



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 02:08 PM EDT

PDB ID : 6AZ3
EMDB ID : EMD-7025
Title : Cryo-EM structure of of the large subunit of Leishmania ribosome bound to paromomycin
Authors : Shalev-Benami, M.; Zhang, Y.; Rozenberg, H.; Nobe, Y.; Taoka, M.; Matzov, D.; Zimmerman, E.; Bashan, A.; Isobe, T.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.
Deposited on : 2017-09-09
Resolution : 2.50 Å(reported)

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) : 2.39

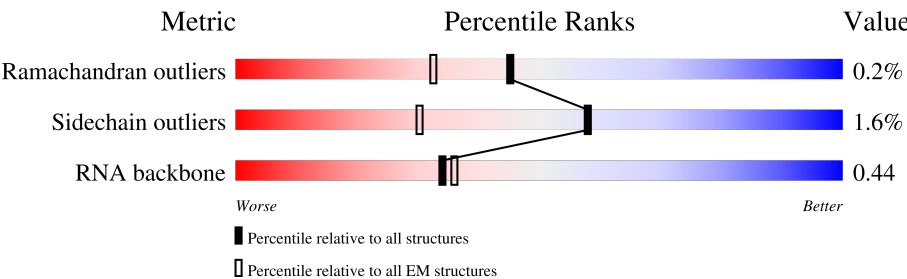
1 Overall quality at a glance

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	254	<div> <div>96%</div> </div>
2	B	402	<div> <div>98%</div> </div>
3	C	366	<div> <div>98%</div> </div>
4	D	168	<div> <div>22%</div> <div>98%</div> </div>
5	E	186	<div> <div>100%</div> </div>
6	F	195	<div> <div>8%</div> <div>69%</div> <div>30%</div> </div>
7	G	348	<div> <div>61%</div> <div>37%</div> </div>
8	H	221	<div> <div>6%</div> <div>97%</div> </div>

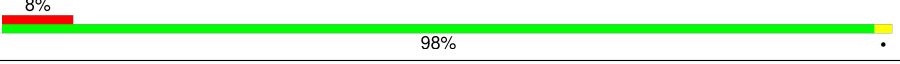
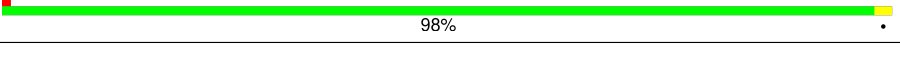
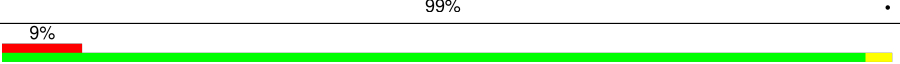
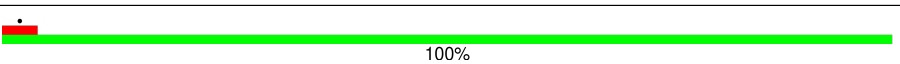
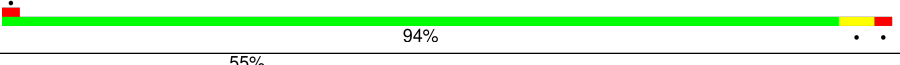
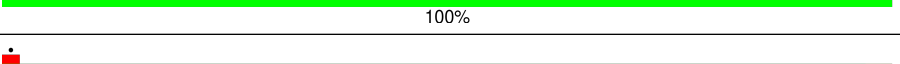
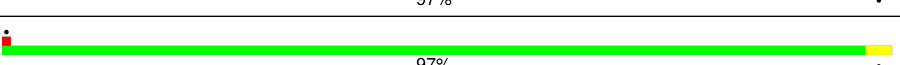



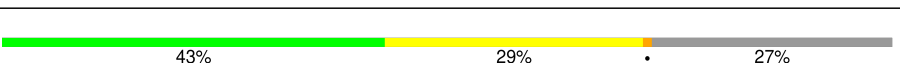
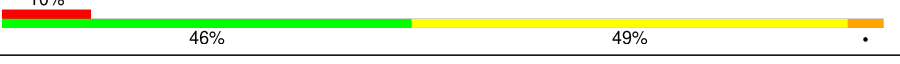





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Mol	Chain	Length	Quality of chain
9	I	212	
10	J	134	
11	K	149	
12	L	144	
13	M	203	
14	N	213	
15	O	305	
16	P	197	
17	Q	189	
18	R	178	
19	S	154	
20	T	154	
21	U	121	
22	V	118	
23	W	121	
24	X	65	
25	Y	132	
26	Z	140	
27	a	125	
28	b	68	
29	c	227	
30	d	92	
31	e	119	
32	f	130	
33	g	125	

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Mol	Chain	Length	Quality of chain
34	h	125	
35	i	97	
36	j	80	
37	k	76	
38	l	50	
39	m	50	
40	n	33	
41	o	90	
42	p	96	
43	1	1778	
44	2	1526	
45	3	211	
46	4	183	
47	5	133	
48	6	71	
49	7	171	
50	8	118	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 126561 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 ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	254	Total	C	N	O	S	7	0
			1985	1235	412	327	11		

- Molecule 2 is a protein called ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	402	Total	C	N	O	S	10	0
			3226	2036	644	533	13		

- Molecule 3 is a protein called Ribosomal protein L1a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	366	Total	C	N	O	S	2	0
			2824	1761	563	485	15		

- Molecule 4 is a protein called 60S ribosomal protein L11 (L5, L16).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1220	774	229	209	8		

- Molecule 5 is a protein called 60S ribosomal protein L9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	186	Total	C	N	O	S	0	0
			1448	917	268	257	6		

- Molecule 6 is a protein called ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	137	Total	C	N	O	S	0	0
			1004	637	185	180	2		

- Molecule 7 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	220	Total	C	N	O	S	2	0
			1746	1099	351	289	7		

- Molecule 8 is a protein called ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	221	Total	C	N	O	S	3	0
			1781	1128	360	286	7		

- Molecule 9 is a protein called ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	212	Total	C	N	O	S	0	0
			1647	1026	331	282	8		

- Molecule 10 is a protein called 60S ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	134	Total	C	N	O	S	0	0
			1001	634	190	171	6		

- Molecule 11 is a protein called Probable 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	149	Total	C	N	O	S	1	0
			1164	726	231	201	6		

- Molecule 12 is a protein called 60S ribosomal protein L27A/L29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	144	Total	C	N	O	S	0	0
			1126	708	226	186	6		

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	203	Total	C	N	O	S	0	0
			1714	1080	362	264	8		

- Molecule 14 is a protein called 60S ribosomal protein L10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	190	Total	C	N	O	S	0	0
			1454	924	285	233	12		

- Molecule 15 is a protein called 60S ribosomal protein L5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	252	Total	C	N	O	S	3	0
			1976	1259	376	336	5		

- Molecule 16 is a protein called 60S ribosomal protein L18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	197	Total	C	N	O	S	0	0
			1539	968	307	258	6		

- Molecule 17 is a protein called Ribosomal protein L19e family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	189	Total	C	N	O	S	0	0
			1452	899	313	235	5		

- Molecule 18 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	178	Total	C	N	O	S	0	0
			1454	927	280	242	5		

- Molecule 19 is a protein called 60S ribosomal protein L21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	154	Total	C	N	O	S	0	0
			1208	767	238	199	4		

- Molecule 20 is a protein called 60S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	154	Total	C	N	O	S	0	0
			1236	773	245	207	11		

- Molecule 21 is a protein called 60S ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	121	Total	C	N	O	S	0	0
			934	605	167	159	3		

- Molecule 22 is a protein called 60S ribosomal protein L23a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	118	Total	C	N	O	S	1	0
			928	590	173	162	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	27	ALA	-	expression tag	UNP A0A3S7WPH7

- Molecule 23 is a protein called ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	121	Total	C	N	O	S	0	0
			971	605	200	162	4		

- Molecule 24 is a protein called ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	65	Total	C	N	O	S	0	0
			553	363	107	79	4		

- Molecule 25 is a protein called Ribosomal L27e family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	132	Total	C	N	O	S	1	0
			1039	666	205	165	3		

- Molecule 26 is a protein called 60S ribosomal protein L28, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	140	Total	C	N	O	S	0	0
			1067	650	226	186	5		

- Molecule 27 is a protein called 60S_ribosomal_protein_L35_putative/GeneDB:LmjF.26.2330/GeneDB:LmjF.26.2340.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	125	Total	C	N	O	S	0	0
			985	615	205	163	2		

- Molecule 28 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	68	Total	C	N	O	S	0	0
			539	330	124	84	1		

- Molecule 29 is a protein called 60S ribosomal protein L7 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	227	Total	C	N	O	S	0	0
			1809	1152	349	297	11		

- Molecule 30 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	92	Total	C	N	O	S	0	0
			691	430	126	130	5		

- Molecule 31 is a protein called 60S ribosomal subunit protein L31, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	119	Total	C	N	O	S	0	0
			936	595	183	156	2		

- Molecule 32 is a protein called 60S_ribosomal_protein_L32/GeneDB:LmjF.21.1720.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	130	Total	C	N	O	S	1	0
			1048	659	210	175	4		

- Molecule 33 is a protein called Ribosomal protein L35Ae family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	125	Total	C	N	O	S	0	0
			998	623	209	161	5		

- Molecule 34 is a protein called 60S ribosomal protein L34, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	125	Total	C	N	O	S	1	0
			1010	623	221	160	6		

- Molecule 35 is a protein called 60S ribosomal protein L36, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	97	Total	C	N	O	S	0	0
			760	482	153	123	2		

- Molecule 36 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	80	Total	C	N	O	S	0	0
			663	403	152	102	6		

- Molecule 37 is a protein called Ribosomal L38e family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	76	Total	C	N	O	S	0	0
			575	361	110	101	3		

- Molecule 38 is a protein called 60S ribosomal protein L39, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	50	Total	C	N	O	S	0	0
			440	285	91	63	1		

- Molecule 39 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	50	Total	C	N	O	S	0	0
			393	248	80	58	7		

- Molecule 40 is a protein called ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	33	Total	C	N	O	S	0	0
			280	172	69	37	2		

- Molecule 41 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	90	Total	C	N	O	S	0	0
			696	432	144	114	6		

- Molecule 42 is a protein called 60S ribosomal protein L44, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	96	Total	C	N	O	S	0	0
			756	478	153	120	5		

- Molecule 43 is a RNA chain called rRNA alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1	1620	Total	C	N	O	P	0	0
			34631	15467	6334	11211	1619		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	A	deletion	GB 322500086
1	?	-	A	deletion	GB 322500086

- Molecule 44 is a RNA chain called rRNA beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2	1078	Total	C	N	O	P	0	0
			22996	10290	4137	7491	1078		

- Molecule 45 is a RNA chain called rRNA gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3	177	Total	C	N	O	P	0	0
			3751	1677	657	1240	177		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	U	deletion	GB 322500086
3	196	C	A	conflict	GB 322500086

- Molecule 46 is a RNA chain called rRNA delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	183	Total	C	N	O	P	0	0
			3906	1742	706	1275	183		

- Molecule 47 is a RNA chain called rRNA epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5	97	Total	C	N	O	P	0	0
			2075	925	379	674	97		

- Molecule 48 is a RNA chain called rRNA zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	6	71	Total	C	N	O	P	0	0
			1477	659	265	482	71		

- Molecule 49 is a RNA chain called rRNA 5.8S.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	163	Total	C	N	O	P	0	0
			3465	1552	616	1135	162		

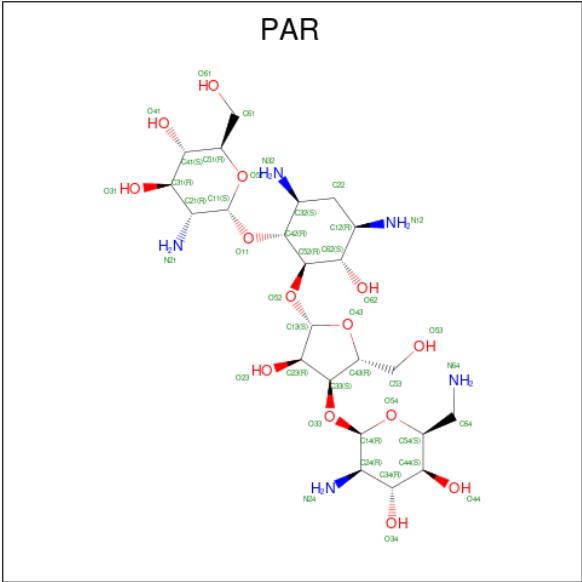
- Molecule 50 is a RNA chain called rRNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	118	Total	C	N	O	P	0	0
			2511	1123	448	822	118		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	14	U	C	conflict	GB 1229082190

- Molecule 51 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				AltConf
51	1	1	Total	C	N	O	0
			42	23	5	14	
			Total	C	N	O	
			42	23	5	14	
			Total	C	N	O	
51	1	1	Total	C	N	O	0
			42	23	5	14	
			Total	C	N	O	
			42	23	5	14	
			Total	C	N	O	
51	2	1	Total	C	N	O	0
			42	23	5	14	
			Total	C	N	O	
			42	23	5	14	
			Total	C	N	O	
51	2	1	Total	C	N	O	0
			42	23	5	14	
			Total	C	N	O	
			42	23	5	14	
			Total	C	N	O	
51	7	1	Total	C	N	O	0
			42	23	5	14	
			Total	C	N	O	
			42	23	5	14	
			Total	C	N	O	

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	1	21	Total	Mg	0
			21	21	
52	2	8	Total	Mg	0
			8	8	

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Mol	Chain	Residues	Atoms		AltConf
52	3	1	Total 1	Mg 1	0
52	4	1	Total 1	Mg 1	0
52	5	1	Total 1	Mg 1	0
52	7	2	Total 2	Mg 2	0

- Molecule 53 is water.

