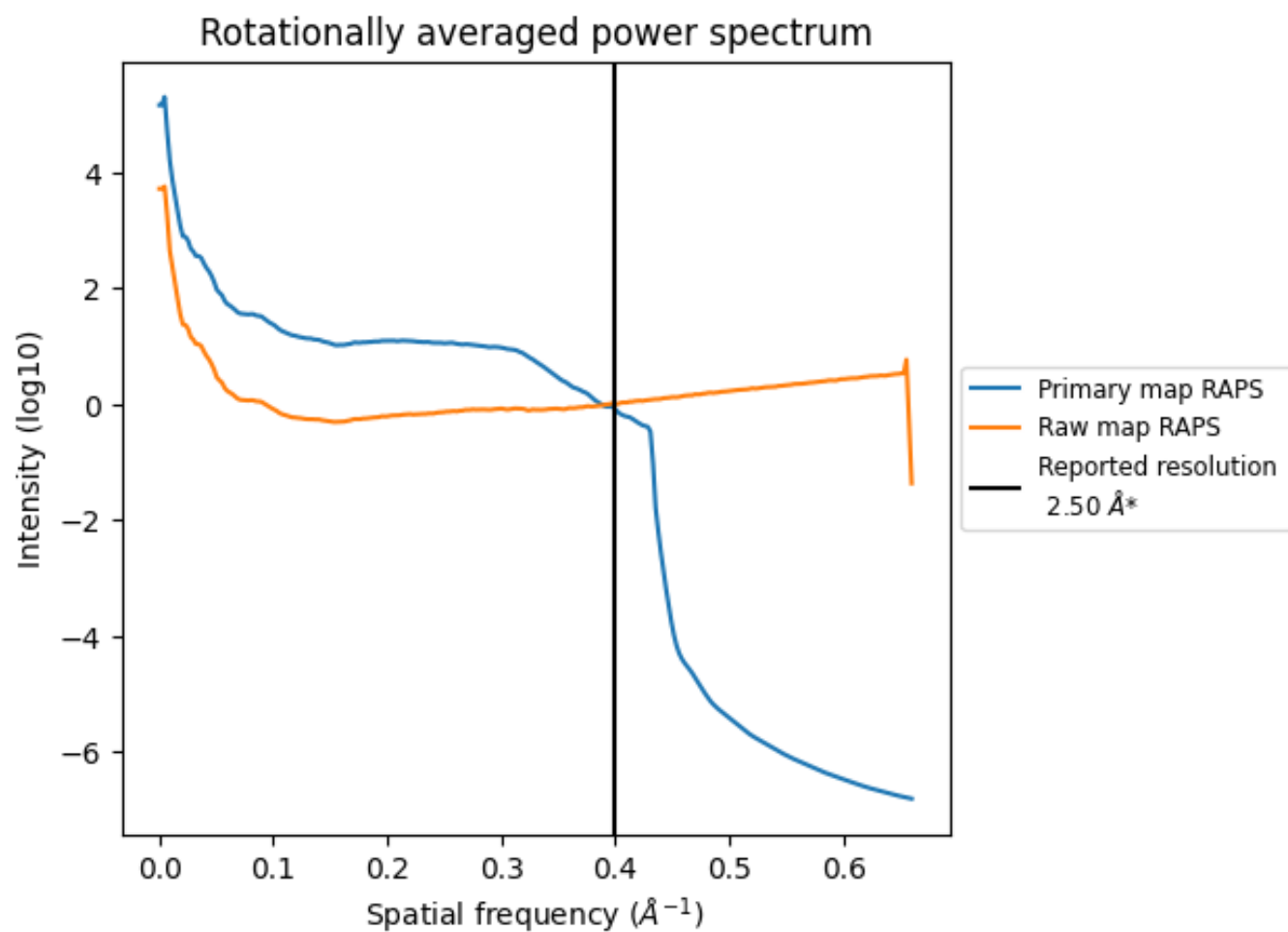
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 828 nm³; this corresponds to an approximate mass of 748 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 ⓘ

