



wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 08:55 AM EST

PDB ID : 8B6C
EMDB ID : EMD-15863
Title : Cryo-EM structure of ribosome-Sec61 in complex with cyclotriazadisulfonamide derivative CK147
Authors : Pauwels, E.; Shewakramani, N.R.; De Wijngaert, B.; Vermeire, K.; Das, K.
Deposited on : 2022-09-26
Resolution : 2.79 Å (reported)
Based on initial models : 6MTE, 3J7Q

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

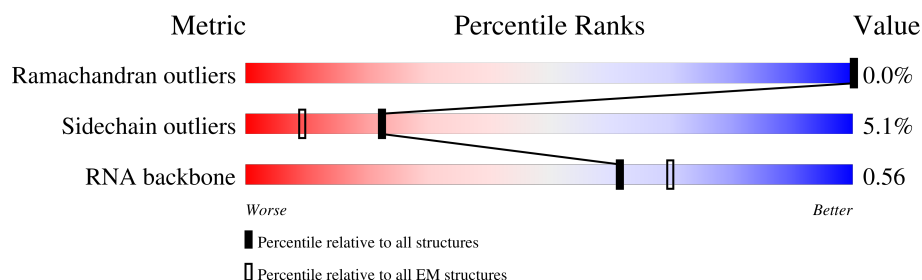
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 2.79 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.





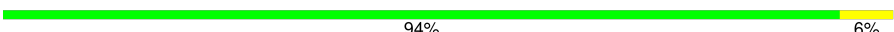

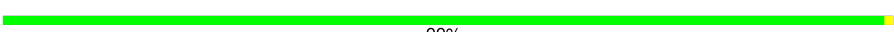







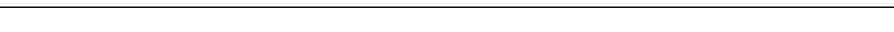

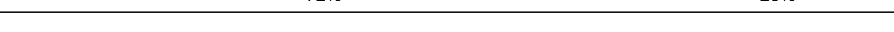
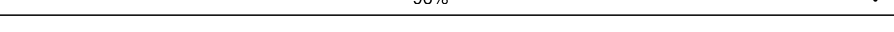
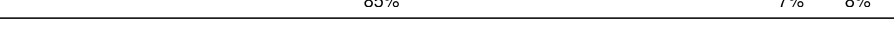

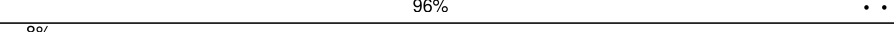

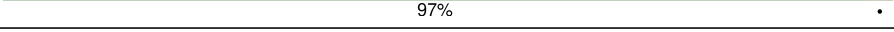
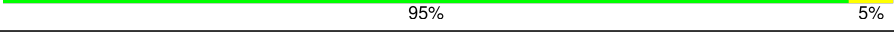
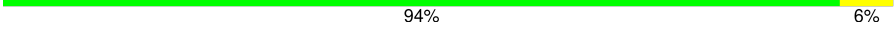
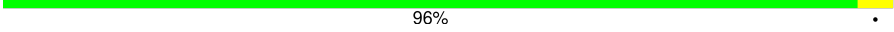
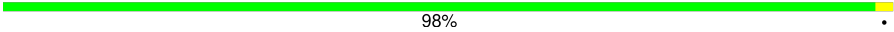
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	T	159	
2	5	4808	
3	F	225	
4	D	293	
5	S	176	
6	b	245	
7	B	394	
8	d	107	

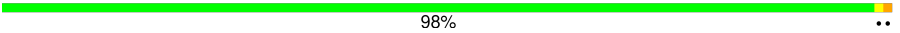


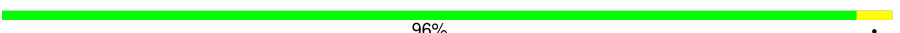










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Mol	Chain	Length	Quality of chain
9	8	156	
10	G	319	
11	J	170	
12	c	98	
13	j	86	
14	A	257	
15	I	214	
16	q	68	
17	p	91	
18	V	131	
19	m	52	
20	l	50	
21	P	153	
22	E	291	
23	Q	188	
24	R	196	
25	W	157	
26	O	203	
27	K	476	
28	C	362	
29	o	103	
30	r	124	
31	f	109	
32	e	128	
33	Z	135	

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Mol	Chain	Length	Quality of chain
34	a	147	 98% ..
35	g	114	 92% 8% .
36	k	70	 90% 9% .
37	H	190	 96% .
38	L	211	 97% .
39	7	120	 90% 10%
40	N	203	 95% 5%
41	i	105	 89% 9% .
42	h	122	 94% 6%
43	M	138	 98% .
44	Y	134	 87% 13%
45	X	118	 95% 5% .
46	U	99	 88% 12%
47	n	25	 76% 24%

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 139959 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 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	3619	Total	C	N	O	P	0	0
			77665	34619	14204	25223	3619		

- Molecule 3 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 4 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 5 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 6 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 7 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 8 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 9 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 11 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 12 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 13 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 14 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 15 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 16 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	67	Total	C	N	O	S	0	0
			535	350	93	88	4		

- Molecule 17 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 18 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 19 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	m	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 20 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 21 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 22 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 23 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 24 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 25 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 26 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 27 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	K	444	Total	C	N	O	S	0	0
			3427	2243	555	607	22		

- Molecule 28 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	362	Total	C	N	O	S	0	0
			2884	1813	577	480	14		

- Molecule 29 is a protein called 60S ribosomal protein L36a-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	o	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 31 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 32 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 33 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 34 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 36 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	24	LYS	ASN	conflict	UNP G1U001

- Molecule 37 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 38 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	74	ARG	HIS	conflict	UNP G1TKB3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 39 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 40 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 41 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 42 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 43 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 44 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 45 is a protein called Ribosomal_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 46 is a protein called 60S ribosomal protein L22 (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
46	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 47 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	5	161	Total	Mg	0
			161	161	
48	8	5	Total	Mg	0
			5	5	
48	A	1	Total	Mg	0
			1	1	
48	I	1	Total	Mg	0
			1	1	
48	V	1	Total	Mg	0
			1	1	
48	P	1	Total	Mg	0
			1	1	
48	a	1	Total	Mg	0
			1	1	
48	7	7	Total	Mg	0
			7	7	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

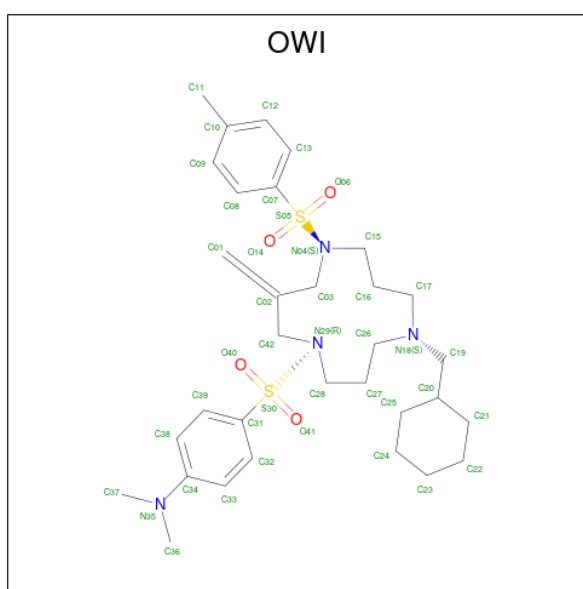
Mol	Chain	Residues	Atoms		AltConf
49	j	1	Total	Zn	0
			1	1	
49	p	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
49	m	1	Total	Zn	0
			1	1	
49	o	1	Total	Zn	0
			1	1	
49	g	1	Total	Zn	0
			1	1	

- Molecule 50 is 4-[[9-(cyclohexylmethyl)-3-methylidene-5-(4-methylphenyl)sulfonyl-1,5,9-triazacyclododec-1-yl]sulfonyl]-{N}, {N}-dimethyl-aniline (three-letter code: OWI) (formula: $C_{32}H_{48}N_4O_4S_2$) (labeled as "Ligand of Interest" by depositor).



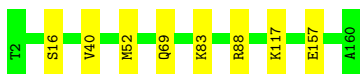
Mol	Chain	Residues	Atoms					AltConf
50	K	1	Total	C	N	O	S	0
			42	32	4	4	2	

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.

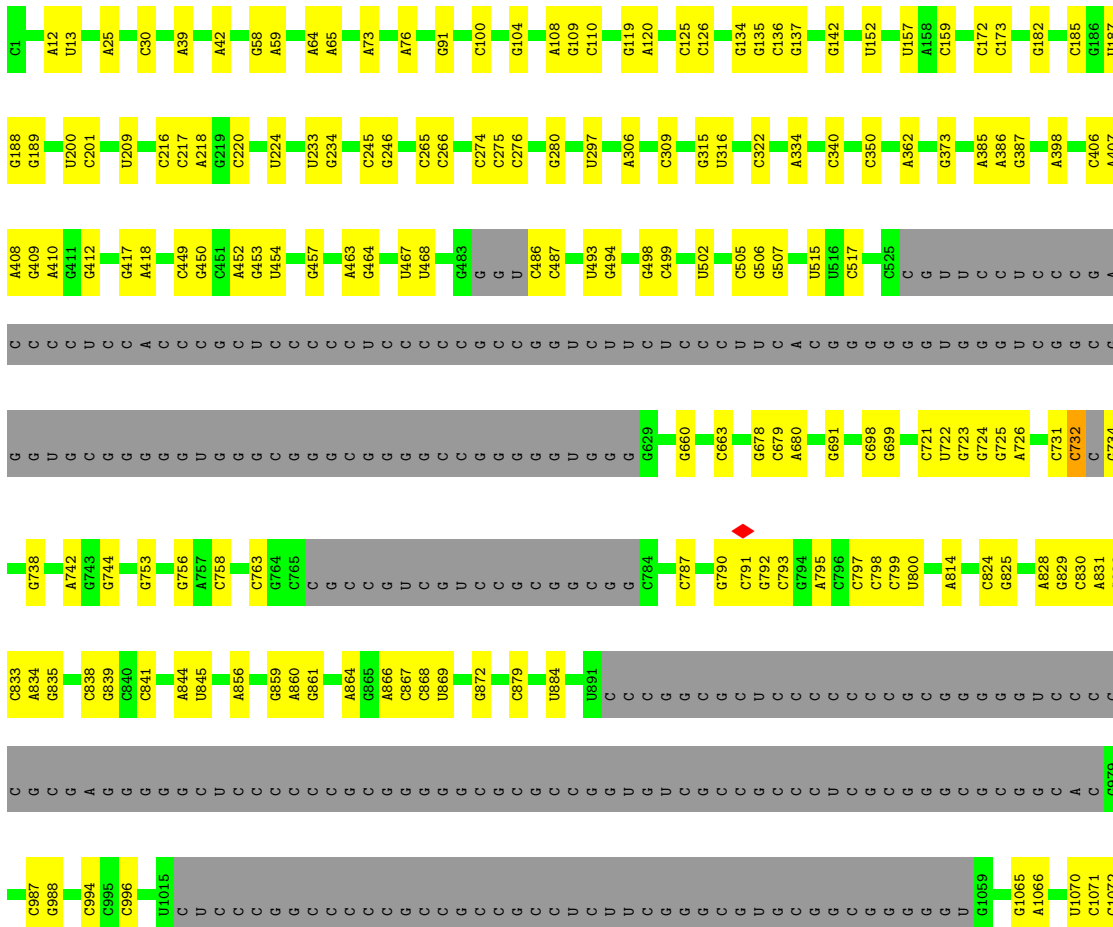
- Molecule 1: 60S ribosomal protein L21

Chain T: 

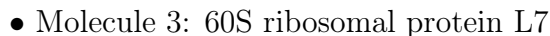


- Molecule 2: 28S rRNA

Chain 5: 







Chain F:  98% .