Mol	Chain	Residues	Atoms		AltConf
53	A	16	Total 16	O 16	0
53	B	11	Total 11	O 11	0
53	C	11	Total 11	O 11	0
53	G	3	Total 3	O 3	0
53	H	7	Total 7	O 7	0
53	I	5	Total 5	O 5	0
53	J	2	Total 2	O 2	0
53	L	5	Total 5	O 5	0
53	M	16	Total 16	O 16	0
53	P	7	Total 7	O 7	0
53	Q	5	Total 5	O 5	0
53	R	2	Total 2	O 2	0
53	S	4	Total 4	O 4	0
53	T	3	Total 3	O 3	0
53	V	4	Total 4	O 4	0

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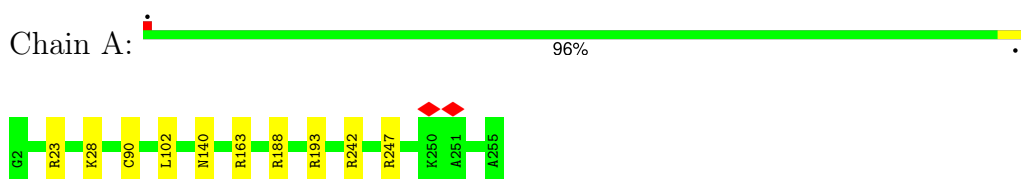
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Mol	Chain	Residues	Atoms		AltConf
53	W	1	Total 1	O 1	0
53	Y	1	Total 1	O 1	0
53	a	1	Total 1	O 1	0
53	c	2	Total 2	O 2	0
53	e	1	Total 1	O 1	0
53	f	3	Total 3	O 3	0
53	g	5	Total 5	O 5	0
53	h	5	Total 5	O 5	0
53	i	1	Total 1	O 1	0
53	j	8	Total 8	O 8	0
53	l	3	Total 3	O 3	0
53	p	6	Total 6	O 6	0
53	1	442	Total 442	O 442	0
53	2	278	Total 278	O 278	0
53	3	26	Total 26	O 26	0
53	4	47	Total 47	O 47	0
53	5	27	Total 27	O 27	0
53	6	2	Total 2	O 2	0
53	7	45	Total 45	O 45	0
53	8	14	Total 14	O 14	0

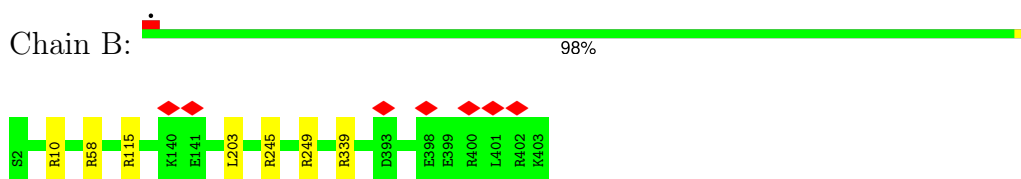
3 Residue-property plots [i](#)

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.

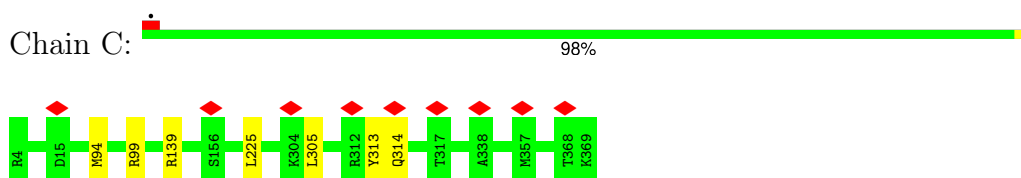
- Molecule 1: ribosomal protein uL2



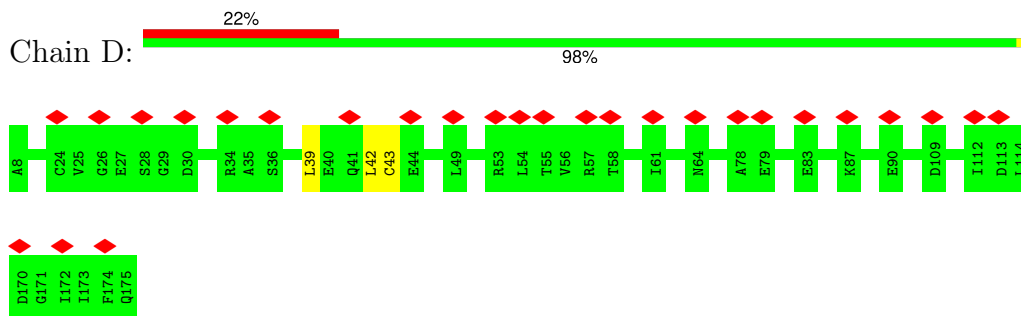
- Molecule 2: ribosomal protein uL3



- Molecule 3: Ribosomal protein L1a, putative



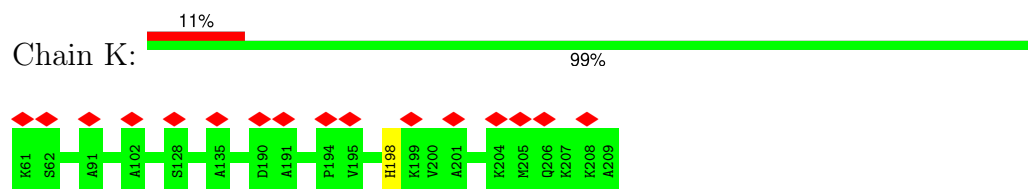
- Molecule 4: 60S ribosomal protein L11 (L5, L16)



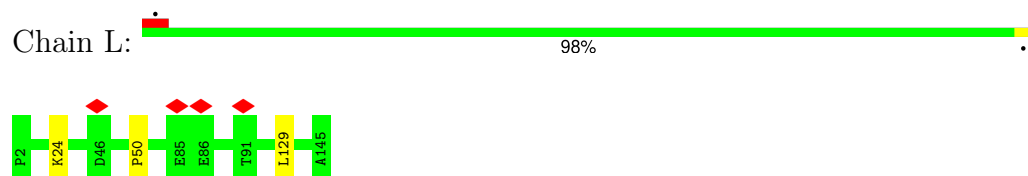
- Molecule 5: 60S ribosomal protein L9, putative



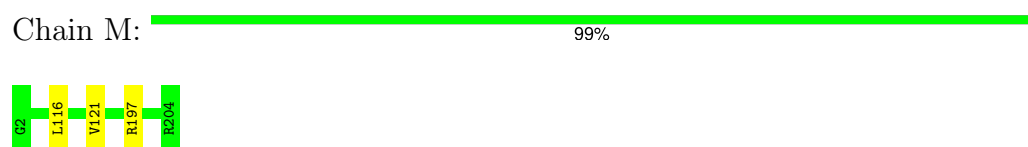
- Molecule 11: Probable 60S ribosomal protein L14



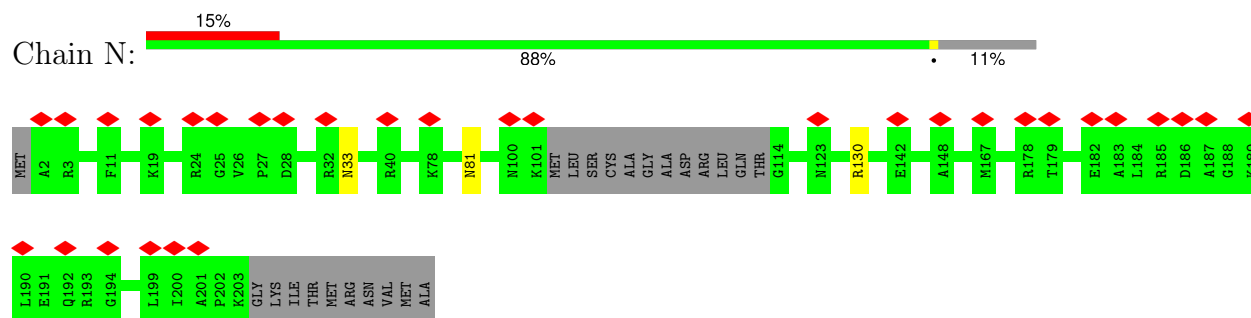
- Molecule 12: 60S ribosomal protein L27A/L29, putative



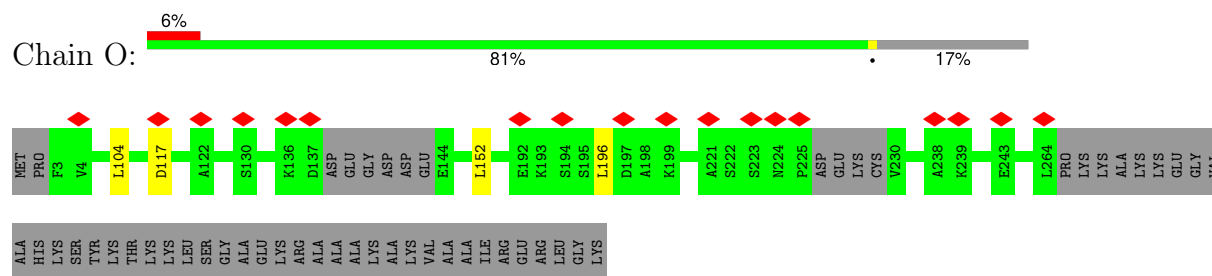
- Molecule 13: Ribosomal protein L15



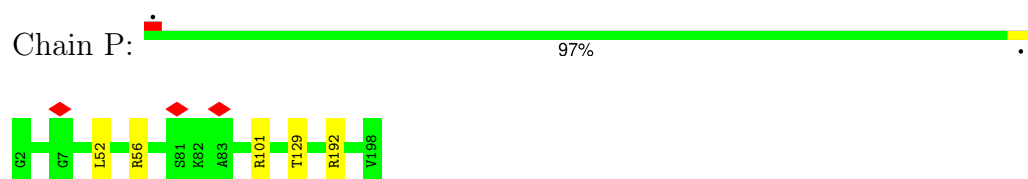
- Molecule 14: 60S ribosomal protein L10, putative



- Molecule 15: 60S ribosomal protein L5, putative

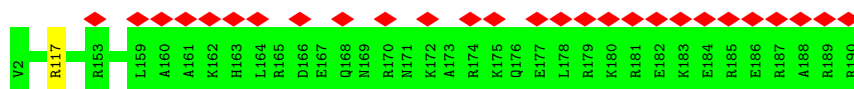


- Molecule 16: 60S ribosomal protein L18, putative



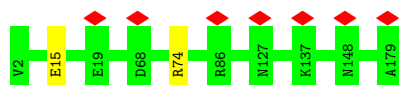
- Molecule 17: Ribosomal protein L19e family protein

Chain Q:  14% 99%



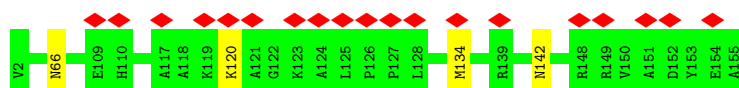
- Molecule 18: 60S ribosomal protein L18a

Chain R:  99%



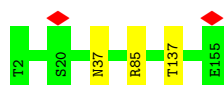
- Molecule 19: 60S ribosomal protein L21, putative

Chain S:  12% 97%



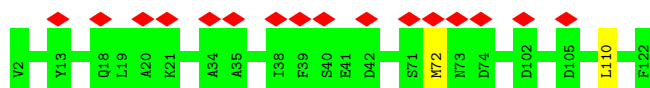
- Molecule 20: 60S ribosomal protein L17, putative

Chain T:  98%



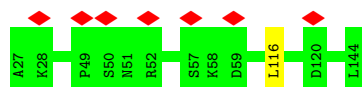
- Molecule 21: 60S ribosomal protein L22, putative

Chain U:  13% 98%



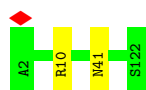
- Molecule 22: 60S ribosomal protein L23a, putative

Chain V:  6% 99%



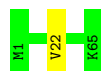
- Molecule 23: ribosomal protein uL24

Chain W:  98%



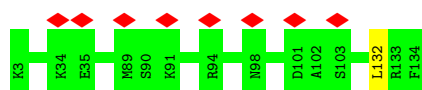
- Molecule 24: ribosomal protein eL24

Chain X: 98%



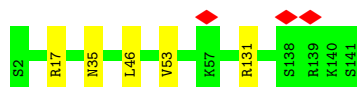
- Molecule 25: Ribosomal L27e family protein

Chain Y: 99%



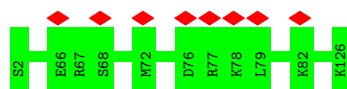
- Molecule 26: 60S ribosomal protein L28, putative

Chain Z: 96%



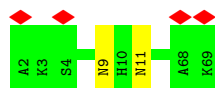
- Molecule 27: 60S_ribosomal_protein_L35_putative/GeneDB:LmjF.26.2330/GeneDB:LmjF.26.2340

Chain a: 100%



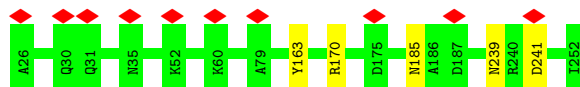
- Molecule 28: 60S ribosomal protein L29

Chain b: 97%

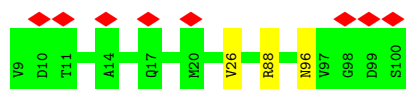


- Molecule 29: 60S ribosomal protein L7 family protein

Chain c: 98%



- Molecule 30: 60S ribosomal protein L30



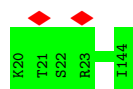
- Molecule 31: 60S ribosomal subunit protein L31, putative



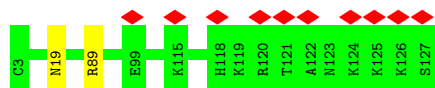
- Molecule 32: 60S_ribosomal_protein_L32/GeneDB:LmjF.21.1720



- Molecule 33: Ribosomal protein L35Ae family protein



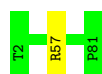
- Molecule 34: 60S ribosomal protein L34, putative



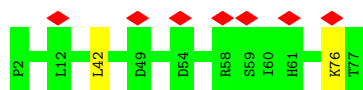
- Molecule 35: 60S ribosomal protein L36, putative



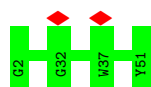
- Molecule 36: 60S ribosomal protein L37



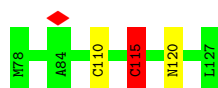
- Molecule 37: Ribosomal L38e family protein



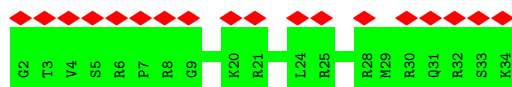
- Molecule 38: 60S ribosomal protein L39, putative



- Molecule 39: Ubiquitin-60S ribosomal protein L40



- Molecule 40: ribosomal protein eL41



- Molecule 41: 60S ribosomal protein L37a



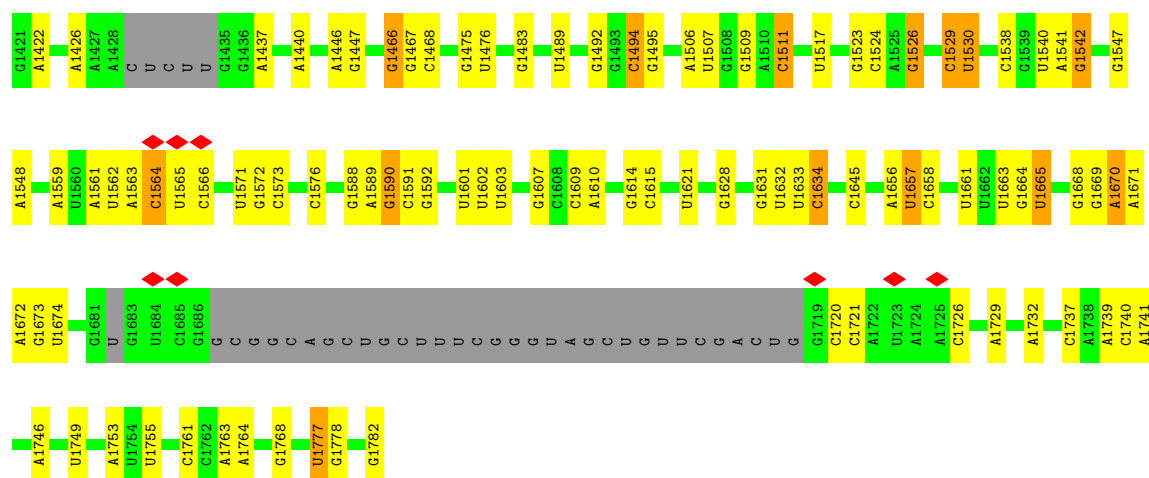
- Molecule 42: 60S ribosomal protein L44, putative