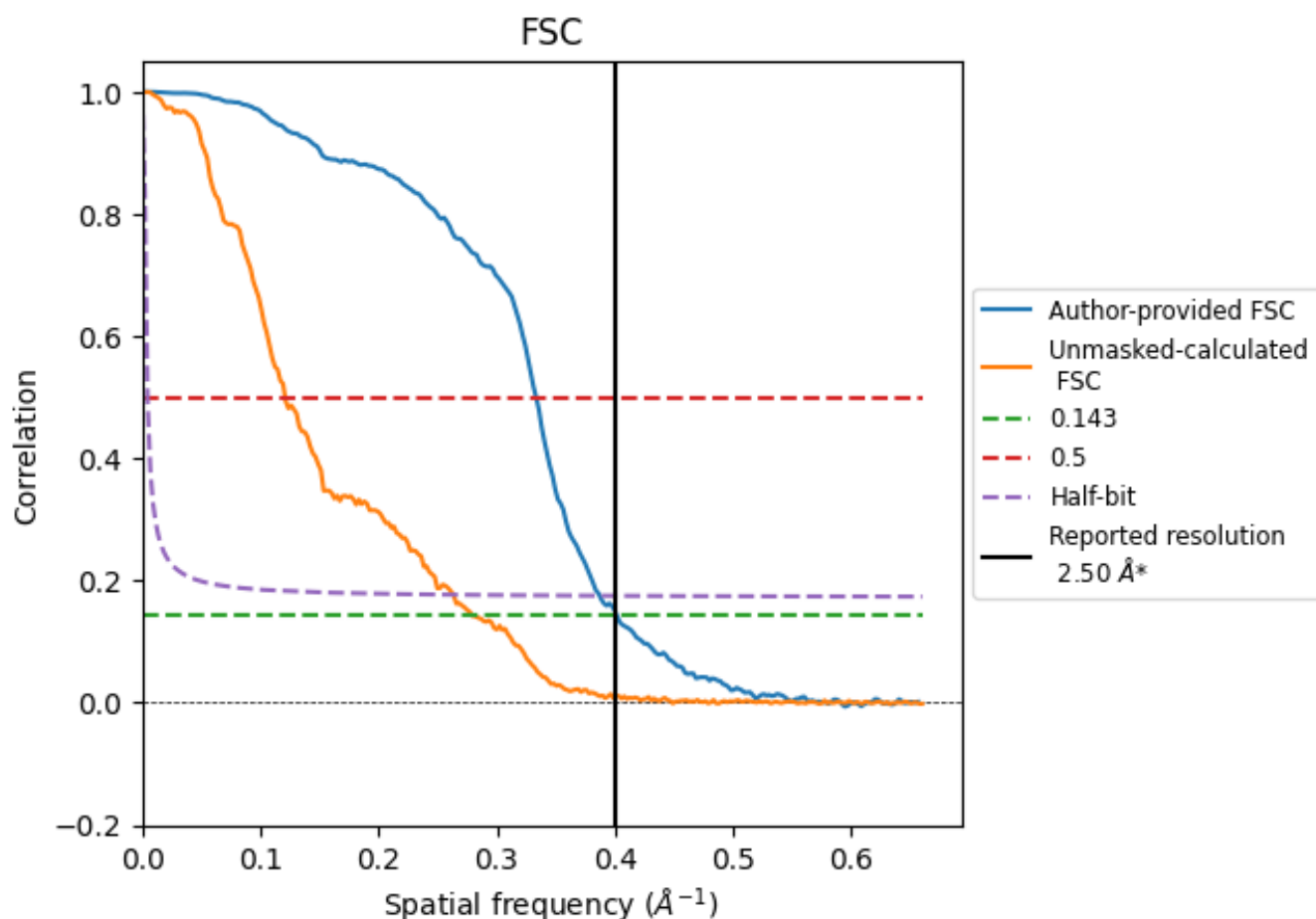


*Reported resolution corresponds to spatial frequency of 0.400 $\text{\AA}^{-1}$

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

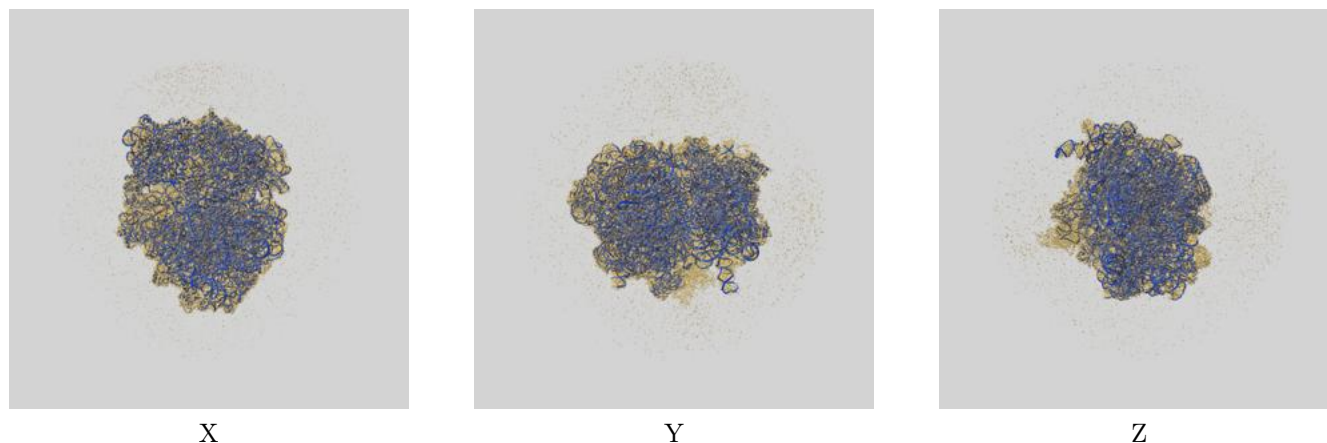
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	3.00	2.58
Unmasked-calculated*	3.58	8.27	3.80