- Molecule 4: Ribosomal_L18_c domain-containing protein

Chain D:  98% .



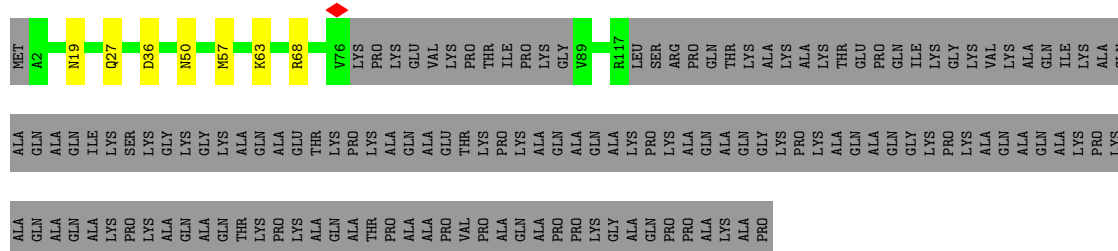
- Molecule 5: 60S ribosomal protein L18a

Chain S:  96% ..



- Molecule 6: 60S ribosomal protein L29

Chain b:  40% . 58%



- Molecule 7: Ribosomal protein L3

Chain B:  98% .




- Molecule 8: 60S ribosomal protein L31

Chain d:  94% 6%



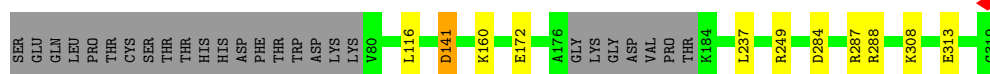
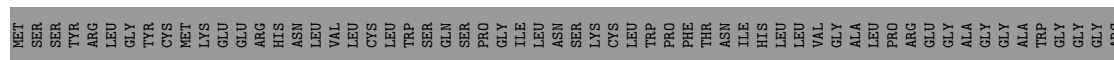
- Molecule 9: 5.8S rRNA

Chain 8:  80% 17% .



- Molecule 10: 60S ribosomal protein L7a

Chain G: 70% 27%



- Molecule 11: 60S ribosomal protein L11

Chain J: 94% 6%



- Molecule 12: 60S ribosomal protein L30

Chain c: 90% 10%



- Molecule 13: Ribosomal protein L37

Chain j: 99% 1%



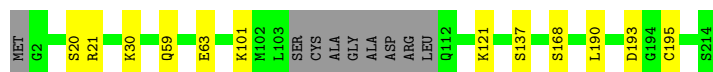
- Molecule 14: Ribosomal protein L8

Chain A: 91% 5%

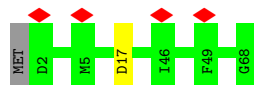


- Molecule 15: Ribosomal protein L10

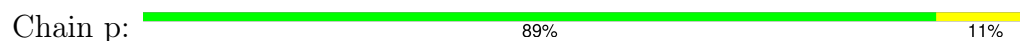
Chain I: 90% 6%



- Molecule 16: Protein transport protein Sec61 subunit gamma



- Molecule 17: 60S ribosomal protein L37a



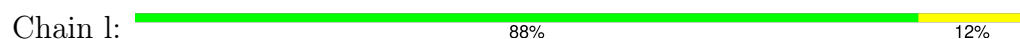
- Molecule 18: 60S ribosomal protein L23



- Molecule 19: 60S ribosomal protein L40



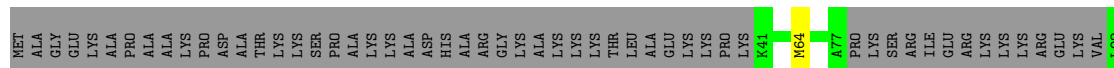
- Molecule 20: 60S ribosomal protein L39-like

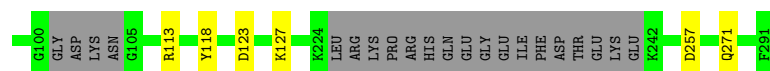


- Molecule 21: 60S ribosomal protein L17



- Molecule 22: 60S ribosomal protein L6





- Molecule 23: eL18

Chain Q: 96%



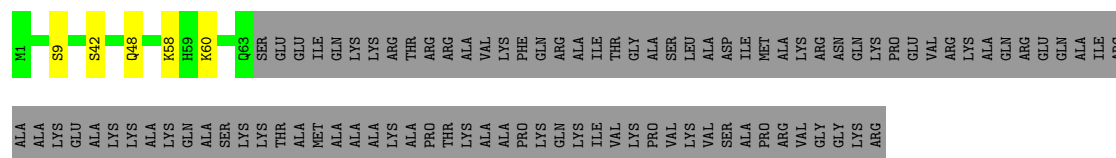
- Molecule 24: 60S ribosomal protein L19

Chain R: 85%



- Molecule 25: Ribosomal protein L24

Chain W: 37%



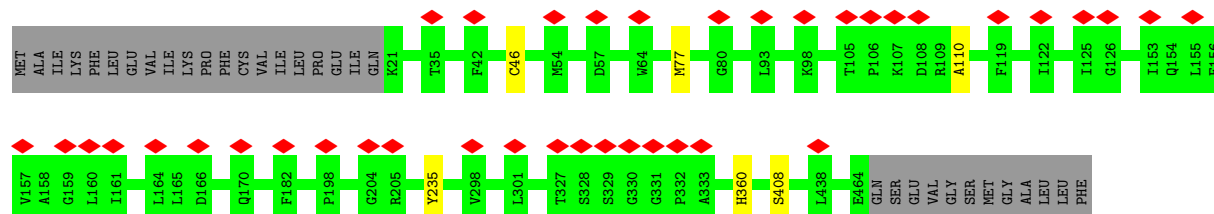
- Molecule 26: 60S ribosomal protein L13a

Chain O: 96%



- Molecule 27: Protein transport protein Sec61 subunit alpha isoform 1

Chain K: 8%



- Molecule 28: 60S ribosomal protein L4

Chain C: 97%



- Molecule 29: 60S ribosomal protein L36a-like



- Molecule 30: 60S ribosomal protein L28



- Molecule 31: 60S ribosomal protein L35a



- Molecule 32: Ribosomal protein L32



- Molecule 33: 60S ribosomal protein L27



- Molecule 34: 60S ribosomal protein L27a

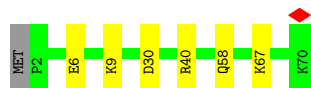
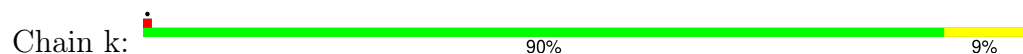


- Molecule 35: 60S ribosomal protein L34





- Molecule 36: 60S ribosomal protein L38



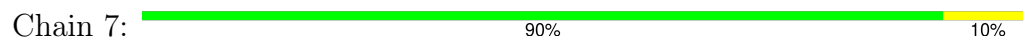
- Molecule 37: 60S ribosomal protein L9



- Molecule 38: 60S ribosomal protein L13



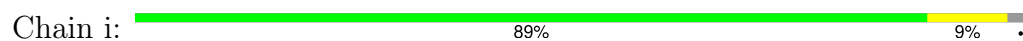
- Molecule 39: 5S rRNA



- Molecule 40: Ribosomal protein L15



- Molecule 41: 60S ribosomal protein L36



- Molecule 42: 60S ribosomal protein L35





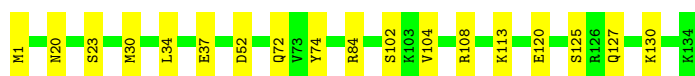
- Molecule 43: 60S ribosomal protein L14

Chain M: 98%



- Molecule 44: Ribosomal protein L26

Chain Y: 87% 13%



- Molecule 45: Ribosomal_L23eN domain-containing protein

Chain X: 95% 5%



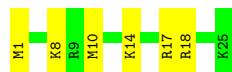
- Molecule 46: 60S ribosomal protein L22 (Fragment)

Chain U: 88% 12%



- Molecule 47: 60S ribosomal protein L41

Chain n: 76% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132229	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.8	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.425	Depositor
Minimum map value	-0.156	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.01581	Depositor
Map size (\AA)	432.96002, 432.96002, 432.96002	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.23, 1.23, 1.23	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: E6G, BGH, B8K, P7G, I4U, OMG, 7MG, MG, 5MC, OWI, B8H, MLZ, ZN, OMC, UR3, P4U, 1MA, E7G, OMU, A2M, PSU

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	T	0.34	0/1326	0.60	0/1770
2	5	0.42	4/85271 (0.0%)	0.79	17/132978 (0.0%)
3	F	0.31	0/1911	0.53	0/2549
4	D	0.33	0/2437	0.56	0/3264
5	S	0.33	0/1501	0.61	2/2012 (0.1%)
6	b	0.31	0/861	0.68	1/1138 (0.1%)
7	B	0.30	0/3240	0.55	0/4339
8	d	0.39	0/903	0.61	0/1216
9	8	0.39	0/3581	0.74	0/5577
10	G	0.33	0/1910	0.61	1/2569 (0.0%)
11	J	0.33	0/1385	0.68	0/1852
12	c	0.31	0/771	0.61	1/1034 (0.1%)
13	j	0.32	0/720	0.60	0/952
14	A	0.37	0/1936	0.61	0/2596
15	I	0.36	0/1702	0.59	1/2272 (0.0%)
16	q	0.30	0/545	0.67	1/728 (0.1%)
17	p	0.34	0/718	0.57	0/953
18	V	0.38	0/993	0.58	0/1332
19	m	0.33	0/425	0.64	0/561
20	l	0.27	0/459	0.59	0/608
21	P	0.33	0/1268	0.62	0/1700
22	E	0.30	0/1762	0.57	0/2362
23	Q	0.31	0/1539	0.63	0/2054
24	R	0.29	0/1524	0.64	0/2013
25	W	0.32	0/541	0.58	0/720
26	O	0.32	0/1662	0.57	0/2222
27	K	0.54	0/3502	0.68	0/4749
28	C	0.35	0/2927	0.58	0/3932
29	o	0.34	0/855	0.61	0/1128
30	r	0.35	0/1010	0.60	0/1354
31	f	0.33	0/895	0.61	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.30	0/1071	0.57	0/1429
33	Z	0.35	0/1130	0.61	2/1507 (0.1%)
34	a	0.30	0/1191	0.77	3/1590 (0.2%)
35	g	0.31	0/916	0.62	0/1220
36	k	0.35	0/575	0.70	0/761
37	H	0.32	0/1535	0.61	2/2063 (0.1%)
38	L	0.33	0/1733	0.62	0/2316
39	7	0.39	0/2858	0.75	0/4455
40	N	0.36	0/1746	0.62	0/2338
41	i	0.29	0/841	0.62	0/1112
42	h	0.28	0/1021	0.58	0/1348
43	M	0.33	0/1158	0.60	0/1547
44	Y	0.32	0/1132	0.63	0/1504
45	X	0.31	0/984	0.68	1/1323 (0.1%)
46	U	0.37	0/823	0.82	1/1104 (0.1%)
47	n	0.26	0/240	0.80	0/305
All	All	0.39	4/149034 (0.0%)	0.73	33/219654 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	732	C	O3'-P	25.73	1.92	1.61
2	5	1390	G	O3'-P	23.27	1.89	1.61
2	5	1392	C	O3'-P	-17.11	1.40	1.61
2	5	731	C	O3'-P	-13.81	1.44	1.61