- Molecule 43: rRNA alpha

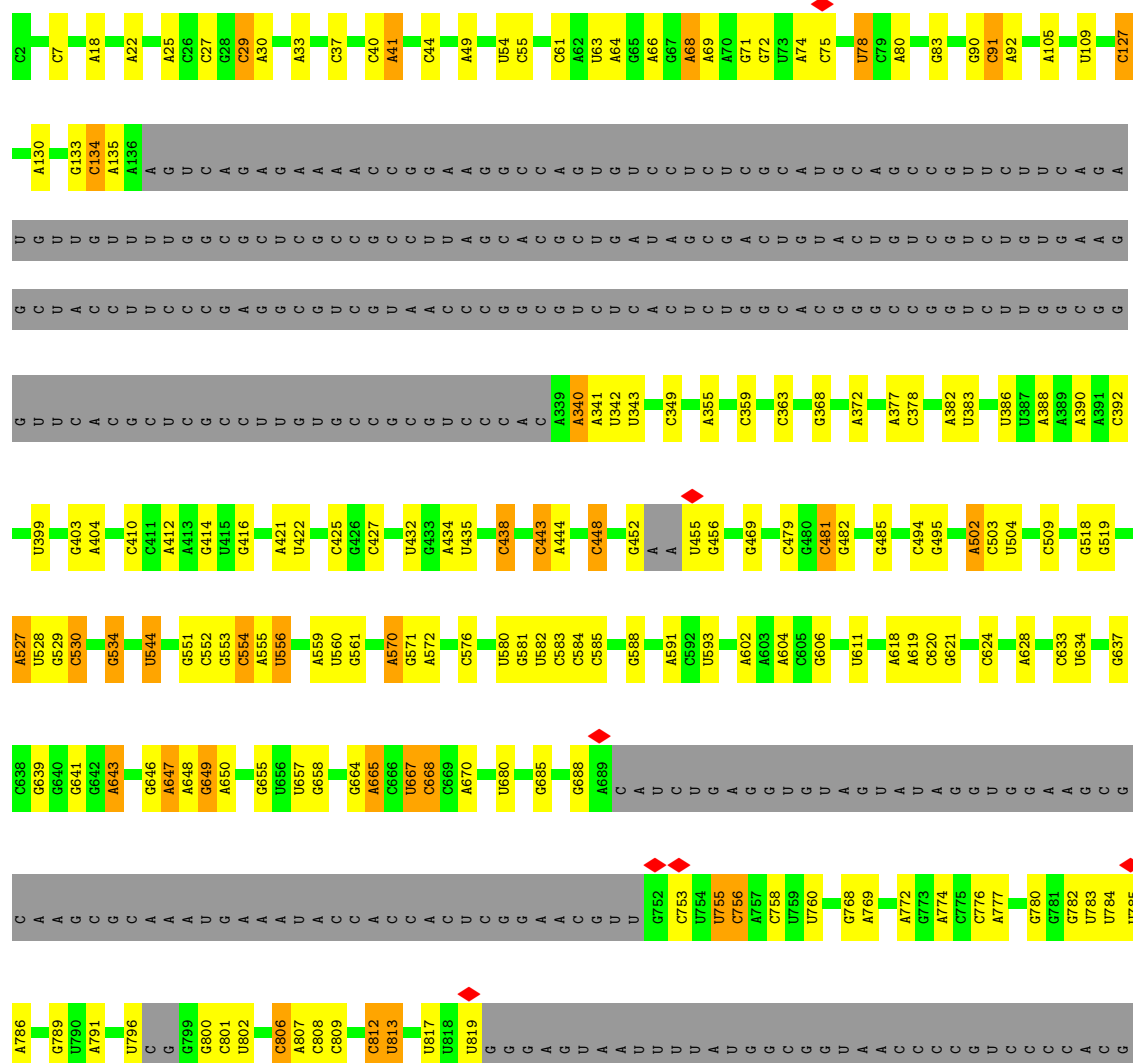


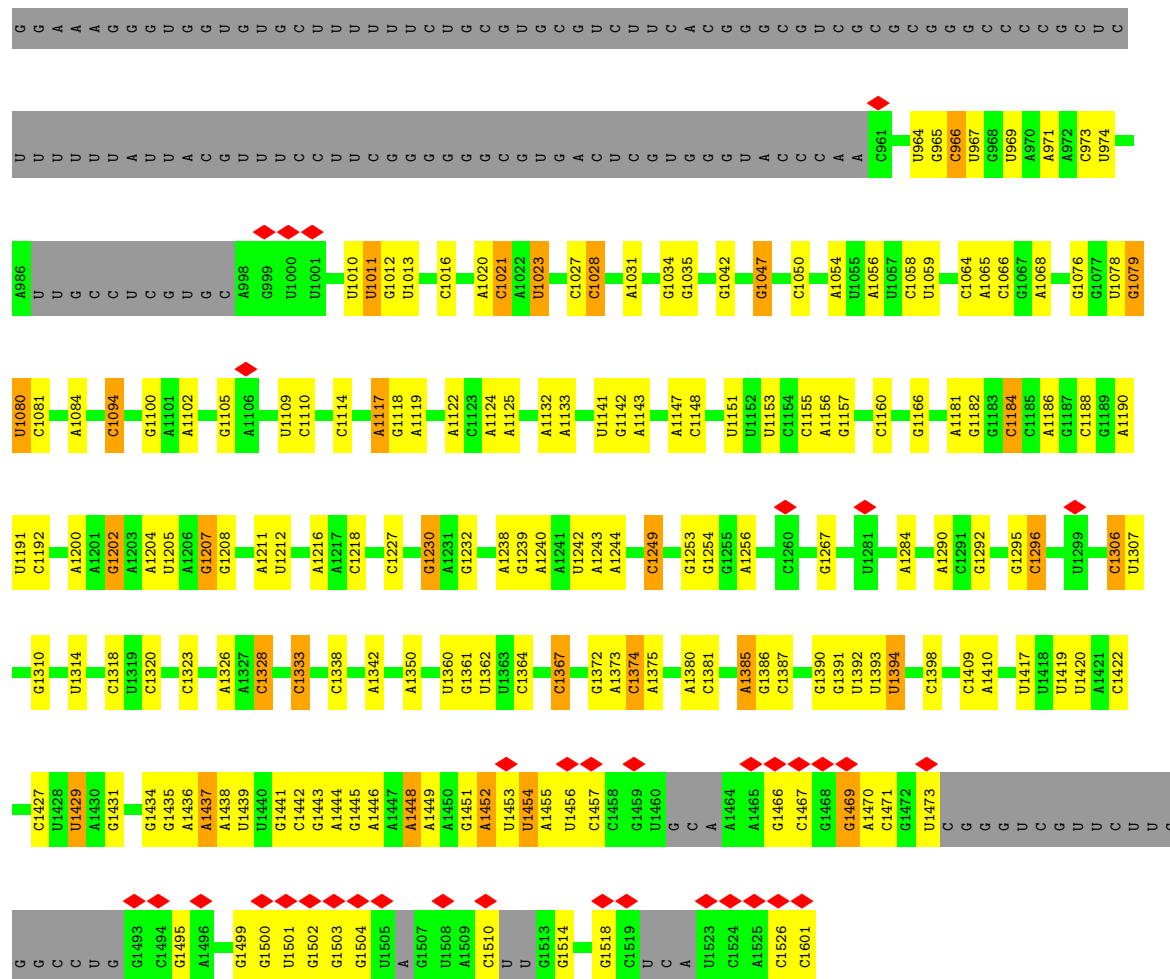




• Molecule 44: rRNA beta

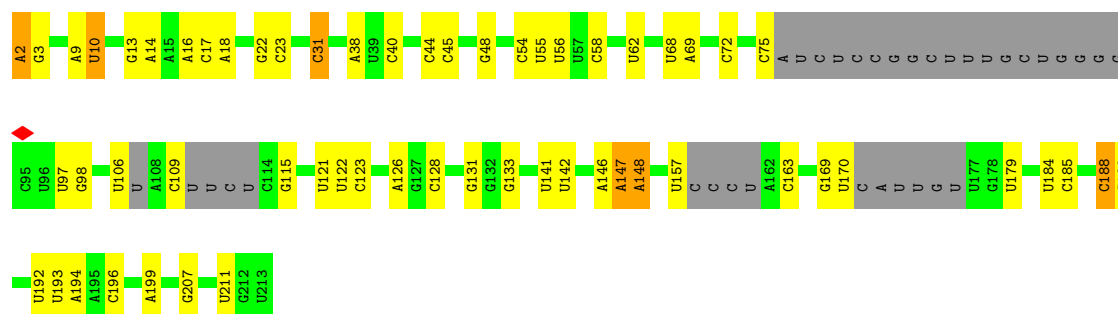
Chain 2: 47% 20% 29%





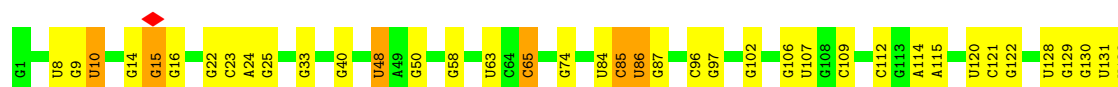
• Molecule 45: rRNA gamma

Chain 3: 56% 25% 16%



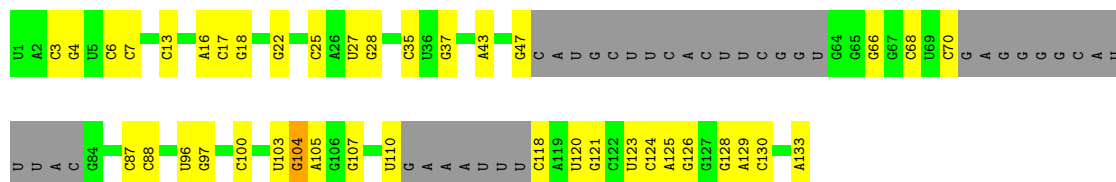
• Molecule 46: rRNA delta

Chain 4: 65% 32%





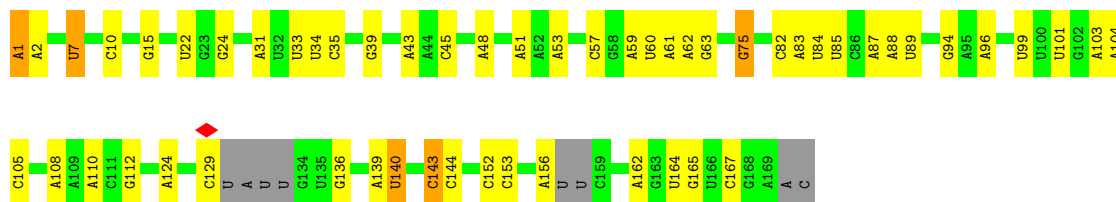
• Molecule 47: rRNA epsilon



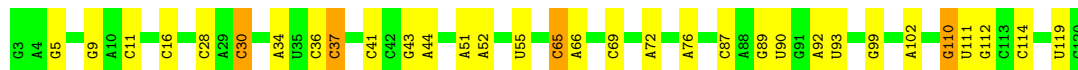
• Molecule 48: rRNA zeta



• Molecule 49: rRNA 5.8S



• Molecule 50: rRNA 5S



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141028	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	-0.407	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	391.68, 391.68, 391.68	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, A2M, MG, OMG, PAR, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.54	0/2042	0.67	1/2735 (0.0%)
2	B	0.48	0/3313	0.68	1/4460 (0.0%)
3	C	0.46	0/2880	0.68	2/3879 (0.1%)
4	D	0.35	0/1242	0.60	0/1678
5	E	0.38	0/1468	0.61	0/1983
6	F	0.40	0/1024	0.63	0/1397
7	G	0.48	1/1777 (0.1%)	0.68	1/2390 (0.0%)
8	H	0.48	1/1825 (0.1%)	0.70	2/2452 (0.1%)
9	I	0.44	0/1680	0.63	1/2257 (0.0%)
10	J	0.49	0/1018	0.69	2/1373 (0.1%)
11	K	0.38	0/1184	0.60	0/1599
12	L	0.48	0/1153	0.68	1/1541 (0.1%)
13	M	0.52	1/1754 (0.1%)	0.67	1/2342 (0.0%)
14	N	0.35	0/1486	0.56	0/2006
15	O	0.41	0/2013	0.67	3/2703 (0.1%)
16	P	0.49	0/1564	0.68	1/2092 (0.0%)
17	Q	0.39	0/1470	0.54	0/1966
18	R	0.47	0/1488	0.64	0/2005
19	S	0.49	0/1235	0.67	0/1663
20	T	0.51	0/1260	0.62	0/1688
21	U	0.39	0/949	0.69	0/1271
22	V	0.44	0/946	0.67	1/1276 (0.1%)
23	W	0.41	0/985	0.65	0/1315
24	X	0.46	0/574	0.59	0/773
25	Y	0.44	0/1064	0.63	1/1430 (0.1%)
26	Z	0.41	0/1082	0.60	0/1452
27	a	0.38	0/996	0.63	0/1333
28	b	0.39	0/550	0.60	0/734
29	c	0.46	0/1842	0.65	1/2473 (0.0%)
30	d	0.39	0/701	0.64	0/953
31	e	0.42	0/951	0.70	1/1274 (0.1%)
32	f	0.50	0/1071	0.67	1/1434 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.51	0/1019	0.66	0/1372
34	h	0.48	0/1029	0.72	0/1370
35	i	0.38	0/774	0.63	2/1036 (0.2%)
36	j	0.52	0/677	0.70	0/904
37	k	0.42	0/583	0.60	1/787 (0.1%)
38	l	0.49	0/453	0.56	0/606
39	m	0.55	1/399 (0.3%)	0.83	2/531 (0.4%)
40	n	0.51	0/284	0.80	0/372
41	o	0.61	2/708 (0.3%)	0.77	1/944 (0.1%)
42	p	0.49	0/769	0.67	1/1021 (0.1%)
43	1	0.89	2/38135 (0.0%)	1.17	279/59442 (0.5%)
44	2	0.86	1/24785 (0.0%)	1.18	187/38608 (0.5%)
45	3	0.83	0/4162	1.21	34/6469 (0.5%)
46	4	0.84	0/4341	1.17	36/6767 (0.5%)
47	5	0.86	0/2317	1.21	26/3604 (0.7%)
48	6	0.64	0/1650	1.12	12/2568 (0.5%)
49	7	0.88	0/3770	1.23	39/5868 (0.7%)
50	8	0.72	0/2807	1.16	29/4371 (0.7%)
All	All	0.73	9/133249 (0.0%)	1.03	670/196567 (0.3%)