*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 3.58 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

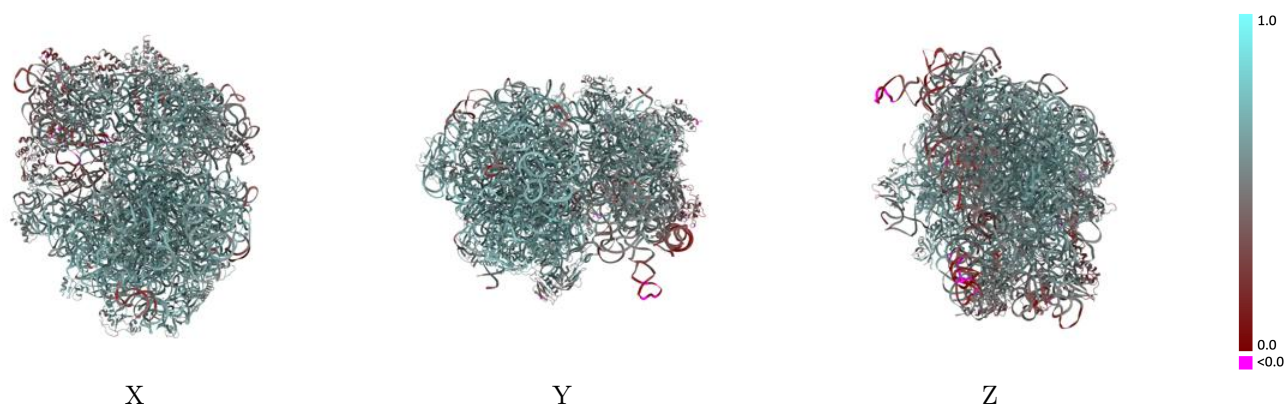
This section contains information regarding the fit between EMDB map EMD-56831 and PDB model 28UL. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