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	731	C	OP1-P-O3'	-26.75	46.34	105.20
34	a	16	SER	N-CA-CB	17.07	136.11	110.50
2	5	731	C	O3'-P-O5'	14.20	130.97	104.00
34	a	15	VAL	N-CA-C	-10.40	82.92	111.00
2	5	732	C	P-O3'-C3'	-8.94	108.97	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles ⓘ

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	T	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
3	F	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
4	D	291/293 (99%)	284 (98%)	7 (2%)	0	100	100
5	S	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
6	b	100/245 (41%)	97 (97%)	3 (3%)	0	100	100
7	B	392/394 (100%)	382 (97%)	10 (3%)	0	100	100
8	d	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
10	G	229/319 (72%)	219 (96%)	10 (4%)	0	100	100
11	J	168/170 (99%)	159 (95%)	9 (5%)	0	100	100
12	c	96/98 (98%)	96 (100%)	0	0	100	100
13	j	84/86 (98%)	84 (100%)	0	0	100	100
14	A	246/257 (96%)	229 (93%)	17 (7%)	0	100	100
15	I	201/214 (94%)	193 (96%)	8 (4%)	0	100	100
16	q	65/68 (96%)	65 (100%)	0	0	100	100
17	p	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
18	V	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
19	m	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
20	l	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
21	P	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
22	E	208/291 (72%)	198 (95%)	9 (4%)	1 (0%)	25	56
23	Q	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
24	R	178/196 (91%)	174 (98%)	4 (2%)	0	100	100
25	W	61/157 (39%)	58 (95%)	3 (5%)	0	100	100
26	O	197/203 (97%)	192 (98%)	5 (2%)	0	100	100
27	K	442/476 (93%)	430 (97%)	11 (2%)	1 (0%)	44	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	C	359/362 (99%)	343 (96%)	16 (4%)	0	100	100
29	o	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
30	r	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
31	f	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
32	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
33	Z	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
34	a	145/147 (99%)	138 (95%)	6 (4%)	1 (1%)	19	48
35	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
36	k	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
37	H	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
38	L	208/211 (99%)	201 (97%)	7 (3%)	0	100	100
40	N	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
41	i	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
42	h	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
43	M	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
44	Y	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
45	X	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
46	U	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
47	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	6861/7436 (92%)	6625 (97%)	233 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	a	16	SER
22	E	118	TYR
27	K	110	ALA

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	T	139/139 (100%)	131 (94%)	8 (6%)	17	45
3	F	196/196 (100%)	192 (98%)	4 (2%)	50	81
4	D	247/247 (100%)	242 (98%)	5 (2%)	50	81
5	S	157/157 (100%)	151 (96%)	6 (4%)	28	62
6	b	84/184 (46%)	78 (93%)	6 (7%)	12	35
7	B	342/342 (100%)	333 (97%)	9 (3%)	41	75
8	d	98/98 (100%)	92 (94%)	6 (6%)	15	43
10	G	200/272 (74%)	189 (94%)	11 (6%)	18	47
11	J	143/143 (100%)	133 (93%)	10 (7%)	12	36
12	c	84/84 (100%)	75 (89%)	9 (11%)	5	17
13	j	73/73 (100%)	72 (99%)	1 (1%)	62	87
14	A	190/199 (96%)	177 (93%)	13 (7%)	13	38
15	I	175/181 (97%)	164 (94%)	11 (6%)	15	42
16	q	58/59 (98%)	58 (100%)	0	100	100
17	p	74/74 (100%)	64 (86%)	10 (14%)	3	10
18	V	101/101 (100%)	94 (93%)	7 (7%)	13	37
19	m	47/47 (100%)	47 (100%)	0	100	100
20	l	47/47 (100%)	41 (87%)	6 (13%)	3	12
21	P	134/134 (100%)	128 (96%)	6 (4%)	23	55
22	E	190/251 (76%)	184 (97%)	6 (3%)	34	68
23	Q	164/165 (99%)	157 (96%)	7 (4%)	25	57
24	R	159/175 (91%)	146 (92%)	13 (8%)	9	29
25	W	55/126 (44%)	50 (91%)	5 (9%)	7	24
26	O	171/173 (99%)	167 (98%)	4 (2%)	45	78
27	K	370/398 (93%)	365 (99%)	5 (1%)	62	87
28	C	301/301 (100%)	289 (96%)	12 (4%)	27	60
29	o	91/91 (100%)	86 (94%)	5 (6%)	18	47
30	r	108/108 (100%)	100 (93%)	8 (7%)	11	33
31	f	88/88 (100%)	84 (96%)	4 (4%)	23	55
32	e	114/114 (100%)	111 (97%)	3 (3%)	41	75
33	Z	117/117 (100%)	108 (92%)	9 (8%)	10	31
34	a	119/119 (100%)	118 (99%)	1 (1%)	79	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	g	98/98 (100%)	89 (91%)	9 (9%)	7	24
36	k	64/65 (98%)	58 (91%)	6 (9%)	7	23
37	H	169/169 (100%)	163 (96%)	6 (4%)	30	64
38	L	175/176 (99%)	170 (97%)	5 (3%)	37	71
40	N	171/171 (100%)	161 (94%)	10 (6%)	17	45
41	i	86/89 (97%)	77 (90%)	9 (10%)	5	18
42	h	109/109 (100%)	102 (94%)	7 (6%)	14	41
43	M	117/117 (100%)	114 (97%)	3 (3%)	41	75
44	Y	124/124 (100%)	106 (86%)	18 (14%)	2	8
45	X	106/106 (100%)	101 (95%)	5 (5%)	22	54
46	U	89/89 (100%)	78 (88%)	11 (12%)	4	13
47	n	24/24 (100%)	18 (75%)	6 (25%)	0	1
All	All	5968/6340 (94%)	5663 (95%)	305 (5%)	22	51

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	L	106	SER
45	X	118	ASP
40	N	80	THR
42	h	88	THR
47	n	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
29	o	36	GLN
45	X	151	ASN
30	r	83	ASN
20	l	20	ASN
27	K	360	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	5	3590/4808 (74%)	695 (19%)	55 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
39	7	119/120 (99%)	12 (10%)	0
9	8	149/156 (95%)	26 (17%)	1 (0%)
All	All	3858/5084 (75%)	733 (18%)	56 (1%)

5 of 733 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	5	12	A
2	5	13	U
2	5	25	A
2	5	30	C
2	5	39	A

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	2028	G
9	8	124	U
2	5	3335	G
2	5	4786	C
2	5	4623	G

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

66 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
2	1MA	5	1266	2	17,25,26	2.62	5 (29%)	17,37,40	1.57	3 (17%)
2	PSU	5	1537	2	18,21,22	2.06	5 (27%)	21,30,33	2.01	4 (19%)
2	OMC	5	3601	2	19,22,23	2.24	5 (26%)	25,31,34	0.97	3 (12%)
2	B8H	5	1799	2	19,22,23	2.06	8 (42%)	21,32,35	2.20	3 (14%)
2	I4U	5	1614	2	20,24,25	2.44	5 (25%)	27,34,37	1.95	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGH	5	3631	2	25,29,30	5.73	12 (48%)	30,43,46	2.44	10 (33%)
2	1MA	5	4161	2	17,25,26	2.56	5 (29%)	17,37,40	1.50	3 (17%)
2	5MC	5	3514	2	19,22,23	2.96	5 (26%)	26,32,35	1.37	3 (11%)
2	A2M	5	1810	48,2	18,25,26	0.91	0	20,36,39	1.33	3 (15%)
2	PSU	5	3461	2	18,21,22	2.05	5 (27%)	21,30,33	1.97	4 (19%)
2	PSU	5	4149	2	18,21,22	1.60	5 (27%)	21,30,33	2.26	6 (28%)
2	B8H	5	3494	2	19,22,23	2.03	7 (36%)	21,32,35	2.06	3 (14%)
2	OMG	5	3524	2	19,26,27	2.60	4 (21%)	21,38,41	1.21	3 (14%)
2	OMU	5	4366	2	19,22,23	3.11	7 (36%)	25,31,34	1.94	6 (24%)
2	OMG	5	4116	2	19,26,27	1.04	1 (5%)	21,38,41	1.39	4 (19%)
19	MLZ	m	72	19	8,9,10	0.49	0	4,9,11	0.53	0
2	B8K	5	4436	2	24,28,29	5.11	7 (29%)	29,42,45	2.41	7 (24%)
2	OMG	5	2207	2	19,26,27	2.59	4 (21%)	21,38,41	1.18	3 (14%)
28	MLZ	C	333	28	8,9,10	0.46	0	4,9,11	0.65	0
2	OMG	5	4240	2	19,26,27	2.58	4 (21%)	21,38,41	1.21	3 (14%)
2	B8K	5	3629	2	24,28,29	5.17	7 (29%)	29,42,45	2.36	7 (24%)
2	5MC	5	4193	2	19,22,23	1.43	3 (15%)	26,32,35	1.38	4 (15%)
2	OMC	5	2208	2	19,22,23	2.24	5 (26%)	25,31,34	0.97	3 (12%)
2	A2M	5	4269	48,2	18,25,26	4.18	5 (27%)	20,36,39	1.81	2 (10%)
2	PSU	5	3496	2	18,21,22	2.02	6 (33%)	21,30,33	1.92	5 (23%)
2	OMC	5	2704	2	19,22,23	2.22	5 (26%)	25,31,34	0.98	2 (8%)
2	A2M	5	3450	2	18,25,26	4.21	5 (27%)	20,36,39	1.66	2 (10%)
2	7MG	5	2365	2	23,26,27	1.41	4 (17%)	27,39,42	2.80	8 (29%)
2	PSU	5	4374	2	18,21,22	2.04	5 (27%)	21,30,33	2.10	4 (19%)
2	A2M	5	1270	2	18,25,26	0.86	0	20,36,39	1.32	3 (15%)
2	OMC	5	2647	2	19,22,23	2.24	5 (26%)	25,31,34	0.97	2 (8%)
2	PSU	5	1632	2	18,21,22	2.00	5 (27%)	21,30,33	2.11	4 (19%)
2	E6G	5	4101	2	19,27,28	1.76	3 (15%)	18,39,42	2.03	3 (16%)
2	E7G	5	1736	2	24,27,28	4.30	7 (29%)	28,40,43	2.25	8 (28%)
2	A2M	5	3557	2	18,25,26	4.17	5 (27%)	20,36,39	1.69	2 (10%)
2	OMG	5	4383	2	19,26,27	2.59	4 (21%)	21,38,41	1.26	3 (14%)
2	OMG	5	2616	2	19,26,27	2.58	4 (21%)	21,38,41	1.24	3 (14%)
2	PSU	5	1638	2	18,21,22	2.03	5 (27%)	21,30,33	2.06	4 (19%)
2	OMC	5	3433	2	19,22,23	2.23	4 (21%)	25,31,34	0.97	2 (8%)
2	OMG	5	1580	48,2	19,26,27	1.12	1 (5%)	21,38,41	1.14	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	5	3447	2	18,21,22	2.00	5 (27%)	21,30,33	2.00	4 (19%)
2	PSU	5	4277	2	18,21,22	1.98	5 (27%)	21,30,33	2.03	4 (19%)
2	P7G	5	1848	2	24,28,29	5.05	6 (25%)	25,41,44	1.13	1 (4%)
2	OMG	5	1477	2	19,26,27	2.60	6 (31%)	21,38,41	1.24	3 (14%)
2	A2M	5	3455	2	18,25,26	4.18	5 (27%)	20,36,39	1.71	2 (10%)
2	OMG	5	1260	2	19,26,27	2.57	5 (26%)	21,38,41	1.20	3 (14%)
2	PSU	5	4188	2	18,21,22	2.06	6 (33%)	21,30,33	2.11	5 (23%)
2	OMC	5	2265	48,2	19,22,23	2.22	5 (26%)	25,31,34	0.97	2 (8%)
2	P7G	5	3612	2	24,28,29	5.12	6 (25%)	25,41,44	1.13	1 (4%)
2	A2M	5	398	2	18,25,26	4.20	5 (27%)	20,36,39	1.67	2 (10%)
2	OMG	5	4369	2	19,26,27	2.59	4 (21%)	21,38,41	1.23	3 (14%)
2	P4U	5	1292	2	21,24,25	2.42	7 (33%)	28,33,36	1.61	3 (10%)
2	B8H	5	4042	2	19,22,23	2.05	8 (42%)	21,32,35	2.20	3 (14%)
2	A2M	5	1489	48,2	18,25,26	4.21	5 (27%)	20,36,39	1.80	2 (10%)
2	PSU	5	2351	2	18,21,22	2.02	5 (27%)	21,30,33	1.95	4 (19%)
2	PSU	5	4196	48,2	18,21,22	1.99	6 (33%)	21,30,33	2.06	4 (19%)
2	PSU	5	4039	2	18,21,22	2.02	5 (27%)	21,30,33	2.06	4 (19%)
2	OMC	5	3619	2	19,22,23	2.23	5 (26%)	25,31,34	0.98	3 (12%)
2	UR3	5	4276	2	19,22,23	1.01	1 (5%)	26,32,35	1.82	5 (19%)
2	OMU	5	4052	2	19,22,23	3.12	7 (36%)	25,31,34	1.91	6 (24%)
2	OMC	5	4282	2	19,22,23	0.95	1 (5%)	25,31,34	1.08	1 (4%)
2	7MG	5	1560	2	23,26,27	4.56	6 (26%)	27,39,42	2.23	8 (29%)
2	PSU	5	4246	2	18,21,22	2.02	5 (27%)	21,30,33	2.10	5 (23%)
2	PSU	5	4382	2	18,21,22	2.02	5 (27%)	21,30,33	2.11	5 (23%)
2	OMG	5	2267	2	19,26,27	1.03	1 (5%)	21,38,41	1.27	3 (14%)
2	A2M	5	1479	2	18,25,26	4.17	5 (27%)	20,36,39	2.35	3 (15%)