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
2	B	0	1
3	C	0	1
6	F	0	1
15	O	0	1
31	e	0	1
39	m	0	1
All	All	0	6

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	m	115	CYS	CB-SG	7.29	1.94	1.82
44	2	1601	C	C1'-N1	6.34	1.58	1.48
41	o	42	CYS	CB-SG	5.97	1.92	1.82
13	M	121	VAL	CB-CG2	-5.42	1.41	1.52
7	G	141	VAL	CB-CG2	-5.41	1.41	1.52

The worst 5 of 670 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	966	C	N1-C2-O2	12.51	126.41	118.90
44	2	966	C	C2-N1-C1'	12.15	132.17	118.80
43	1	256	U	C2-N1-C1'	11.99	132.09	117.70
47	5	104	G	N7-C8-N9	11.16	118.68	113.10
43	1	778	C	N3-C2-O2	-11.06	114.16	121.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	115[B]	ARG	Mainchain
3	C	313	TYR	Peptide
6	F	102	THR	Peptide
15	O	117	ASP	Peptide
31	e	123	ASP	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/254 (102%)	247 (95%)	13 (5%)	0	100	100
2	B	410/402 (102%)	387 (94%)	23 (6%)	0	100	100
3	C	366/366 (100%)	340 (93%)	25 (7%)	1 (0%)	37	56
4	D	166/168 (99%)	147 (89%)	17 (10%)	2 (1%)	11	21
5	E	184/186 (99%)	171 (93%)	13 (7%)	0	100	100
6	F	133/195 (68%)	120 (90%)	13 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	218/348 (63%)	206 (94%)	11 (5%)	1 (0%)	25	44
8	H	222/221 (100%)	212 (96%)	10 (4%)	0	100	100
9	I	210/212 (99%)	188 (90%)	20 (10%)	2 (1%)	13	25
10	J	132/134 (98%)	119 (90%)	13 (10%)	0	100	100
11	K	148/149 (99%)	133 (90%)	15 (10%)	0	100	100
12	L	142/144 (99%)	127 (89%)	14 (10%)	1 (1%)	19	35
13	M	201/203 (99%)	195 (97%)	6 (3%)	0	100	100
14	N	186/213 (87%)	179 (96%)	7 (4%)	0	100	100
15	O	249/305 (82%)	232 (93%)	17 (7%)	0	100	100
16	P	195/197 (99%)	182 (93%)	13 (7%)	0	100	100
17	Q	187/189 (99%)	180 (96%)	7 (4%)	0	100	100
18	R	176/178 (99%)	153 (87%)	22 (12%)	1 (1%)	22	39
19	S	152/154 (99%)	138 (91%)	14 (9%)	0	100	100
20	T	152/154 (99%)	138 (91%)	14 (9%)	0	100	100
21	U	119/121 (98%)	103 (87%)	15 (13%)	1 (1%)	16	31
22	V	117/118 (99%)	109 (93%)	8 (7%)	0	100	100
23	W	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
24	X	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
25	Y	131/132 (99%)	128 (98%)	3 (2%)	0	100	100
26	Z	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
27	a	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
28	b	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
29	c	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
30	d	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
31	e	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	14	28
32	f	129/130 (99%)	123 (95%)	6 (5%)	0	100	100
33	g	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
34	h	124/125 (99%)	117 (94%)	7 (6%)	0	100	100
35	i	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
36	j	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
37	k	74/76 (97%)	71 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	l	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
39	m	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
40	n	31/33 (94%)	28 (90%)	3 (10%)	0	100	100
41	o	88/90 (98%)	79 (90%)	9 (10%)	0	100	100
42	p	94/96 (98%)	84 (89%)	9 (10%)	1 (1%)	12	23
All	All	6329/6652 (95%)	5911 (93%)	407 (6%)	11 (0%)	45	64

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	43	CYS
9	I	68	VAL
31	e	124	ALA
3	C	314	GLN
4	D	42	LEU

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	A	204/198 (103%)	191 (94%)	13 (6%)	14	30
2	B	333/340 (98%)	325 (98%)	8 (2%)	44	70
3	C	291/297 (98%)	287 (99%)	4 (1%)	62	83
4	D	114/146 (78%)	113 (99%)	1 (1%)	75	90
5	E	160/169 (95%)	160 (100%)	0	100	100
6	F	100/154 (65%)	99 (99%)	1 (1%)	73	88
7	G	178/292 (61%)	173 (97%)	5 (3%)	38	65
8	H	184/187 (98%)	179 (97%)	5 (3%)	40	67
9	I	167/175 (95%)	164 (98%)	3 (2%)	54	78
10	J	105/107 (98%)	103 (98%)	2 (2%)	52	77
11	K	116/125 (93%)	114 (98%)	2 (2%)	56	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	114/114 (100%)	113 (99%)	1 (1%)	75	90
13	M	179/179 (100%)	178 (99%)	1 (1%)	84	94
14	N	138/179 (77%)	135 (98%)	3 (2%)	47	73
15	O	193/242 (80%)	193 (100%)	0	100	100
16	P	163/163 (100%)	159 (98%)	4 (2%)	42	69
17	Q	130/166 (78%)	129 (99%)	1 (1%)	79	91
18	R	156/157 (99%)	155 (99%)	1 (1%)	84	94
19	S	123/128 (96%)	119 (97%)	4 (3%)	33	59
20	T	130/133 (98%)	127 (98%)	3 (2%)	45	72
21	U	91/106 (86%)	90 (99%)	1 (1%)	70	87
22	V	97/102 (95%)	97 (100%)	0	100	100
23	W	105/105 (100%)	103 (98%)	2 (2%)	52	77
24	X	58/60 (97%)	57 (98%)	1 (2%)	56	79
25	Y	104/113 (92%)	104 (100%)	0	100	100
26	Z	108/113 (96%)	103 (95%)	5 (5%)	23	45
27	a	98/115 (85%)	98 (100%)	0	100	100
28	b	54/56 (96%)	52 (96%)	2 (4%)	29	55
29	c	180/189 (95%)	176 (98%)	4 (2%)	47	73
30	d	77/81 (95%)	74 (96%)	3 (4%)	27	52
31	e	101/104 (97%)	98 (97%)	3 (3%)	36	63
32	f	108/111 (97%)	105 (97%)	3 (3%)	38	65
33	g	101/103 (98%)	101 (100%)	0	100	100
34	h	104/108 (96%)	102 (98%)	2 (2%)	52	77
35	i	77/81 (95%)	77 (100%)	0	100	100
36	j	67/68 (98%)	66 (98%)	1 (2%)	60	82
37	k	60/69 (87%)	59 (98%)	1 (2%)	56	79
38	l	44/46 (96%)	44 (100%)	0	100	100
39	m	41/44 (93%)	39 (95%)	2 (5%)	21	42
40	n	28/31 (90%)	28 (100%)	0	100	100
41	o	70/72 (97%)	69 (99%)	1 (1%)	62	83
42	p	77/83 (93%)	76 (99%)	1 (1%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5128/5611 (91%)	5034 (98%)	94 (2%)	58 78

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	S	134	MET
28	b	9	ASN
20	T	37	ASN
24	X	22	VAL
29	c	185	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
19	S	142	ASN
28	b	17	HIS
20	T	97	ASN
24	X	14	HIS
29	c	109	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
43	1	1603/1778 (90%)	438 (27%)	18 (1%)
44	2	1067/1526 (69%)	287 (26%)	17 (1%)
45	3	172/211 (81%)	45 (26%)	3 (1%)
46	4	182/183 (99%)	47 (25%)	2 (1%)
47	5	93/133 (69%)	30 (32%)	0
48	6	70/71 (98%)	34 (48%)	4 (5%)
49	7	161/171 (94%)	39 (24%)	2 (1%)
50	8	117/118 (99%)	25 (21%)	1 (0%)
All	All	3465/4191 (82%)	945 (27%)	47 (1%)

5 of 945 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
43	1	4	G
43	1	16	G
43	1	20	G
43	1	24	A

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Mol	Chain	Res	Type
43	1	29	C

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	2	648	A
45	3	2	A
44	2	755	U
44	2	1437	A
45	3	188	C

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

68 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	$\# Z > 2$
43	OMU	1	1253	43	19,22,23	0.62	0	25,31,34	0.80	1 (4%)
43	A2M	1	955	43	18,25,26	1.64	3 (16%)	20,36,39	1.23	2 (10%)
43	OMU	1	48	43	19,22,23	0.69	0	25,31,34	1.05	2 (8%)
43	A2M	1	1541	43,44	18,25,26	1.62	3 (16%)	20,36,39	1.06	2 (10%)
44	OMG	2	534	44	19,26,27	1.29	2 (10%)	21,38,41	1.47	5 (23%)
44	OMG	2	1047	44	19,26,27	1.27	2 (10%)	21,38,41	1.39	2 (9%)
43	OMG	1	959	43	19,26,27	1.28	2 (10%)	21,38,41	1.34	4 (19%)
44	OMC	2	359	44	19,22,23	1.05	1 (5%)	25,31,34	1.11	3 (12%)
44	A2M	2	604	43,44	18,25,26	1.47	3 (16%)	20,36,39	0.95	0
44	OMG	2	655	44	19,26,27	1.38	2 (10%)	21,38,41	1.46	3 (14%)
44	OMC	2	1160	44	19,22,23	0.94	1 (5%)	25,31,34	1.15	3 (12%)
43	OMU	1	847	43	19,22,23	0.49	0	25,31,34	1.06	2 (8%)
44	OMC	2	1318	44	19,22,23	0.99	2 (10%)	25,31,34	1.28	3 (12%)
44	A2M	2	1385	44	18,25,26	1.47	2 (11%)	20,36,39	1.27	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	OMG	7	75	49	19,26,27	1.22	2 (10%)	21,38,41	1.50	5 (23%)
49	A2M	7	162	49,43	18,25,26	1.63	3 (16%)	20,36,39	1.24	2 (10%)
44	OMG	2	1079	44	19,26,27	1.25	2 (10%)	21,38,41	1.58	5 (23%)
49	A2M	7	43	49	18,25,26	1.43	2 (11%)	20,36,39	1.14	1 (5%)
45	OMU	3	10	45	19,22,23	0.65	0	25,31,34	1.04	2 (8%)
44	OMU	2	560	44	19,22,23	0.59	0	25,31,34	1.07	2 (8%)
44	A2M	2	665	44	18,25,26	1.74	3 (16%)	20,36,39	1.14	1 (5%)
43	A2M	1	678	43,44	18,25,26	1.49	2 (11%)	20,36,39	1.01	1 (5%)
43	OMC	1	695	43	19,22,23	0.81	0	25,31,34	0.99	1 (4%)
44	OMC	2	1249	44	19,22,23	1.04	1 (5%)	25,31,34	1.18	2 (8%)
44	A2M	2	1068	44	18,25,26	1.41	3 (16%)	20,36,39	1.07	1 (5%)
43	OMU	1	1661	43	19,22,23	0.62	0	25,31,34	0.88	1 (4%)
43	OMG	1	1526	43	19,26,27	1.38	2 (10%)	21,38,41	1.46	6 (28%)
44	A2M	2	382	44	18,25,26	0.83	0	20,36,39	1.19	2 (10%)
44	A2M	2	628	44	18,25,26	1.52	1 (5%)	20,36,39	0.95	1 (5%)
44	A2M	2	1186	44	18,25,26	1.64	4 (22%)	20,36,39	1.44	2 (10%)
44	A2M	2	572	44	18,25,26	1.41	1 (5%)	20,36,39	1.14	2 (10%)
44	A2M	2	527	44	18,25,26	1.73	4 (22%)	20,36,39	2.21	6 (30%)
44	A2M	2	570	43,44	18,25,26	1.33	1 (5%)	20,36,39	1.41	3 (15%)
44	OMG	2	1230	44	19,26,27	1.43	2 (10%)	21,38,41	1.17	2 (9%)
44	OMC	2	1398	44	19,22,23	0.92	1 (5%)	25,31,34	1.07	2 (8%)
44	OMG	2	1254	44	19,26,27	1.20	2 (10%)	21,38,41	1.57	5 (23%)
43	OMG	1	856	43	19,26,27	1.24	2 (10%)	21,38,41	1.59	2 (9%)
44	OMG	2	1232	44	19,26,27	1.26	2 (10%)	21,38,41	1.34	3 (14%)
43	OMU	1	845	43	19,22,23	0.55	0	25,31,34	0.96	2 (8%)
43	OMG	1	1628	43	19,26,27	1.25	2 (10%)	21,38,41	1.54	5 (23%)
44	OMU	2	73	44	19,22,23	0.63	0	25,31,34	0.86	0
43	A2M	1	927	43	18,25,26	1.59	2 (11%)	20,36,39	1.20	2 (10%)
44	OMU	2	667	44	19,22,23	0.60	0	25,31,34	1.22	2 (8%)
43	OMU	1	1107	43	19,22,23	0.66	0	25,31,34	1.01	2 (8%)
43	OMC	1	1529	43	19,22,23	1.02	2 (10%)	25,31,34	1.14	2 (8%)
43	OMG	1	1190	43	19,26,27	1.43	3 (15%)	21,38,41	1.55	2 (9%)
43	A2M	1	697	43	18,25,26	1.55	3 (16%)	20,36,39	1.27	3 (15%)
44	OMC	2	443	44	19,22,23	0.83	0	25,31,34	1.26	4 (16%)
43	OMG	1	1542	43,44	19,26,27	1.24	2 (10%)	21,38,41	1.47	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	A2M	1	69	43	18,25,26	1.46	3 (16%)	20,36,39	1.31	2 (10%)
44	A2M	2	1373	44	18,25,26	1.73	3 (16%)	20,36,39	1.17	2 (10%)
43	A2M	1	858	43	18,25,26	1.66	2 (11%)	20,36,39	2.07	3 (15%)
44	OMG	2	71	44	19,26,27	1.36	3 (15%)	21,38,41	1.43	4 (19%)
49	OMU	7	7	49,43	19,22,23	0.49	0	25,31,34	1.03	2 (8%)
43	A2M	1	437	43	18,25,26	1.35	2 (11%)	20,36,39	0.84	0
44	OMU	2	1078	44	19,22,23	0.62	1 (5%)	25,31,34	1.09	2 (8%)
44	OMG	2	641	44	19,26,27	1.42	2 (10%)	21,38,41	1.49	5 (23%)
44	A2M	2	591	44	18,25,26	1.59	2 (11%)	20,36,39	0.99	0
44	OMG	2	1361	44	19,26,27	1.33	2 (10%)	21,38,41	1.46	4 (19%)
46	OMG	4	74	46	19,26,27	1.23	2 (10%)	21,38,41	1.48	4 (19%)
44	OMC	2	583	44	19,22,23	0.98	1 (5%)	25,31,34	1.07	2 (8%)
44	OMU	2	1420	44	19,22,23	0.52	0	25,31,34	0.89	2 (8%)
43	A2M	1	681	43	18,25,26	1.53	3 (16%)	20,36,39	1.11	3 (15%)
44	A2M	2	502	44	18,25,26	0.80	0	20,36,39	1.44	3 (15%)
43	OMU	1	1371	43	19,22,23	1.18	1 (5%)	25,31,34	1.74	6 (24%)
44	OMU	2	1360	44	19,22,23	0.48	0	25,31,34	1.02	2 (8%)
43	A2M	1	235	43	18,25,26	1.52	2 (11%)	20,36,39	1.26	2 (10%)
44	OMU	2	1153	44	19,22,23	0.55	0	25,31,34	0.87	2 (8%)