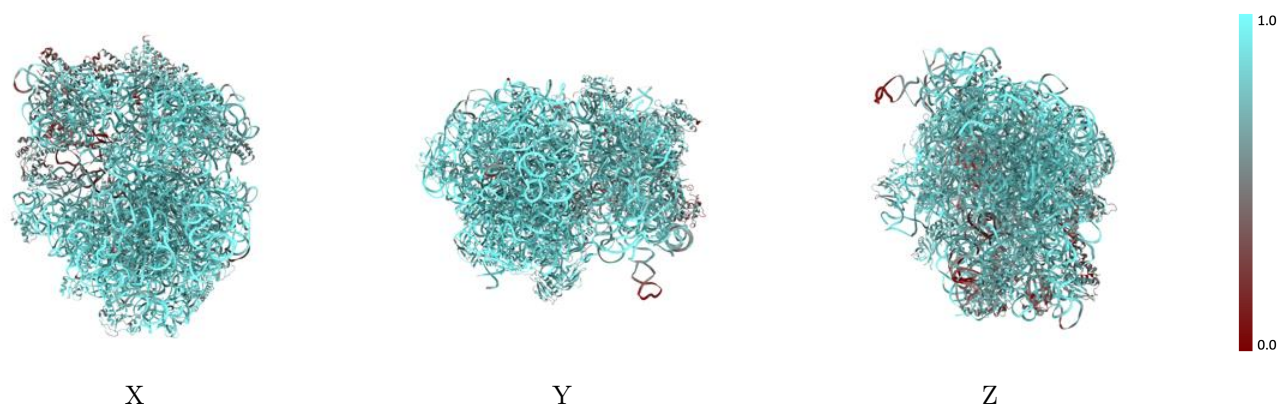
The images above show the 3D surface view of the map at the recommended contour level 0.0507 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