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
2	1MA	5	1266	2	-	0/3/25/26	0/3/3/3
2	PSU	5	1537	2	-	2/7/25/26	0/2/2/2
2	OMC	5	3601	2	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B8H	5	1799	2	-	0/7/25/26	0/2/2/2
2	I4U	5	1614	2	-	1/9/29/30	0/2/2/2
2	BGH	5	3631	2	-	2/13/43/44	0/3/3/3
2	1MA	5	4161	2	-	1/3/25/26	0/3/3/3
2	5MC	5	3514	2	-	0/7/25/26	0/2/2/2
2	A2M	5	1810	48,2	-	0/5/27/28	0/3/3/3
2	PSU	5	3461	2	-	2/7/25/26	0/2/2/2
2	PSU	5	4149	2	-	2/7/25/26	0/2/2/2
2	B8H	5	3494	2	-	2/7/25/26	0/2/2/2
2	OMG	5	3524	2	-	2/5/27/28	0/3/3/3
2	OMU	5	4366	2	-	1/9/27/28	0/2/2/2
2	OMG	5	4116	2	-	1/5/27/28	0/3/3/3
19	MLZ	m	72	19	-	1/7/8/10	-
2	B8K	5	4436	2	-	0/11/41/42	0/3/3/3
2	OMG	5	2207	2	-	2/5/27/28	0/3/3/3
28	MLZ	C	333	28	-	0/7/8/10	-
2	OMG	5	4240	2	-	3/5/27/28	0/3/3/3
2	B8K	5	3629	2	-	3/11/41/42	0/3/3/3
2	5MC	5	4193	2	-	4/7/25/26	0/2/2/2
2	OMC	5	2208	2	-	0/9/27/28	0/2/2/2
2	A2M	5	4269	48,2	-	3/5/27/28	0/3/3/3
2	PSU	5	3496	2	-	3/7/25/26	0/2/2/2
2	OMC	5	2704	2	-	1/9/27/28	0/2/2/2
2	A2M	5	3450	2	-	0/5/27/28	0/3/3/3
2	7MG	5	2365	2	-	0/7/37/38	0/3/3/3
2	PSU	5	4374	2	-	0/7/25/26	0/2/2/2
2	A2M	5	1270	2	-	3/5/27/28	0/3/3/3
2	OMC	5	2647	2	-	1/9/27/28	0/2/2/2
2	PSU	5	1632	2	-	1/7/25/26	0/2/2/2
2	E6G	5	4101	2	-	4/6/28/29	0/3/3/3
2	E7G	5	1736	2	-	3/9/39/40	0/3/3/3
2	A2M	5	3557	2	-	1/5/27/28	0/3/3/3
2	OMG	5	4383	2	-	3/5/27/28	0/3/3/3
2	OMG	5	2616	2	-	1/5/27/28	0/3/3/3
2	PSU	5	1638	2	-	0/7/25/26	0/2/2/2
2	OMC	5	3433	2	-	4/9/27/28	0/2/2/2
2	OMG	5	1580	48,2	-	0/5/27/28	0/3/3/3
2	PSU	5	3447	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	5	4277	2	-	0/7/25/26	0/2/2/2
2	P7G	5	1848	2	-	0/10/40/41	0/3/3/3
2	OMG	5	1477	2	-	0/5/27/28	0/3/3/3
2	A2M	5	3455	2	-	0/5/27/28	0/3/3/3
2	OMG	5	1260	2	-	1/5/27/28	0/3/3/3
2	PSU	5	4188	2	-	0/7/25/26	0/2/2/2
2	OMC	5	2265	48,2	-	2/9/27/28	0/2/2/2
2	P7G	5	3612	2	-	3/10/40/41	0/3/3/3
2	A2M	5	398	2	-	1/5/27/28	0/3/3/3
2	OMG	5	4369	2	-	1/5/27/28	0/3/3/3
2	P4U	5	1292	2	-	4/10/29/30	0/2/2/2
2	B8H	5	4042	2	-	2/7/25/26	0/2/2/2
2	A2M	5	1489	48,2	-	2/5/27/28	0/3/3/3
2	PSU	5	2351	2	-	0/7/25/26	0/2/2/2
2	PSU	5	4196	48,2	-	4/7/25/26	0/2/2/2
2	PSU	5	4039	2	-	2/7/25/26	0/2/2/2
2	OMC	5	3619	2	-	1/9/27/28	0/2/2/2
2	UR3	5	4276	2	-	0/7/25/26	0/2/2/2
2	OMU	5	4052	2	-	3/9/27/28	0/2/2/2
2	OMC	5	4282	2	-	2/9/27/28	0/2/2/2
2	7MG	5	1560	2	-	0/7/37/38	0/3/3/3
2	PSU	5	4246	2	-	5/7/25/26	0/2/2/2
2	PSU	5	4382	2	-	3/7/25/26	0/2/2/2
2	OMG	5	2267	2	-	2/5/27/28	0/3/3/3
2	A2M	5	1479	2	-	2/5/27/28	0/3/3/3

The worst 5 of 312 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3629	B8K	C8-N9	-22.47	1.31	1.45
2	5	3631	BGH	C8-N9	-22.39	1.31	1.45
2	5	4436	B8K	C8-N9	-22.15	1.31	1.45
2	5	3612	P7G	C8-N9	-21.39	1.32	1.45
2	5	1848	P7G	C8-N9	-21.09	1.32	1.45

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	2365	7MG	N9-C4-N3	9.54	139.43	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1479	A2M	C4'-O4'-C1'	-8.42	102.21	109.92
2	5	1614	I4U	O4-C4-C5	8.34	121.37	115.45
2	5	4149	PSU	N1-C2-N3	6.94	122.49	115.17
2	5	1799	B8H	N3-C2-N1	6.72	121.71	115.22

There are no chirality outliers.

5 of 97 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	5	1260	OMG	C1'-C2'-O2'-CM2
2	5	1270	A2M	C1'-C2'-O2'-CM'
2	5	1292	P4U	N3-C4-O4-C41
2	5	1292	P4U	O4'-C4'-C5'-O5'
2	5	1537	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 183 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
50	OWI	K	501	-	45,45,45	2.20	12 (26%)	62,64,64	2.87	14 (22%)

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
50	OWI	K	501	-	-	26/52/60/60	0/3/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	K	501	OWI	S05-N04	6.76	1.72	1.63
50	K	501	OWI	S30-N29	6.53	1.72	1.63
50	K	501	OWI	C31-S30	5.60	1.84	1.76
50	K	501	OWI	C07-S05	4.87	1.83	1.76
50	K	501	OWI	C34-N35	3.84	1.46	1.37

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	K	501	OWI	O41-S30-O40	-12.28	100.43	119.59
50	K	501	OWI	O14-S05-O06	-11.97	100.91	119.59
50	K	501	OWI	O41-S30-N29	7.07	113.34	106.69
50	K	501	OWI	O14-S05-N04	6.19	112.52	106.69
50	K	501	OWI	O06-S05-N04	4.63	111.04	106.69