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
43	OMU	1	1253	43	-	2/9/27/28	0/2/2/2
43	A2M	1	955	43	-	0/5/27/28	0/3/3/3
43	OMU	1	48	43	-	2/9/27/28	0/2/2/2
43	A2M	1	1541	43,44	-	0/5/27/28	0/3/3/3
44	OMG	2	534	44	-	2/5/27/28	0/3/3/3
44	OMG	2	1047	44	-	2/5/27/28	0/3/3/3
43	OMG	1	959	43	-	2/5/27/28	0/3/3/3
44	OMC	2	359	44	-	0/9/27/28	0/2/2/2
44	A2M	2	604	43,44	-	0/5/27/28	0/3/3/3
44	OMG	2	655	44	-	0/5/27/28	0/3/3/3
44	OMC	2	1160	44	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	OMU	1	847	43	-	0/9/27/28	0/2/2/2
44	OMC	2	1318	44	-	0/9/27/28	0/2/2/2
44	A2M	2	1385	44	-	2/5/27/28	0/3/3/3
49	OMG	7	75	49	-	2/5/27/28	0/3/3/3
49	A2M	7	162	49,43	-	0/5/27/28	0/3/3/3
44	OMG	2	1079	44	-	2/5/27/28	0/3/3/3
49	A2M	7	43	49	-	0/5/27/28	0/3/3/3
45	OMU	3	10	45	-	1/9/27/28	0/2/2/2
44	OMU	2	560	44	-	1/9/27/28	0/2/2/2
44	A2M	2	665	44	-	2/5/27/28	0/3/3/3
43	A2M	1	678	43,44	-	1/5/27/28	0/3/3/3
43	OMC	1	695	43	-	0/9/27/28	0/2/2/2
44	OMC	2	1249	44	-	1/9/27/28	0/2/2/2
44	A2M	2	1068	44	-	0/5/27/28	0/3/3/3
43	OMU	1	1661	43	-	0/9/27/28	0/2/2/2
43	OMG	1	1526	43	-	0/5/27/28	0/3/3/3
44	A2M	2	382	44	-	1/5/27/28	0/3/3/3
44	A2M	2	628	44	-	0/5/27/28	0/3/3/3
44	A2M	2	1186	44	-	0/5/27/28	0/3/3/3
44	A2M	2	572	44	-	0/5/27/28	0/3/3/3
44	A2M	2	527	44	-	0/5/27/28	0/3/3/3
44	A2M	2	570	43,44	-	1/5/27/28	0/3/3/3
44	OMG	2	1230	44	-	2/5/27/28	0/3/3/3
44	OMC	2	1398	44	-	0/9/27/28	0/2/2/2
44	OMG	2	1254	44	-	0/5/27/28	0/3/3/3
43	OMG	1	856	43	-	0/5/27/28	0/3/3/3
44	OMG	2	1232	44	-	0/5/27/28	0/3/3/3
43	OMU	1	845	43	-	0/9/27/28	0/2/2/2
43	OMG	1	1628	43	-	0/5/27/28	0/3/3/3
44	OMU	2	73	44	-	0/9/27/28	0/2/2/2
43	A2M	1	927	43	-	0/5/27/28	0/3/3/3
44	OMU	2	667	44	-	2/9/27/28	0/2/2/2
43	OMU	1	1107	43	-	0/9/27/28	0/2/2/2
43	OMC	1	1529	43	-	1/9/27/28	0/2/2/2
43	OMG	1	1190	43	-	0/5/27/28	0/3/3/3
43	A2M	1	697	43	-	0/5/27/28	0/3/3/3
44	OMC	2	443	44	-	5/9/27/28	0/2/2/2
43	OMG	1	1542	43,44	-	2/5/27/28	0/3/3/3
43	A2M	1	69	43	-	0/5/27/28	0/3/3/3
44	A2M	2	1373	44	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A2M	1	858	43	-	1/5/27/28	0/3/3/3
44	OMG	2	71	44	-	0/5/27/28	0/3/3/3
49	OMU	7	7	49,43	-	2/9/27/28	0/2/2/2
43	A2M	1	437	43	-	0/5/27/28	0/3/3/3
44	OMU	2	1078	44	-	0/9/27/28	0/2/2/2
44	OMG	2	641	44	-	2/5/27/28	0/3/3/3
44	A2M	2	591	44	-	0/5/27/28	0/3/3/3
44	OMG	2	1361	44	-	0/5/27/28	0/3/3/3
46	OMG	4	74	46	-	0/5/27/28	0/3/3/3
44	OMC	2	583	44	-	0/9/27/28	0/2/2/2
44	OMU	2	1420	44	-	0/9/27/28	0/2/2/2
43	A2M	1	681	43	-	3/5/27/28	0/3/3/3
44	A2M	2	502	44	-	2/5/27/28	0/3/3/3
43	OMU	1	1371	43	-	5/9/27/28	0/2/2/2
44	OMU	2	1360	44	-	0/9/27/28	0/2/2/2
43	A2M	1	235	43	-	1/5/27/28	0/3/3/3
44	OMU	2	1153	44	-	0/9/27/28	0/2/2/2

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1	1371	OMU	C2-N1	4.72	1.45	1.38
44	2	665	A2M	O5'-C5'	-4.47	1.31	1.44
44	2	1186	A2M	O5'-C5'	-4.45	1.31	1.44
43	1	681	A2M	O5'-C5'	-4.39	1.31	1.44
43	1	927	A2M	O5'-C5'	-4.38	1.31	1.44

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1	858	A2M	C4'-O4'-C1'	-7.85	102.73	109.92
44	2	527	A2M	C4'-O4'-C1'	-7.39	103.16	109.92
44	2	1186	A2M	C4'-O4'-C1'	-4.66	105.66	109.92
43	1	856	OMG	O6-C6-N1	-4.36	115.44	120.62
43	1	1371	OMU	O2-C2-N1	4.11	128.14	122.80

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1	48	OMU	O4'-C4'-C5'-O5'
43	1	681	A2M	O4'-C4'-C5'-O5'
43	1	959	OMG	O4'-C4'-C5'-O5'
43	1	959	OMG	C3'-C4'-C5'-O5'
43	1	1253	OMU	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 44 ligands modelled in this entry, 34 are monoatomic - leaving 10 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$
51	PAR	2	1705	-	44,45,45	3.59	8 (18%)	63,67,67	1.65	15 (23%)
51	PAR	1	1802	-	44,45,45	3.58	8 (18%)	63,67,67	1.21	7 (11%)
51	PAR	1	1805	-	44,45,45	3.53	8 (18%)	63,67,67	1.60	12 (19%)
51	PAR	2	1703	-	44,45,45	3.63	10 (22%)	63,67,67	1.96	17 (26%)
51	PAR	1	1803	43	44,45,45	3.60	8 (18%)	63,67,67	1.38	7 (11%)
51	PAR	7	201	-	44,45,45	3.58	9 (20%)	63,67,67	1.79	16 (25%)
51	PAR	1	1804	-	44,45,45	3.69	9 (20%)	63,67,67	1.59	12 (19%)
51	PAR	2	1704	-	44,45,45	3.63	8 (18%)	63,67,67	1.28	9 (14%)
51	PAR	2	1702	-	44,45,45	3.60	8 (18%)	63,67,67	1.45	7 (11%)
51	PAR	1	1801	-	44,45,45	3.61	8 (18%)	63,67,67	1.38	9 (14%)

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
51	PAR	2	1705	-	-	11/18/94/94	0/4/4/4
51	PAR	1	1802	-	-	6/18/94/94	0/4/4/4
51	PAR	1	1805	-	-	7/18/94/94	0/4/4/4
51	PAR	2	1703	-	-	9/18/94/94	0/4/4/4
51	PAR	1	1803	43	-	7/18/94/94	0/4/4/4
51	PAR	7	201	-	-	8/18/94/94	0/4/4/4
51	PAR	1	1804	-	-	7/18/94/94	0/4/4/4
51	PAR	2	1704	-	-	6/18/94/94	0/4/4/4
51	PAR	2	1702	-	-	4/18/94/94	0/4/4/4
51	PAR	1	1801	-	-	8/18/94/94	0/4/4/4

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	1	1804	PAR	C13-C23	-16.96	1.31	1.52
51	2	1704	PAR	C13-C23	-16.68	1.31	1.52
51	1	1803	PAR	C13-C23	-16.65	1.31	1.52
51	1	1802	PAR	C13-C23	-16.49	1.31	1.52
51	1	1801	PAR	C13-C23	-16.46	1.32	1.52

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	2	1703	PAR	O52-C13-O43	-5.86	105.38	111.37
51	1	1805	PAR	C41-C31-C21	5.26	119.72	110.99
51	7	201	PAR	C44-C34-C24	4.89	119.11	110.99
51	2	1703	PAR	C22-C12-C62	4.83	117.30	110.08
51	7	201	PAR	O52-C13-O43	4.70	116.17	111.37

There are no chirality outliers.

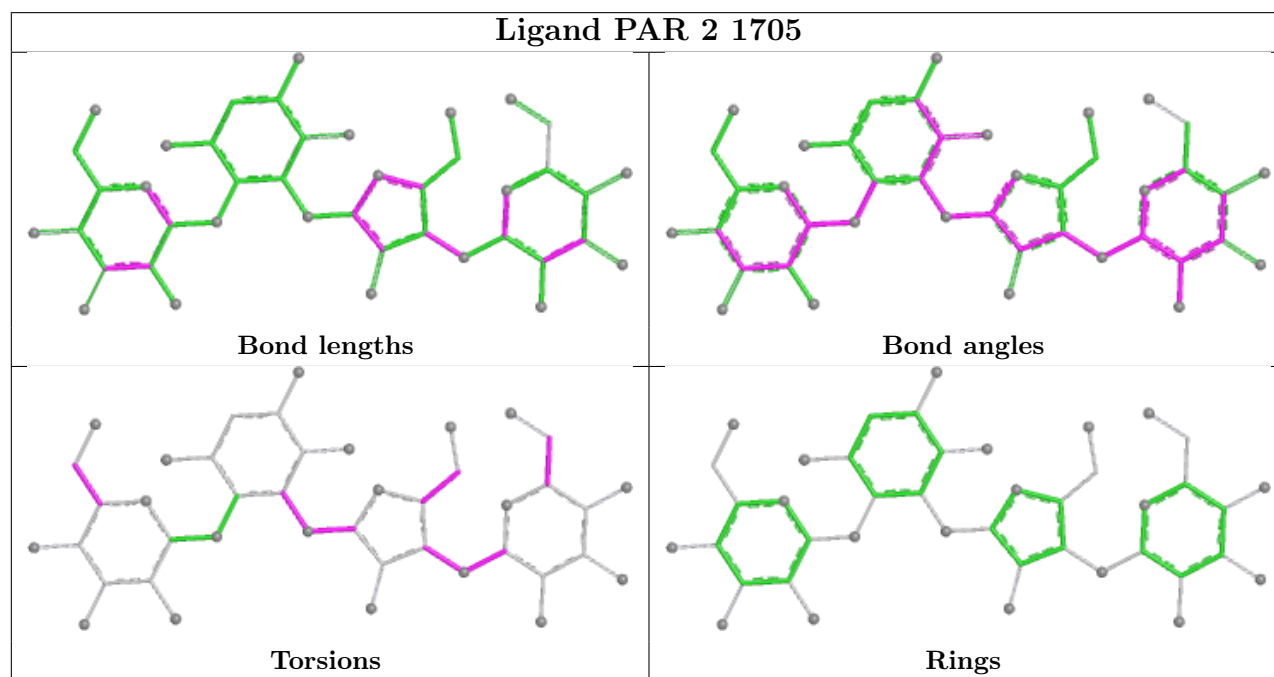
5 of 73 torsion outliers are listed below:

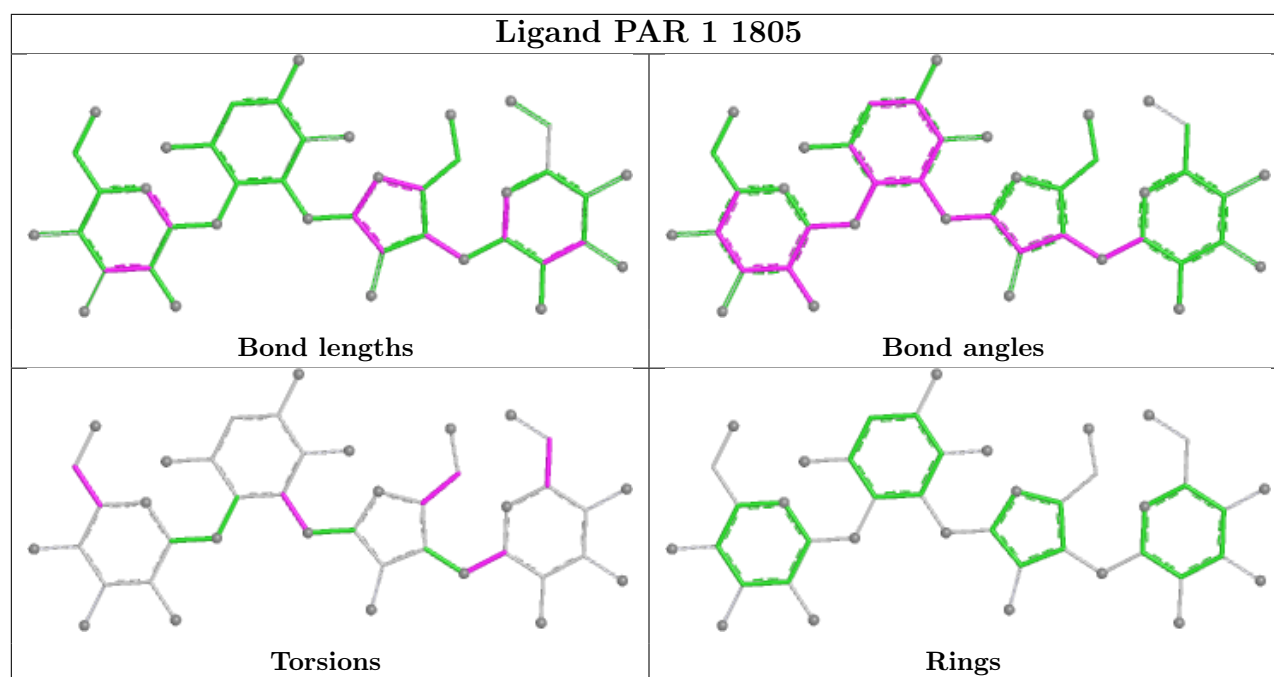
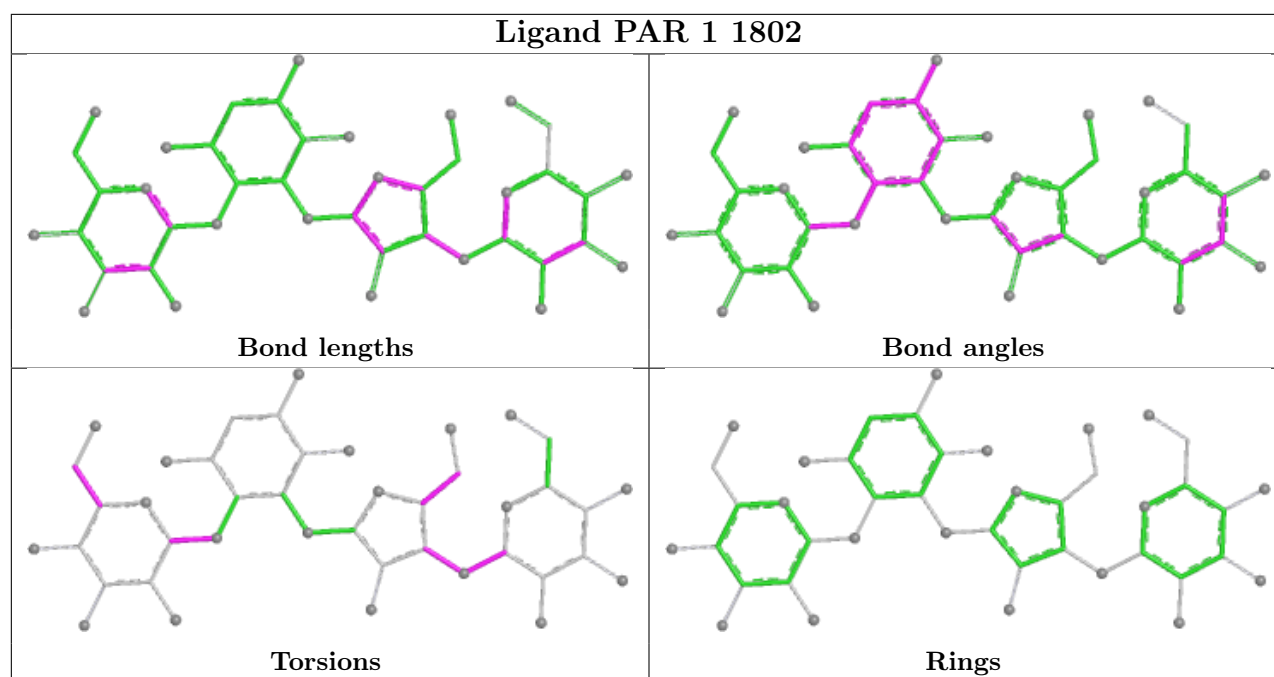
Mol	Chain	Res	Type	Atoms
51	1	1801	PAR	C23-C13-O52-C52
51	1	1802	PAR	C33-C43-C53-O53
51	1	1803	PAR	O54-C54-C64-N64
51	1	1804	PAR	C23-C13-O52-C52
51	1	1805	PAR	C44-C54-C64-N64

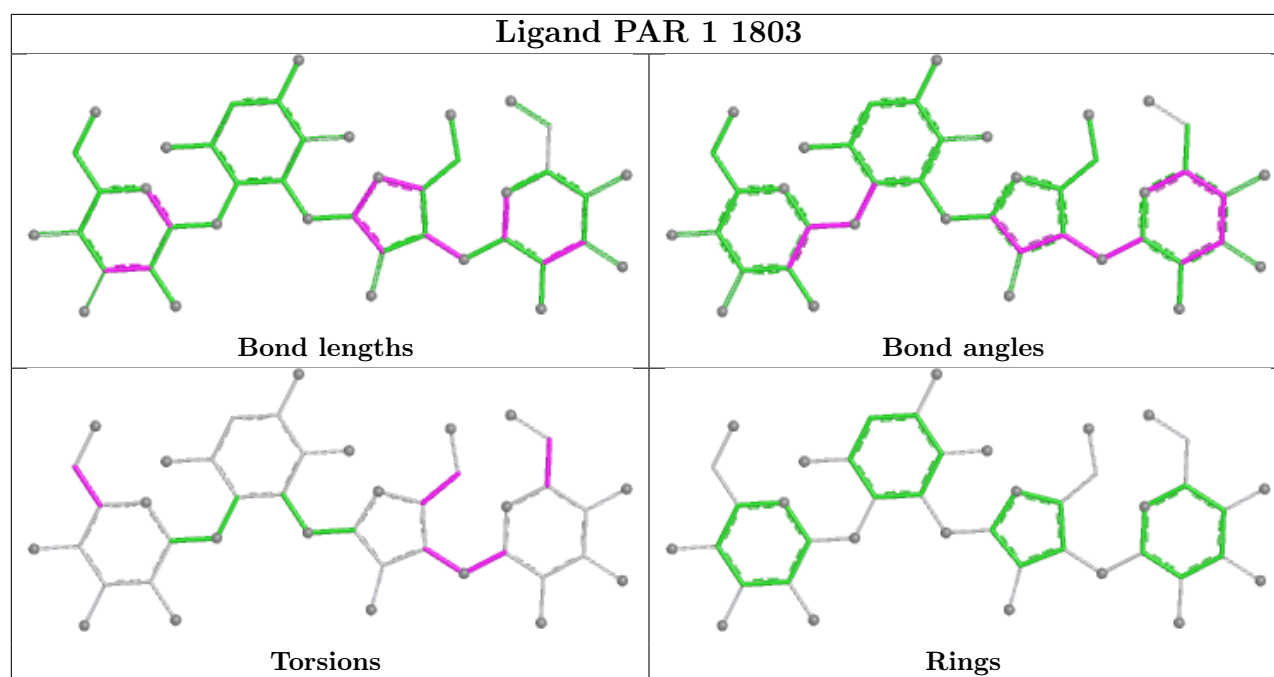
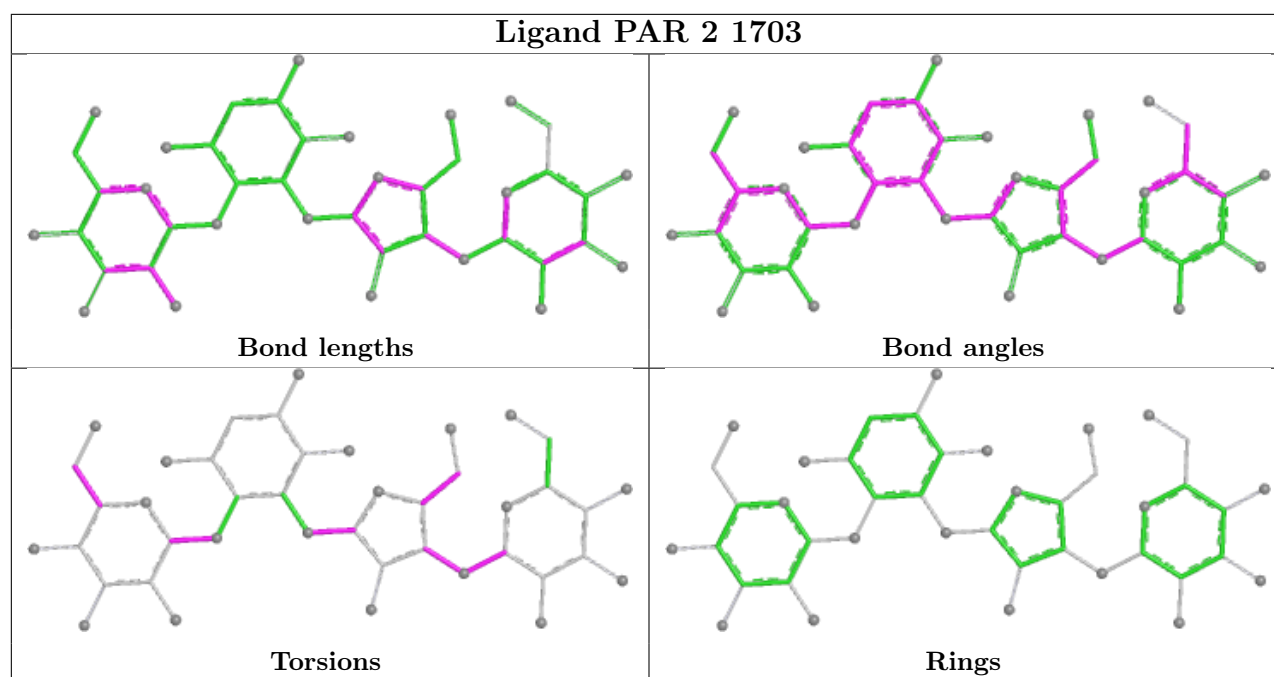
There are no ring outliers.

No monomer is involved in short contacts.

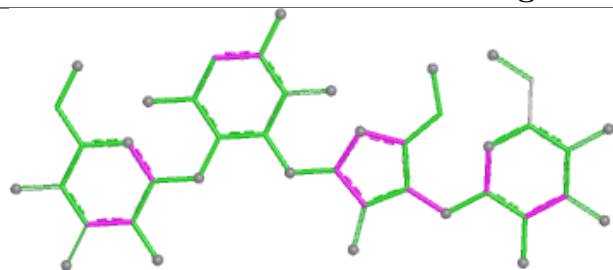
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