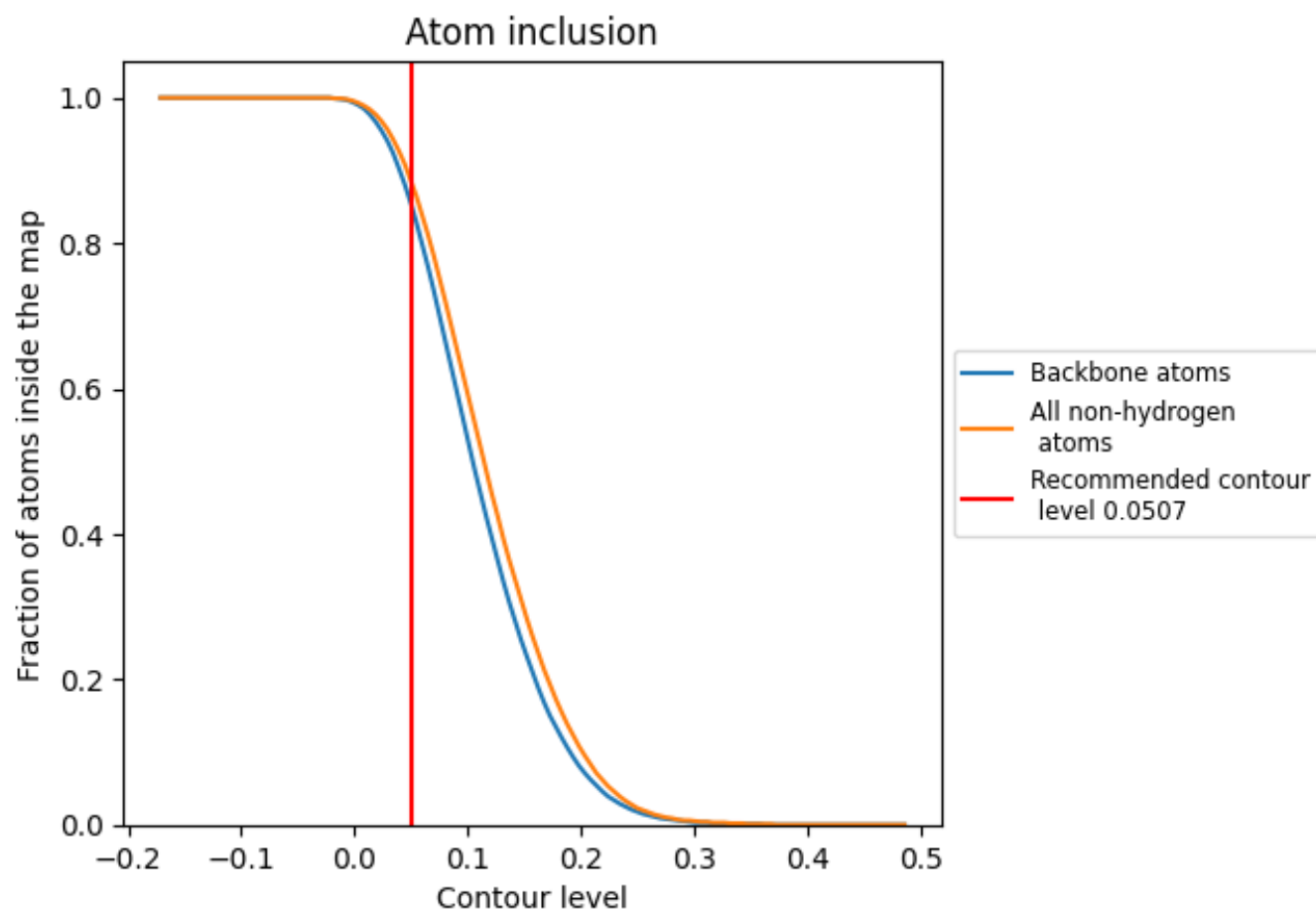
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0507).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0507) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.5840
0	 0.8410	 0.6000
1	 0.9440	 0.6650
2	 0.9610	 0.6700
3	 0.9040	 0.6260
4	 0.5190	 0.3830
A	 0.8860	 0.5460
B	 0.6890	 0.4940
C	 0.6860	 0.5110
D	 0.5230	 0.3930
E	 0.8240	 0.5980
F	 0.7430	 0.5160
G	 0.4070	 0.3180
H	 0.8560	 0.6010
I	 0.6580	 0.4570
J	 0.5510	 0.4220
K	 0.8150	 0.5710
L	 0.7540	 0.5380
M	 0.6320	 0.4440
N	 0.7250	 0.5140
O	 0.8330	 0.5820
P	 0.7330	 0.5030
Q	 0.7470	 0.5270
R	 0.8160	 0.5680
S	 0.6460	 0.4640
T	 0.6990	 0.4860
U	 0.6290	 0.4640
X	 0.7820	 0.5390
Y	 0.4460	 0.3590
Z	 0.8270	 0.4950
a	 0.9660	 0.6350
b	 0.9350	 0.5810
c	 0.9340	 0.6640
d	 0.9210	 0.6440
e	 0.8740	 0.6120



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Chain	Atom inclusion	Q-score
f	 0.5980	 0.4310
g	 0.7650	 0.5120
h	 0.5830	 0.4870
i	 0.9240	 0.6430
j	 0.8880	 0.6380
k	 0.9120	 0.6370
l	 0.8940	 0.6360
m	 0.9580	 0.6620
n	 0.8060	 0.5470
o	 0.8350	 0.6030
p	 0.9470	 0.6690
q	 0.8970	 0.6340
r	 0.8980	 0.6290
s	 0.8670	 0.6050
t	 0.8370	 0.5690
u	 0.8420	 0.5880
v	 0.9020	 0.6370
w	 0.9220	 0.6430
x	 0.8280	 0.5680
y	 0.8970	 0.6250
z	 0.9040	 0.6350