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

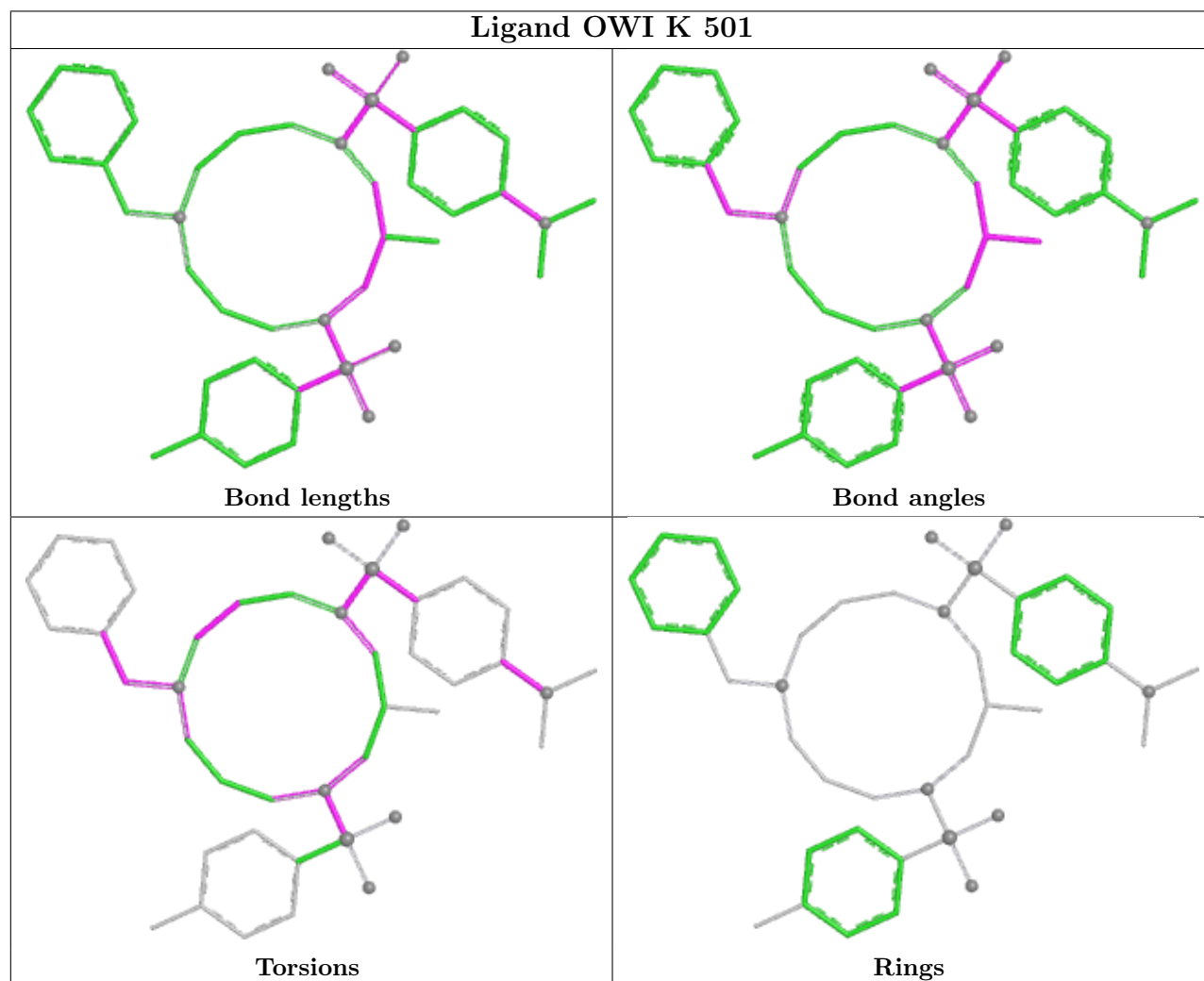
Mol	Chain	Res	Type	Atoms
50	K	501	OWI	C16-C15-N04-S05
50	K	501	OWI	N18-C19-C20-C21
50	K	501	OWI	N18-C19-C20-C25
50	K	501	OWI	C20-C19-N18-C26
50	K	501	OWI	C02-C42-N29-C28

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.

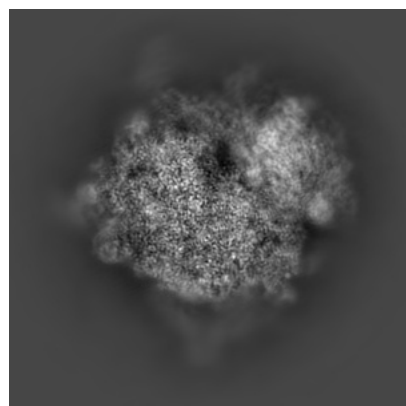
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15863. These allow visual inspection of the internal detail of the map and identification of artifacts.

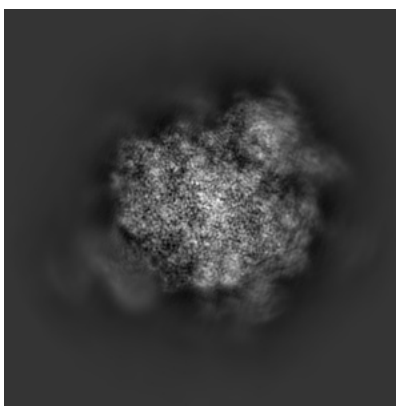
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

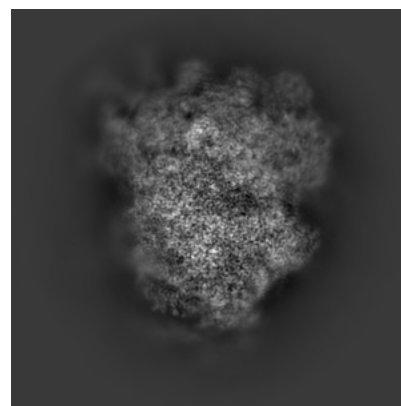
6.1.1 Primary map



X

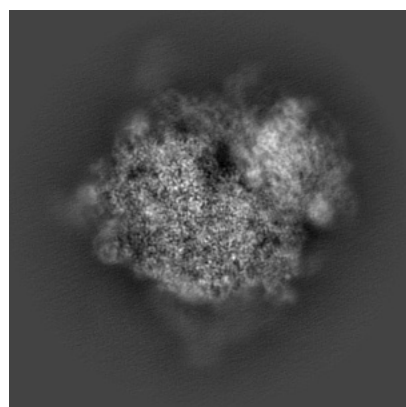


Y

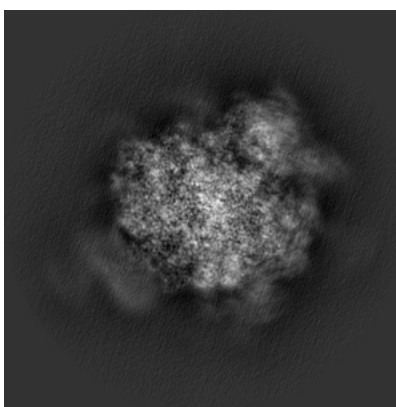


Z

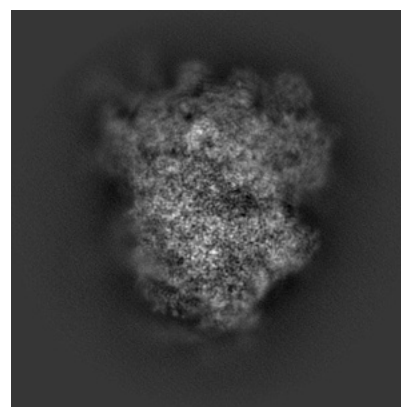
6.1.2 Raw map



X



Y

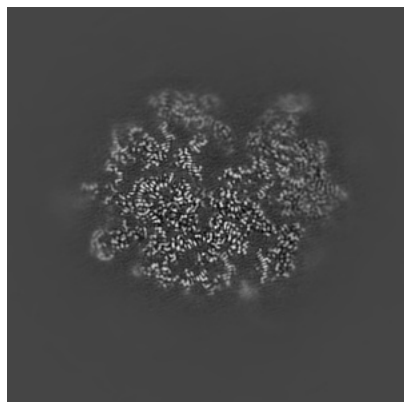


Z

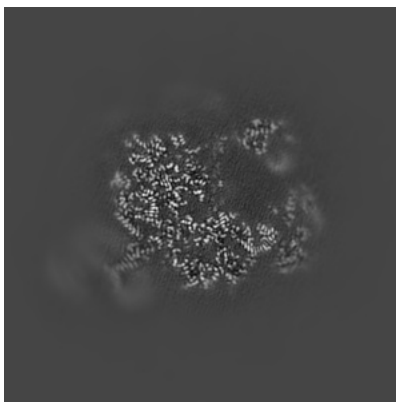
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

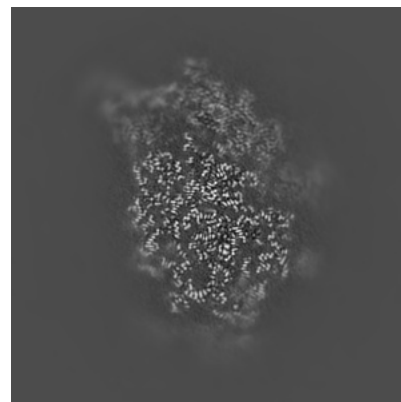
6.2.1 Primary map



X Index: 176

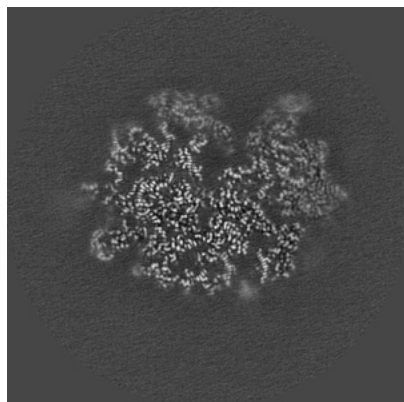


Y Index: 176

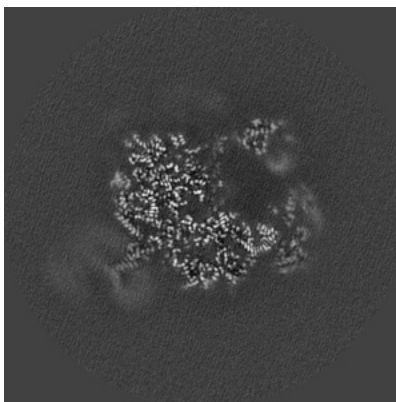


Z Index: 176

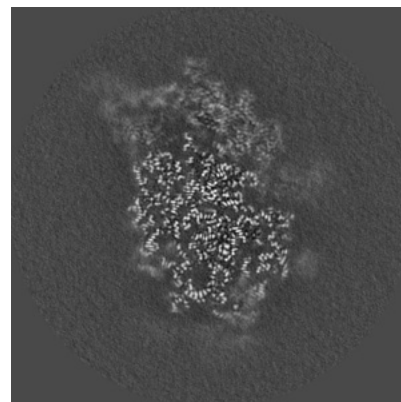
6.2.2 Raw map



X Index: 176



Y Index: 176

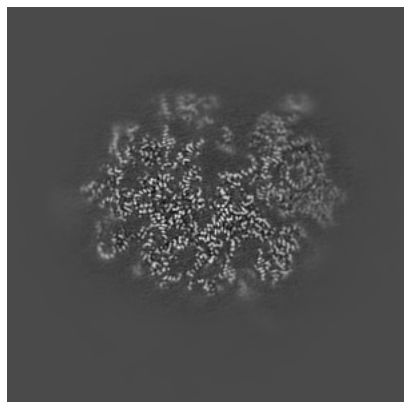


Z Index: 176

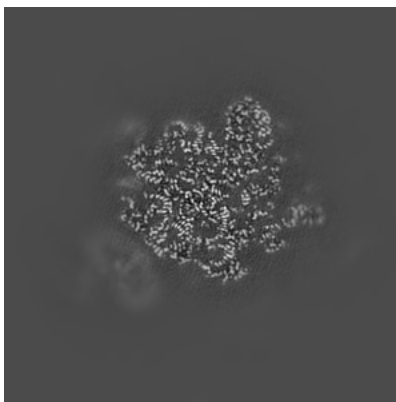
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