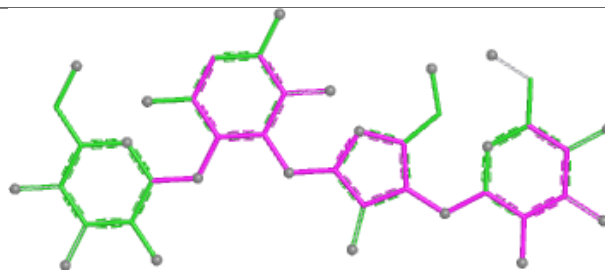




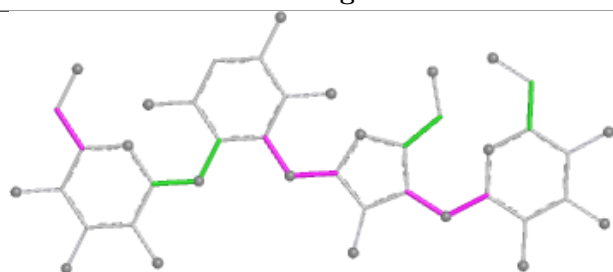
Ligand PAR 7 201



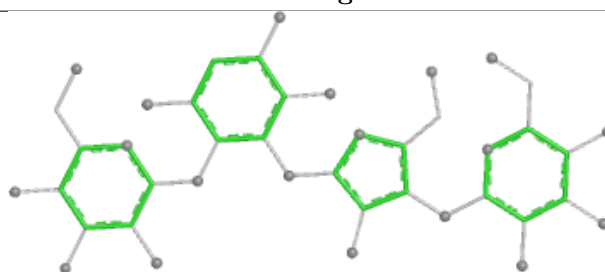
Bond lengths



Bond angles

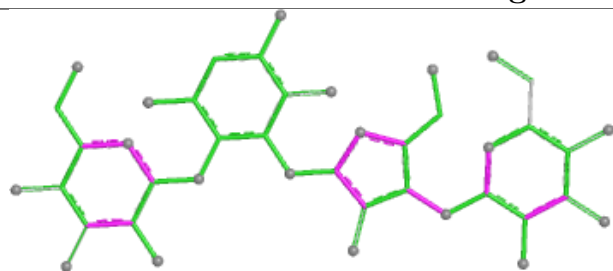


Torsions

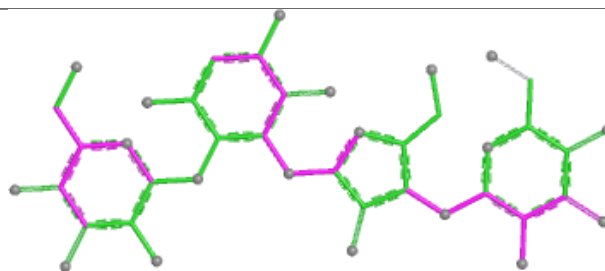


Rings

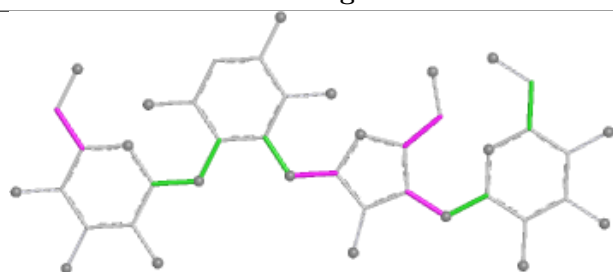
Ligand PAR 1 1804



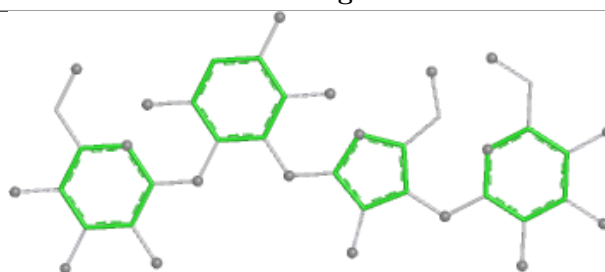
Bond lengths



Bond angles

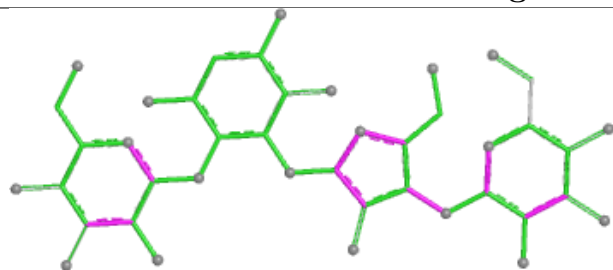


Torsions

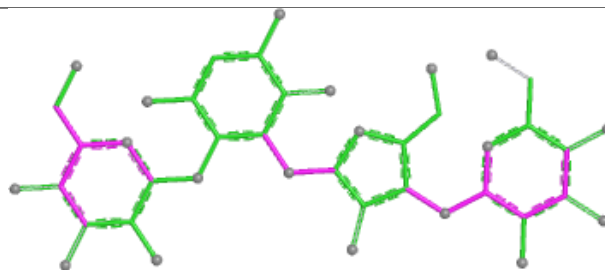


Rings

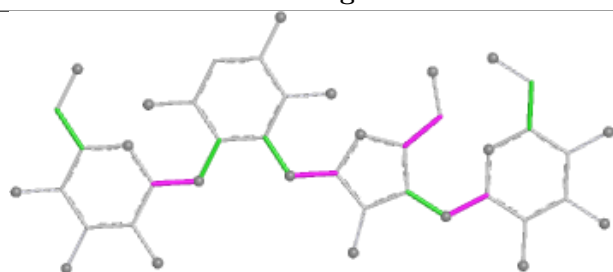
Ligand PAR 2 1704



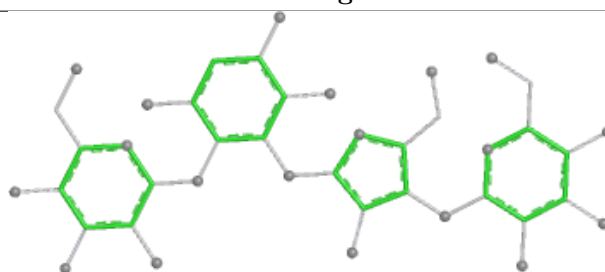
Bond lengths



Bond angles

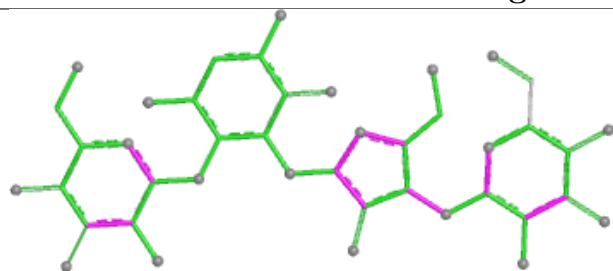


Torsions

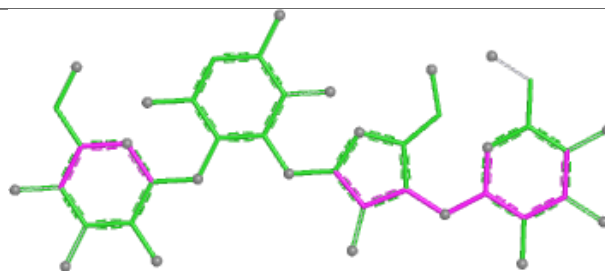


Rings

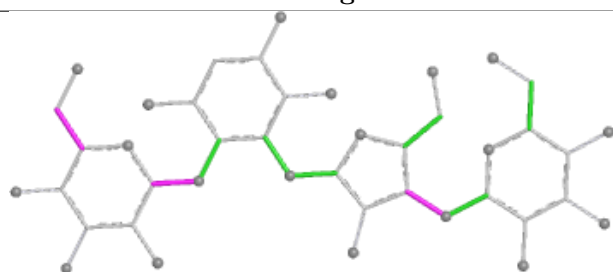
Ligand PAR 2 1702



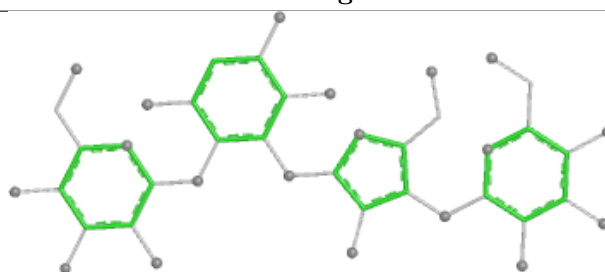
Bond lengths



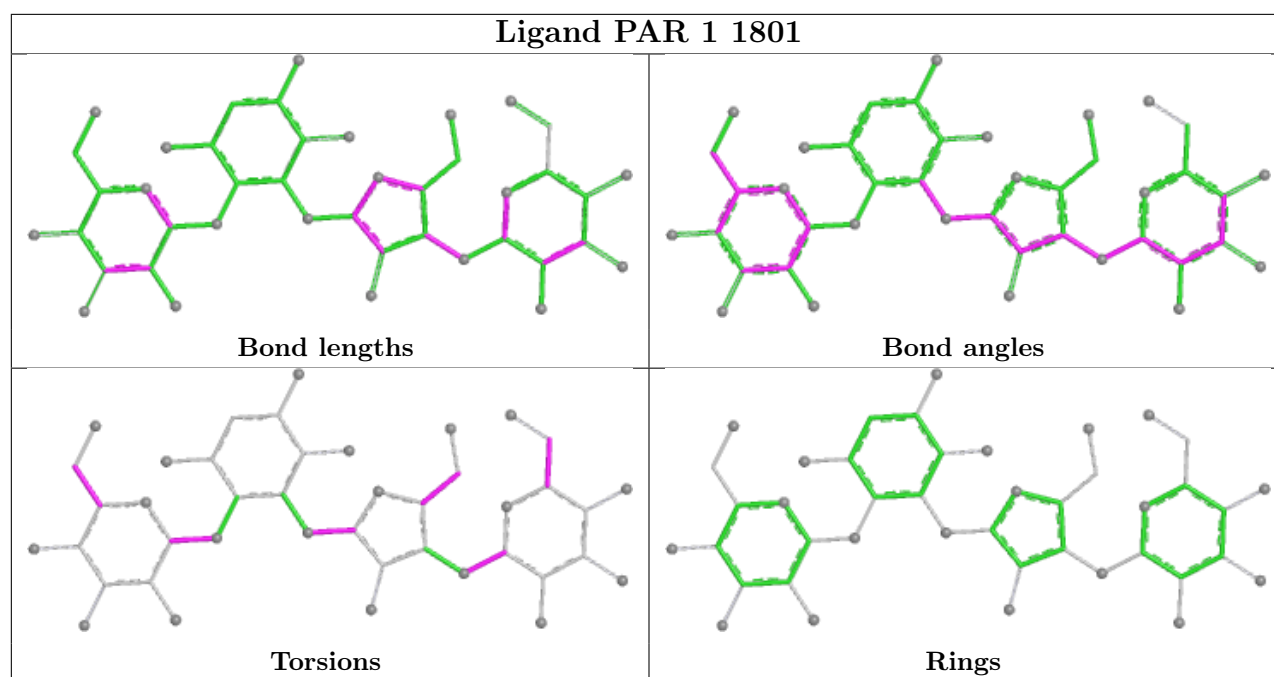
Bond angles



Torsions



Rings



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.

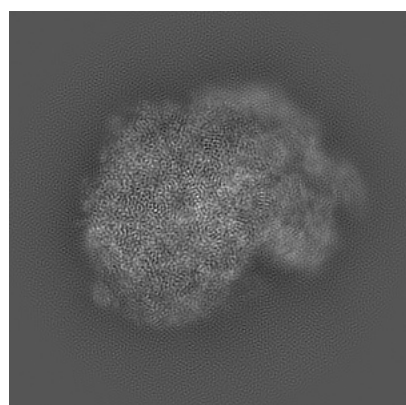
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7025. These allow visual inspection of the internal detail of the map and identification of artifacts.

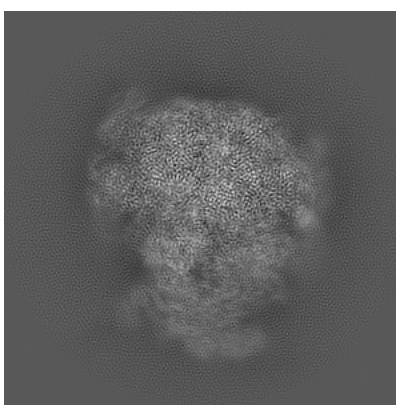
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

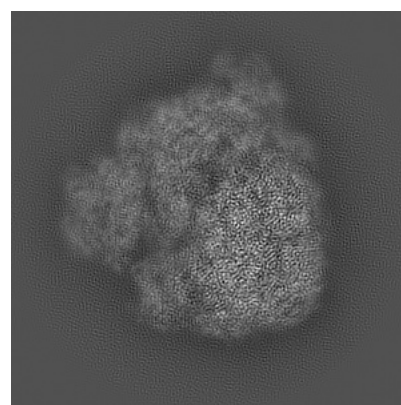
6.1.1 Primary map



X



Y

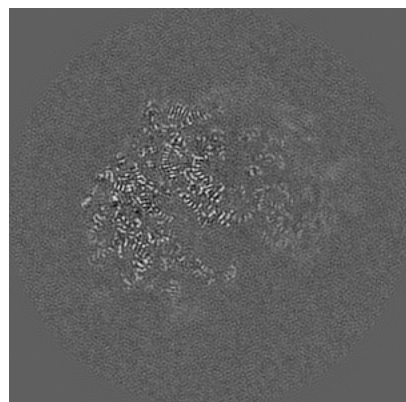


Z

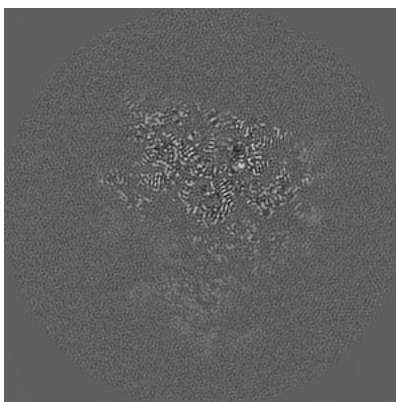
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

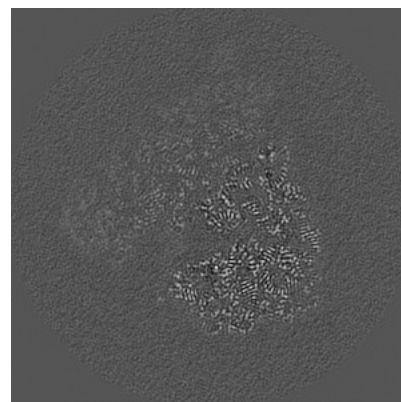
6.2.1 Primary map



X Index: 192



Y Index: 192

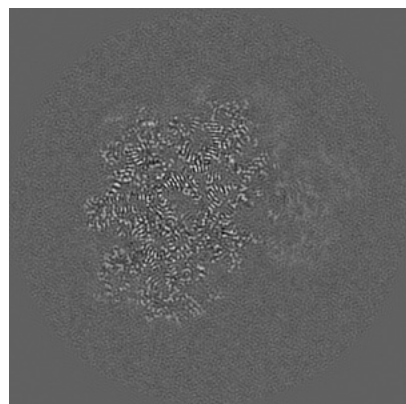


Z Index: 192

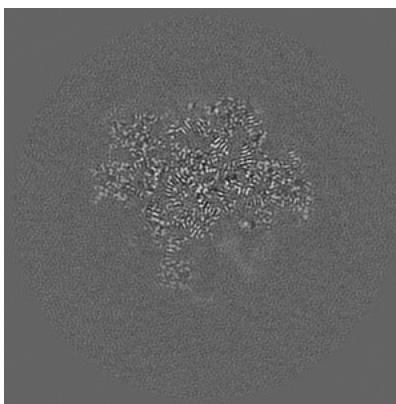
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

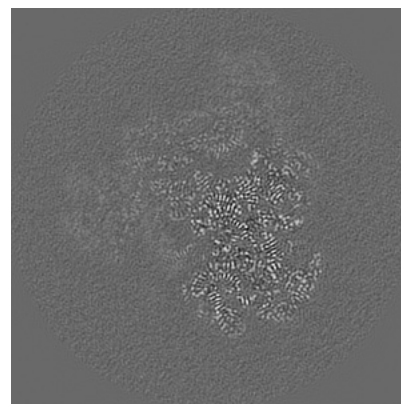
6.3.1 Primary map



X Index: 228



Y Index: 133

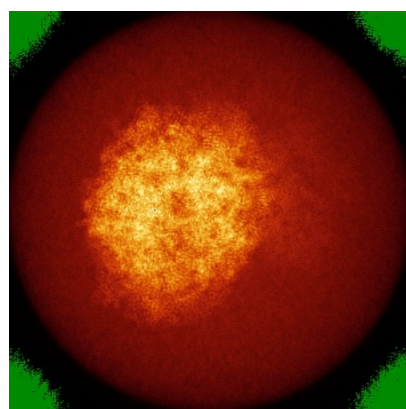


Z Index: 211

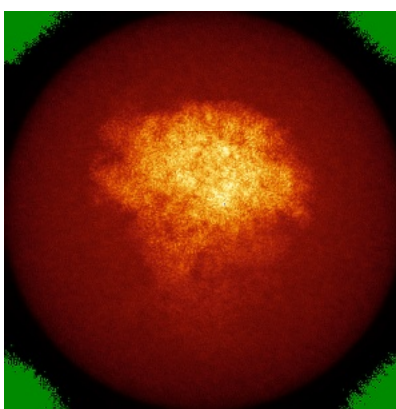
The images above show the largest variance slices of the map in three orthogonal directions.

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

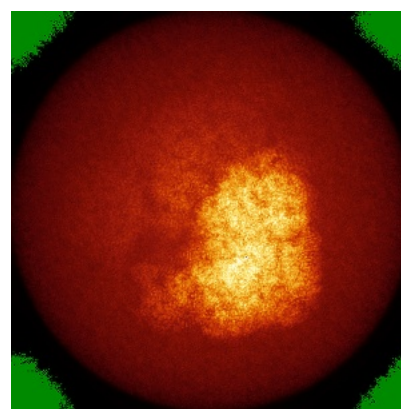
6.4.1 Primary map



X



Y

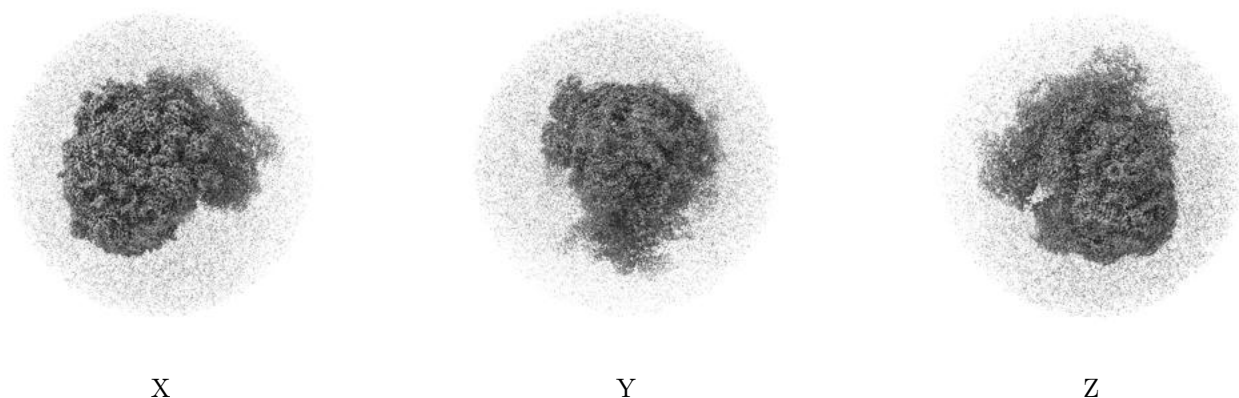


Z

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 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