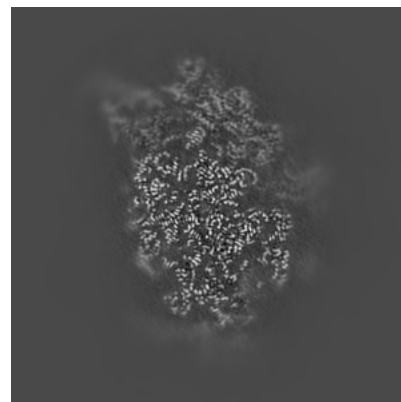
6.3.1 Primary map



X Index: 179

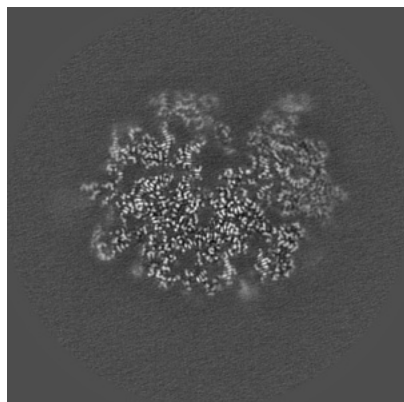


Y Index: 147

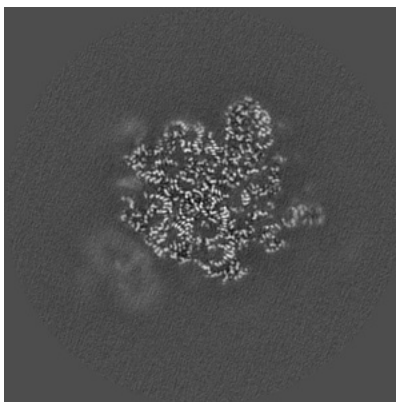


Z Index: 180

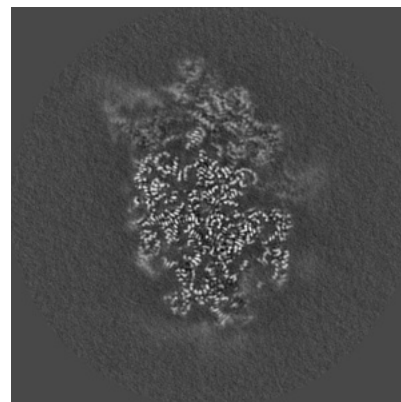
6.3.2 Raw map



X Index: 177



Y Index: 147

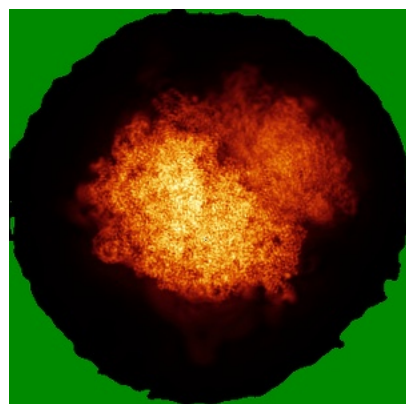


Z Index: 180

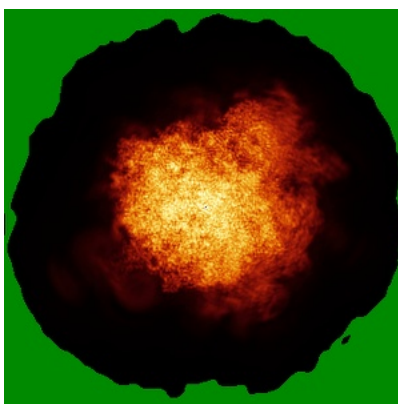
The images above show the largest variance slices of the map in three orthogonal directions.

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

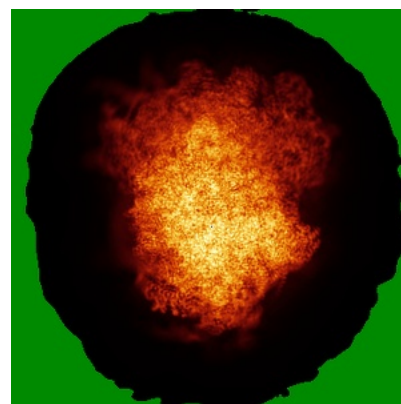
6.4.1 Primary map



X

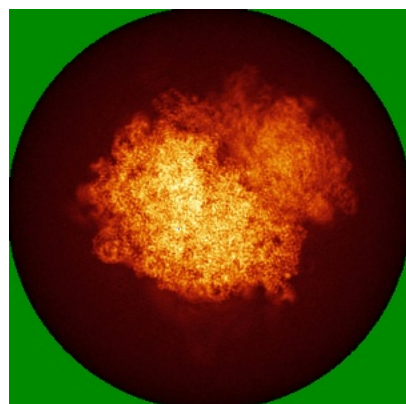


Y

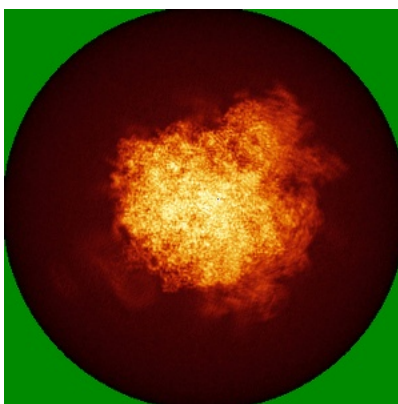


Z

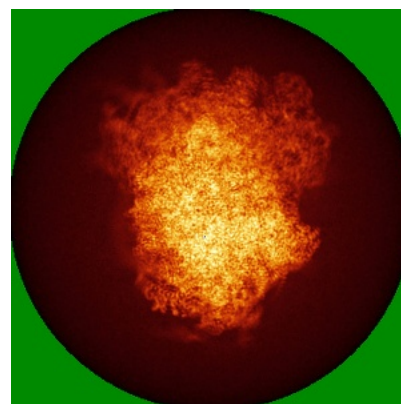
6.4.2 Raw map



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.

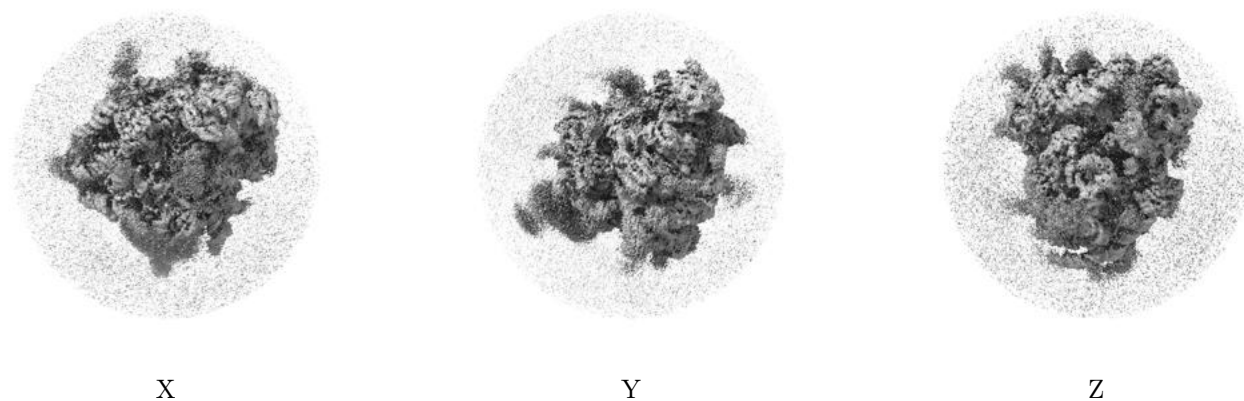
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01581. 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.

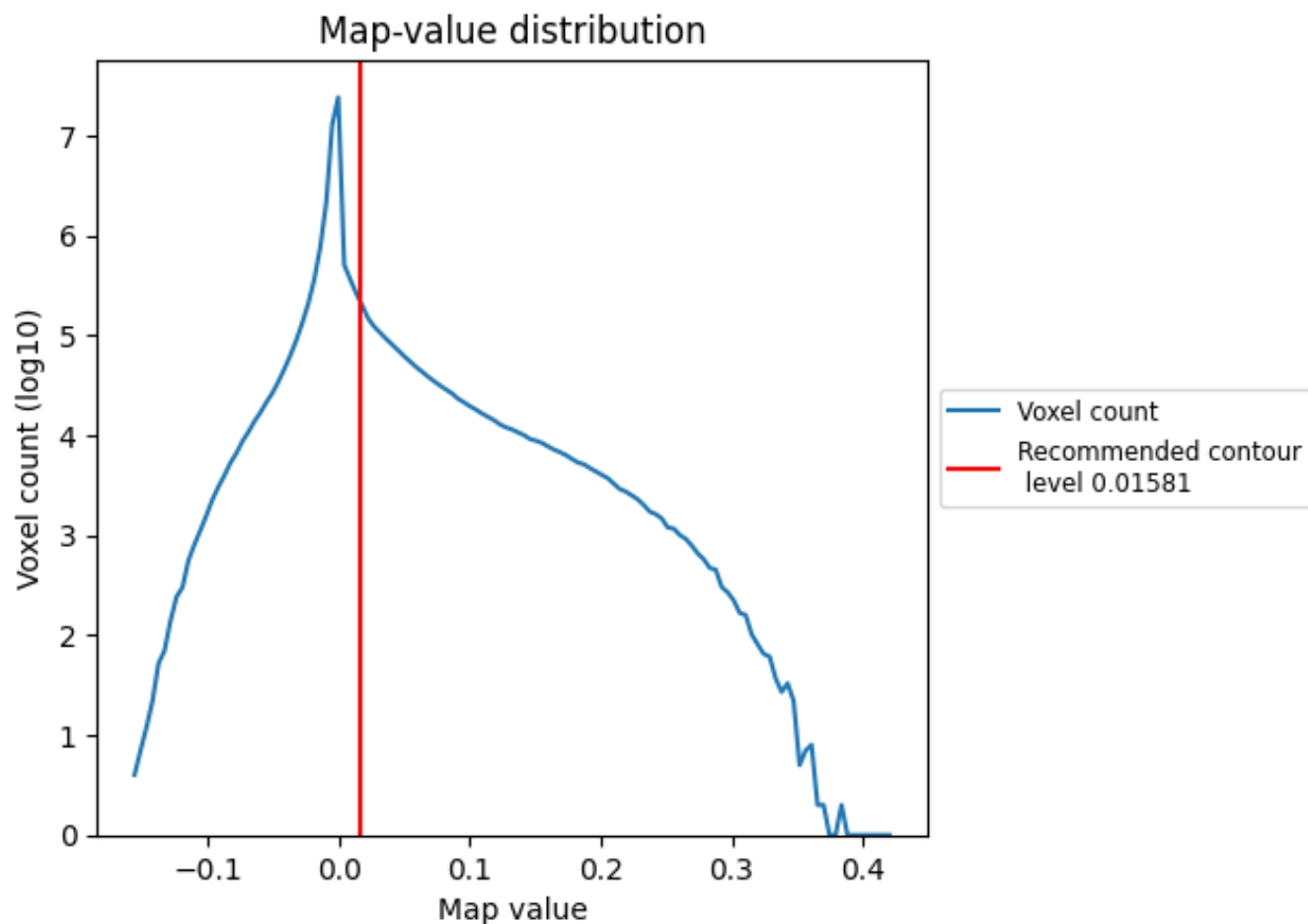
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

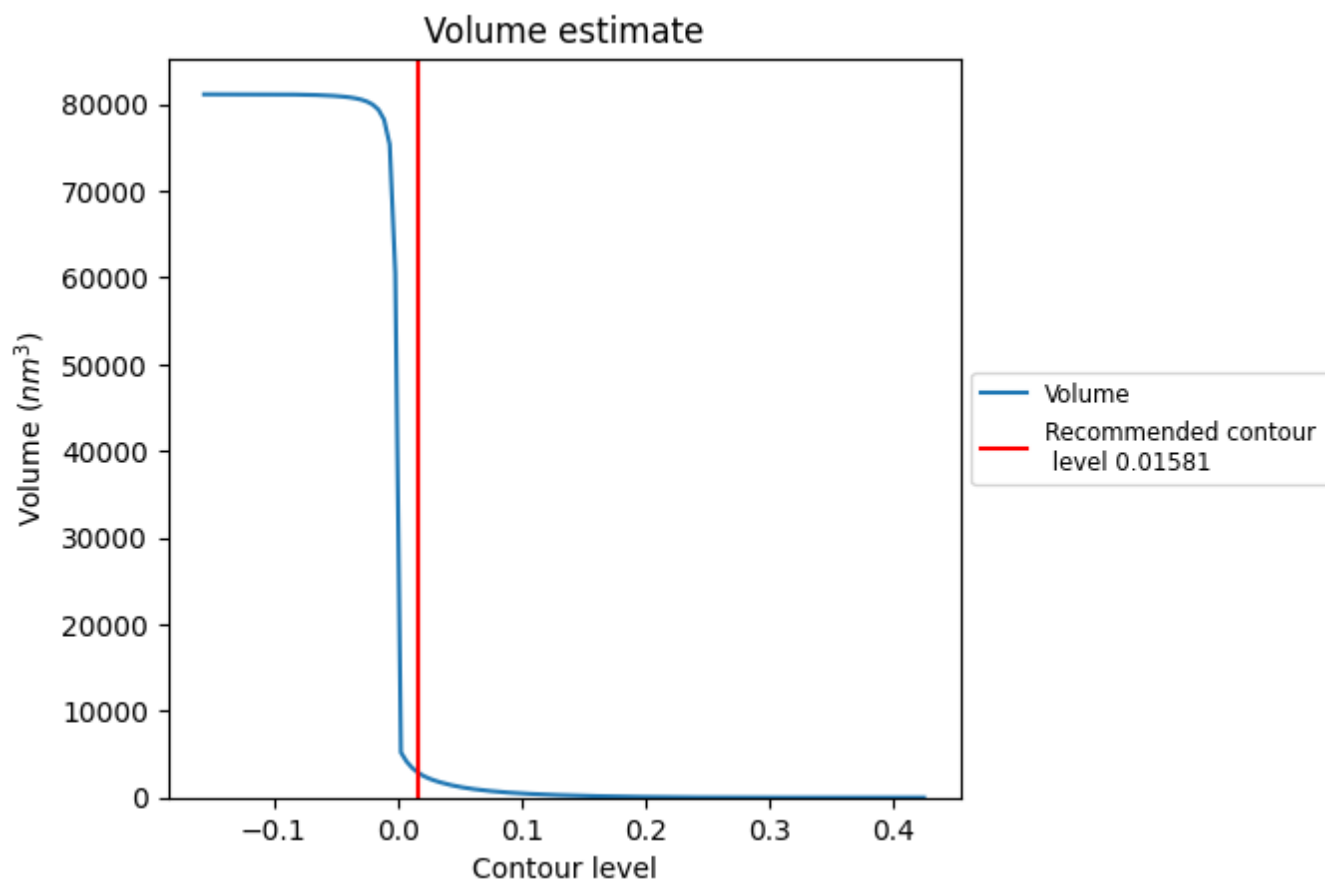
This section contains the results of statistical analysis of the map.

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.

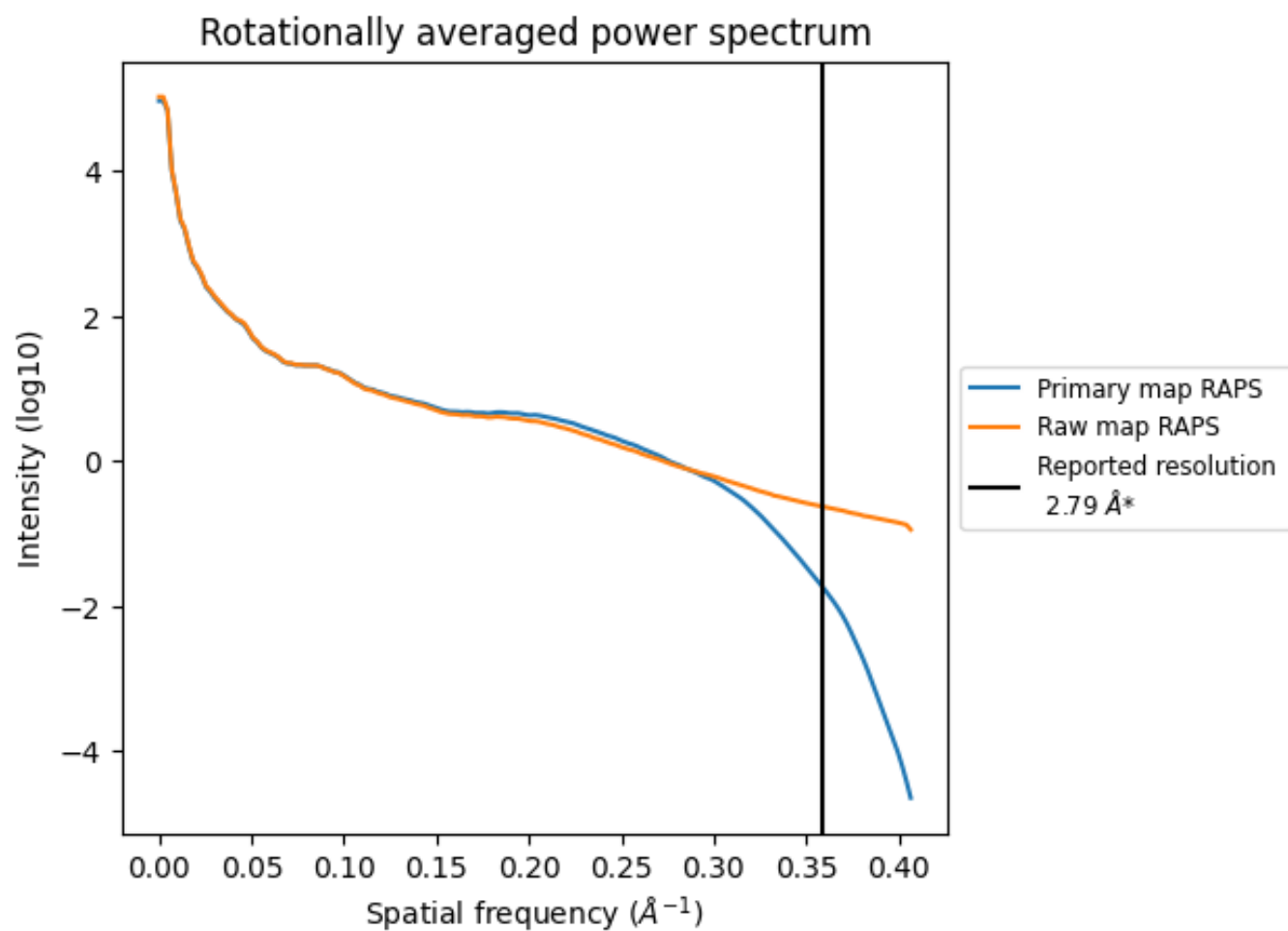
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2951 nm^3 ; this corresponds to an approximate mass of 2665 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 ⓘ

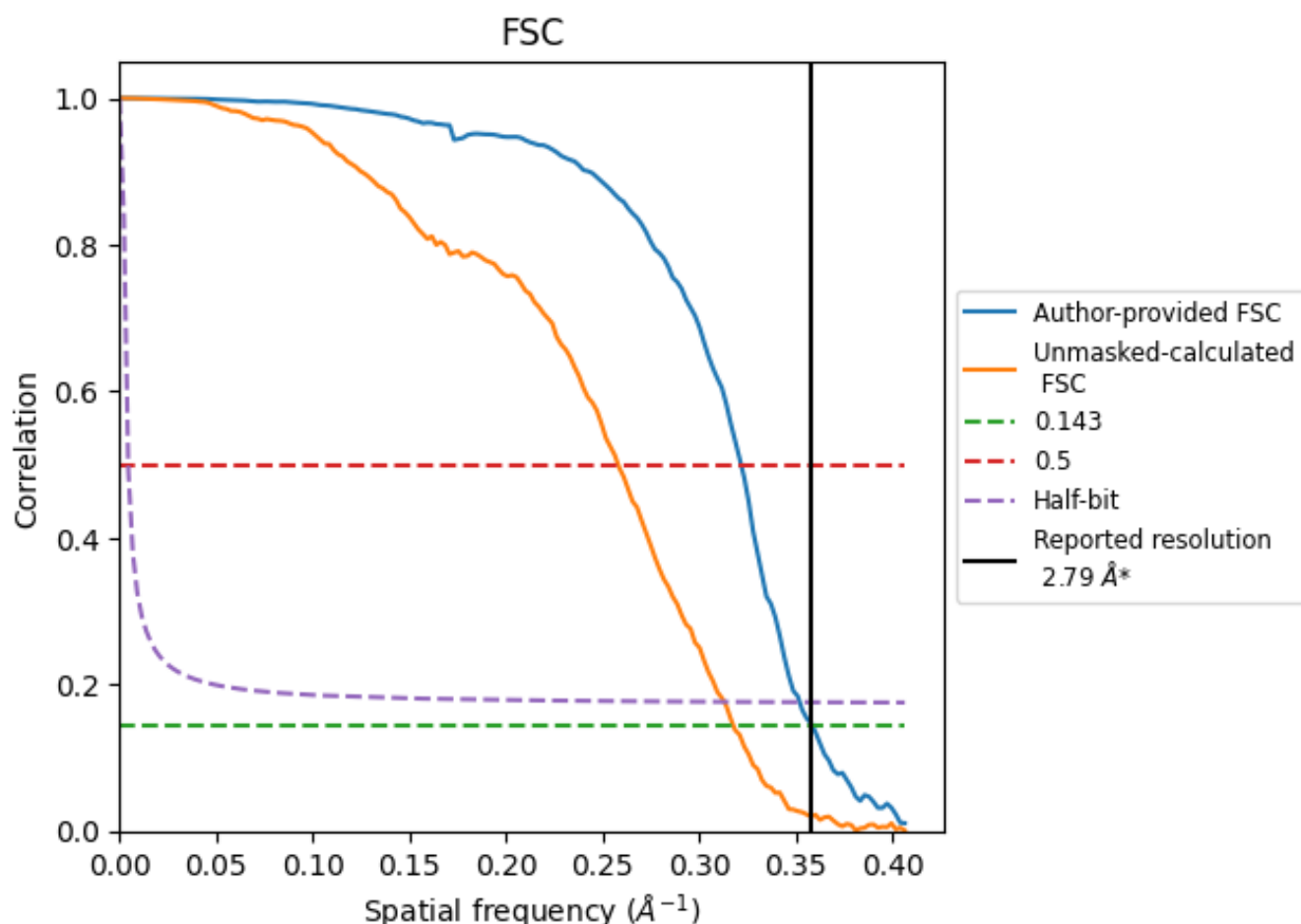


*Reported resolution corresponds to spatial frequency of 0.358 \AA^{-1}

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 0.358 Å⁻¹

8.2 Resolution estimates [i](#)

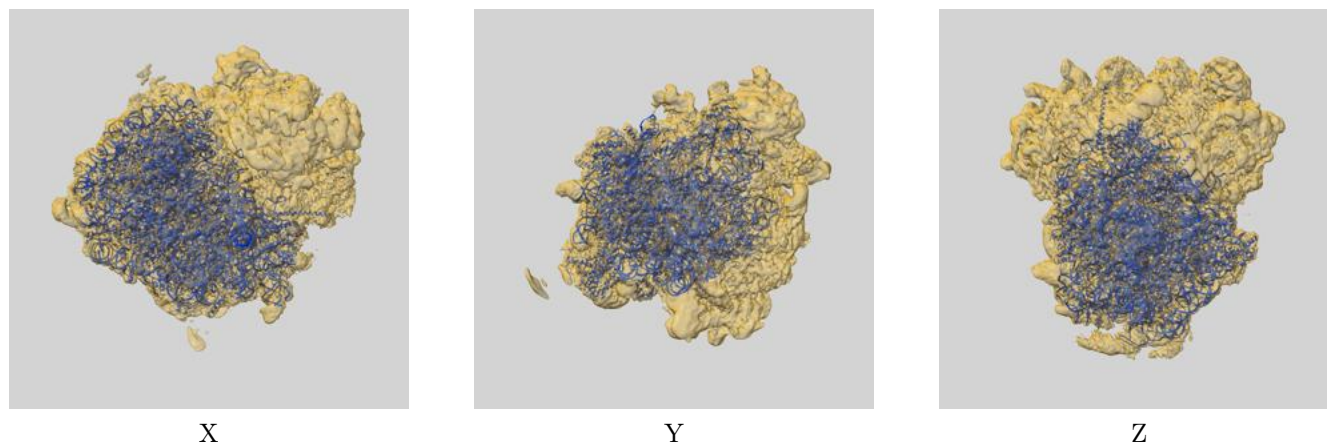
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.11	2.84
Unmasked-calculated*	3.15	3.87	3.19

*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 3.15 differs from the reported value 2.79 by more than 10 %

9 Map-model fit [i](#)

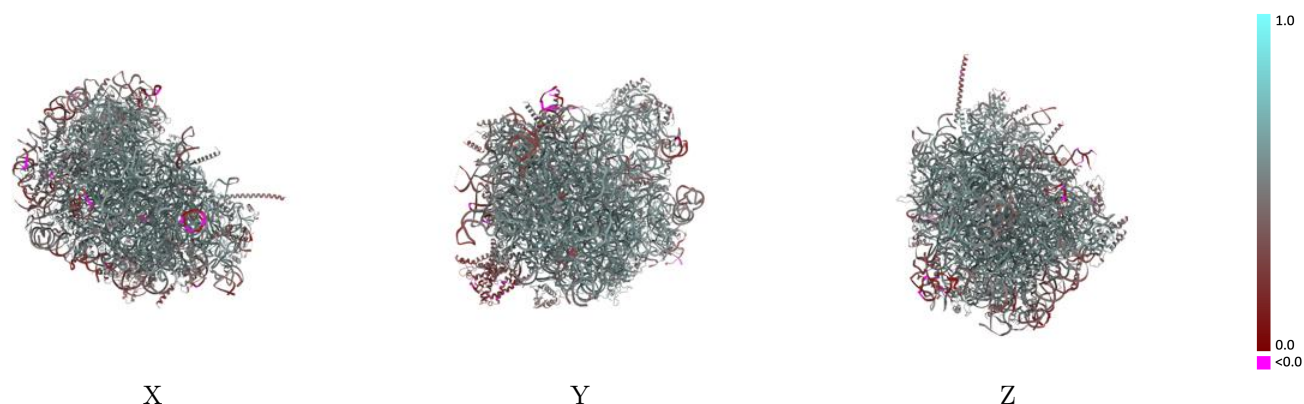
This section contains information regarding the fit between EMDB map EMD-15863 and PDB model 8B6C. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



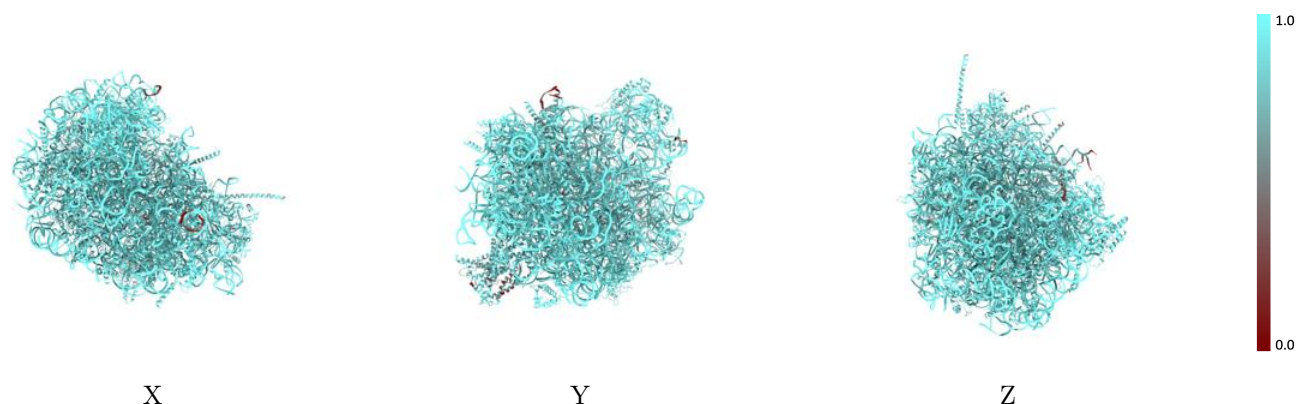
The images above show the 3D surface view of the map at the recommended contour level 0.01581 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



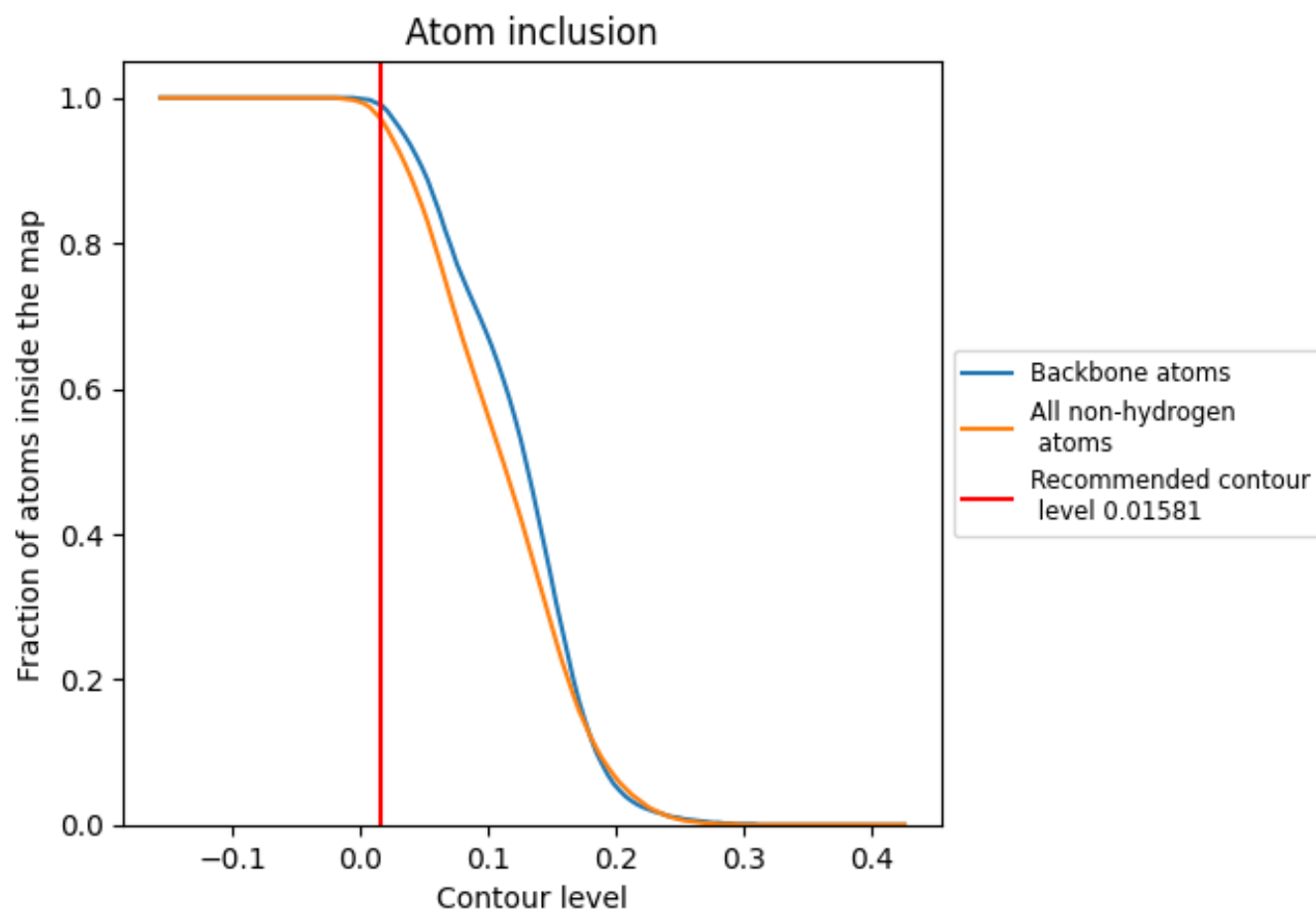
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01581).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.01581) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9710	 0.5160
5	 0.9870	 0.5160
7	 0.9980	 0.5520
8	 0.9950	 0.5410
A	 0.9700	 0.5720
B	 0.9690	 0.5500
C	 0.9660	 0.5490
D	 0.9720	 0.5050
E	 0.9710	 0.5230
F	 0.9590	 0.5510
G	 0.9560	 0.4800
H	 0.9550	 0.5320
I	 0.9590	 0.5400
J	 0.9500	 0.4670
K	 0.7720	 0.2550
L	 0.9370	 0.5110
M	 0.9720	 0.5320
N	 0.9720	 0.5760
O	 0.9750	 0.5530
P	 0.9620	 0.5550
Q	 0.9580	 0.5600
R	 0.9400	 0.4920
S	 0.9720	 0.5580
T	 0.9600	 0.5390
U	 0.9440	 0.4390
V	 0.9560	 0.5610
W	 0.9570	 0.5450
X	 0.9310	 0.5240
Y	 0.9450	 0.5250
Z	 0.9700	 0.5140
a	 0.9750	 0.5680
b	 0.9320	 0.4730
c	 0.9400	 0.4970
d	 0.9510	 0.5230
e	 0.9660	 0.5670



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Chain	Atom inclusion	Q-score
f	 0.9670	 0.5760
g	 0.9450	 0.5440
h	 0.9370	 0.5150
i	 0.9470	 0.4970
j	 0.9780	 0.5790
k	 0.9170	 0.4660
l	 0.9560	 0.5470
m	 0.9520	 0.5540
n	 0.8850	 0.4620
o	 0.9620	 0.5470
p	 0.9420	 0.5400
q	 0.8050	 0.2950
r	 0.9770	 0.5530