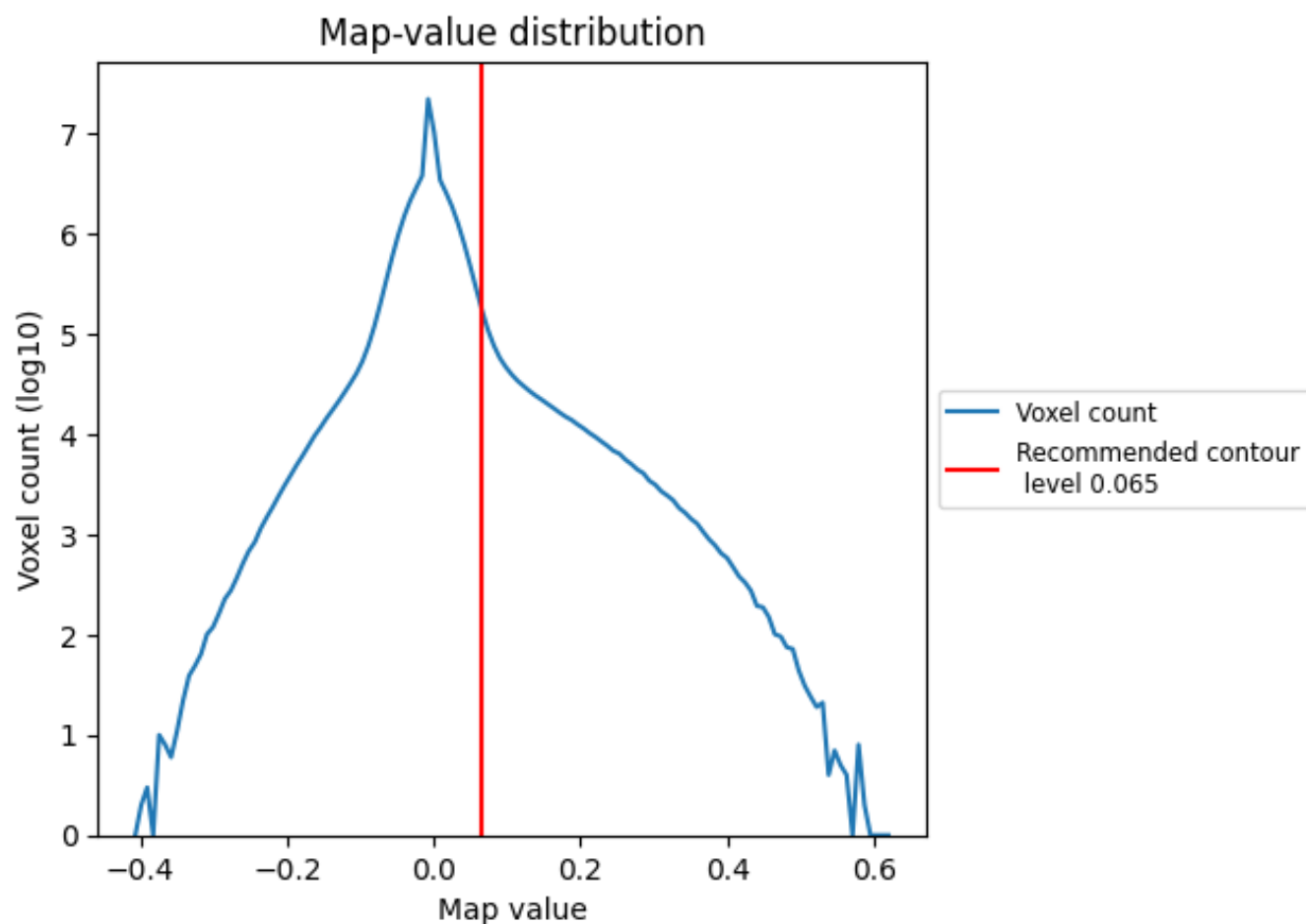
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

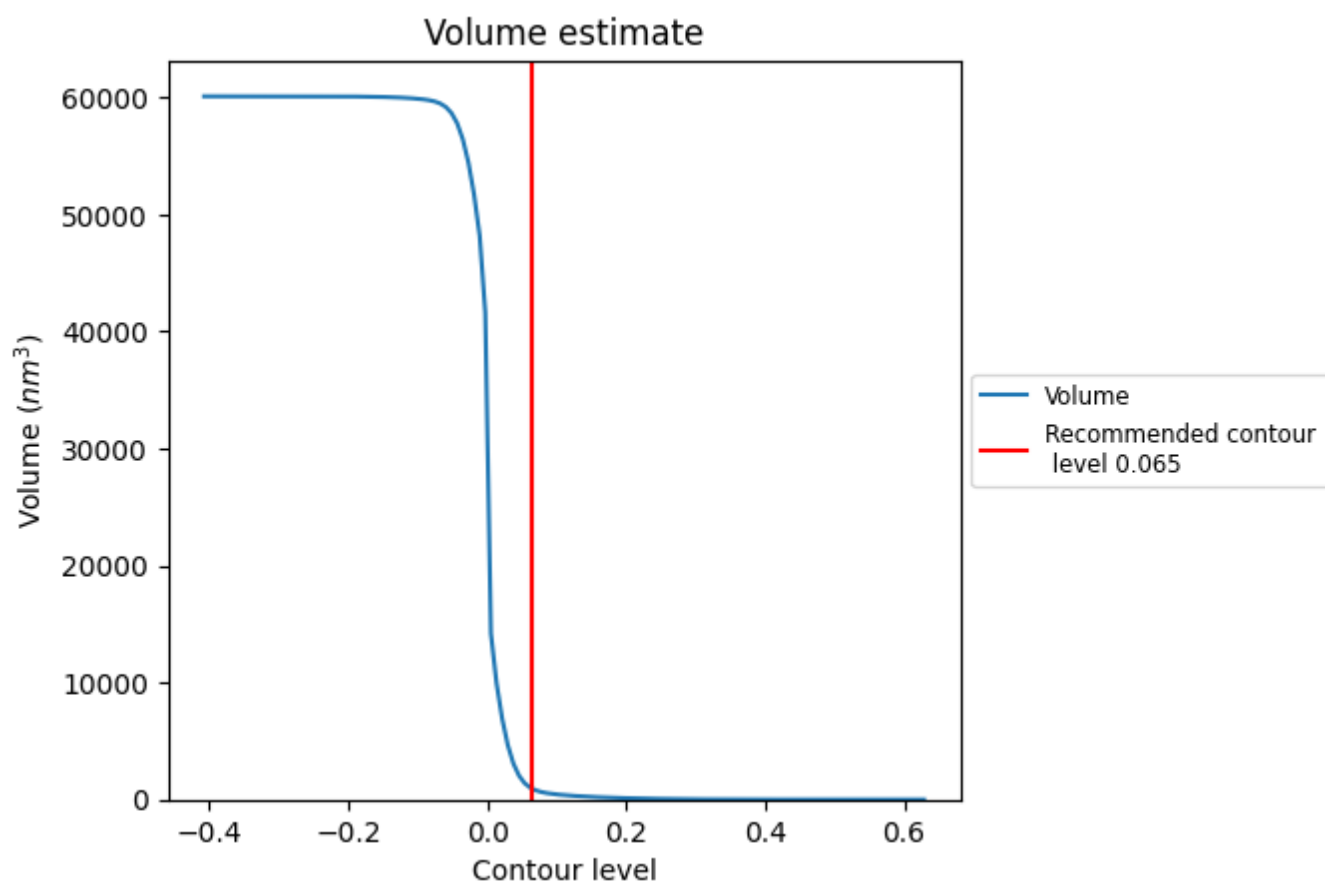
This section contains the results of statistical analysis of the map.

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.

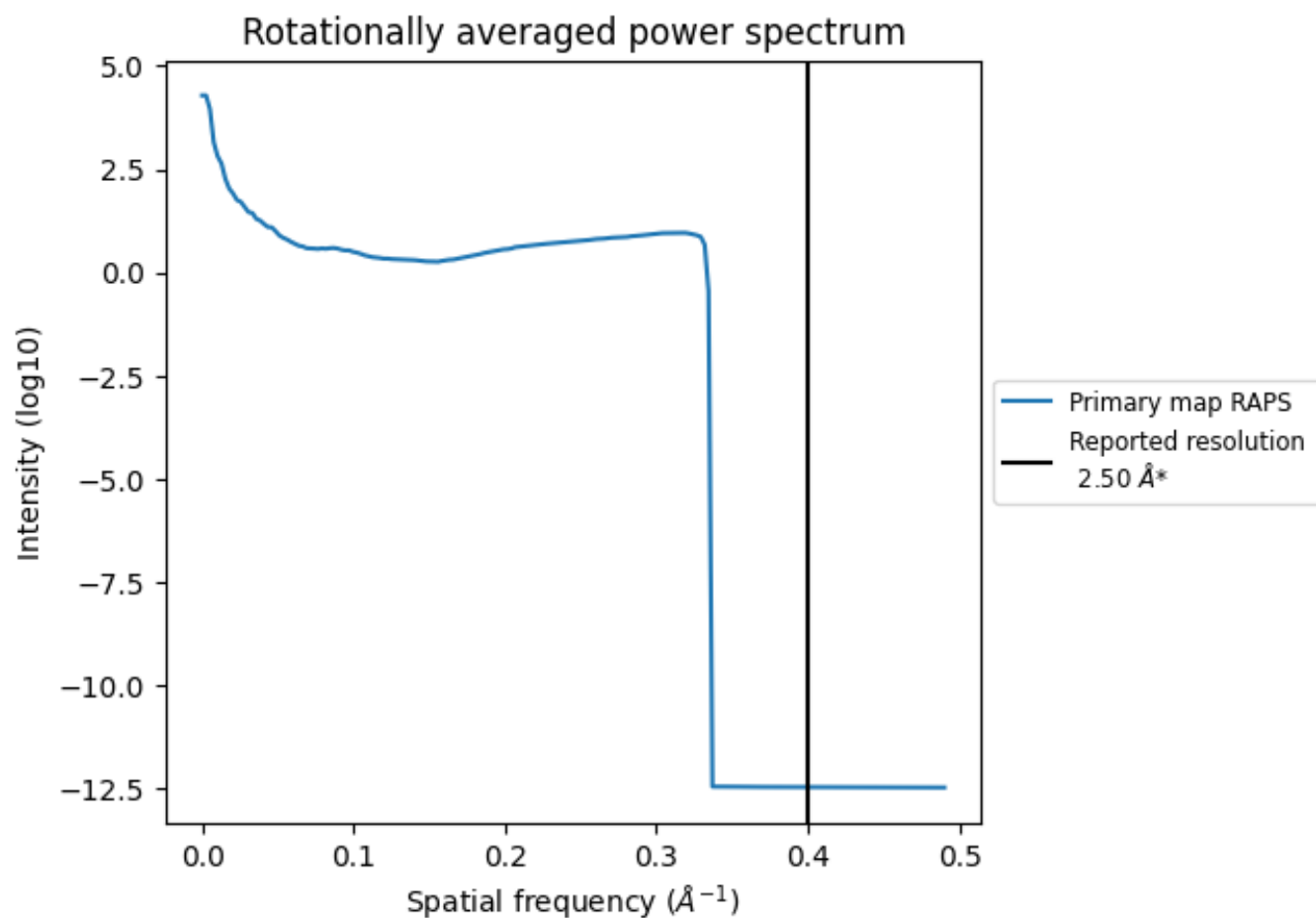
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 933 nm³; this corresponds to an approximate mass of 843 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 Å⁻¹

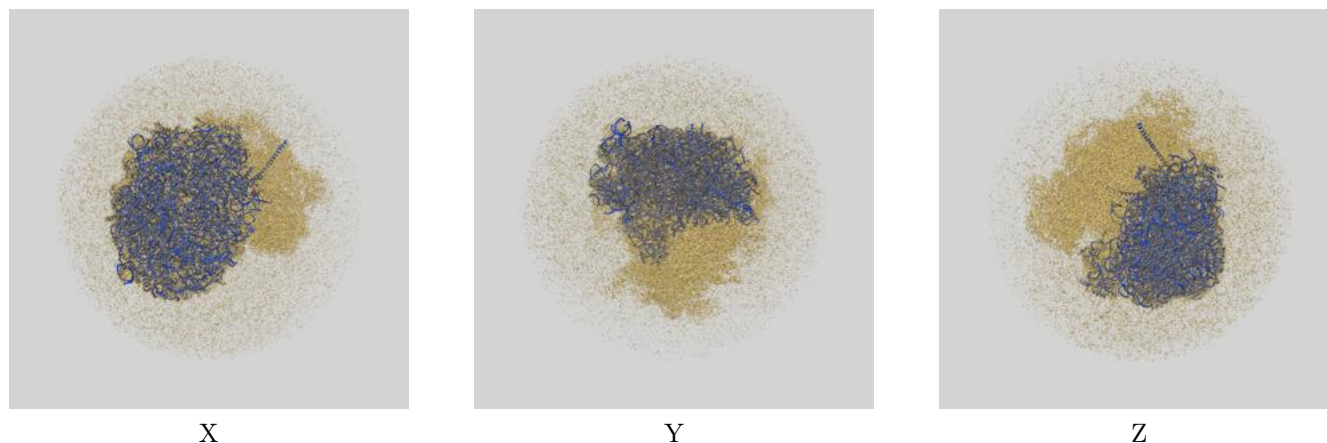
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

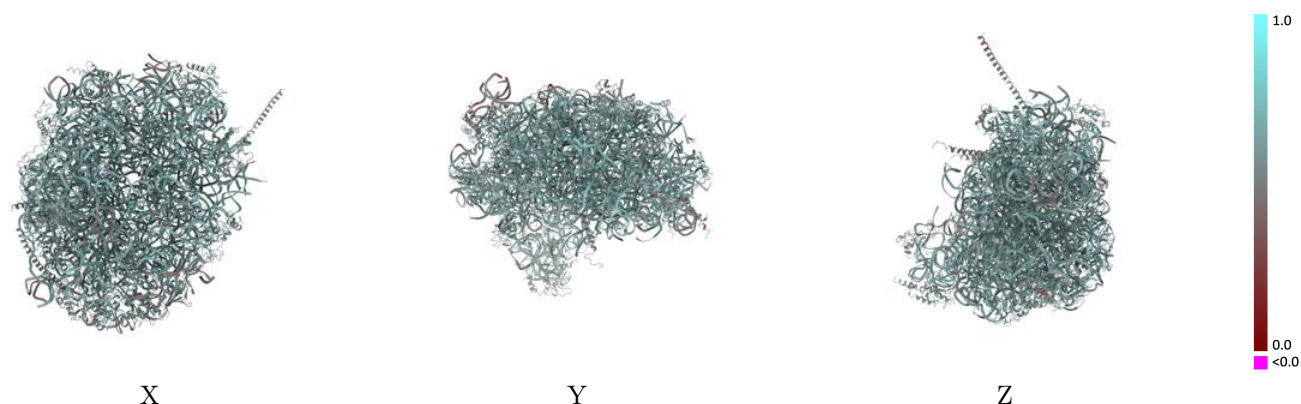
This section contains information regarding the fit between EMDB map EMD-7025 and PDB model 6AZ3. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



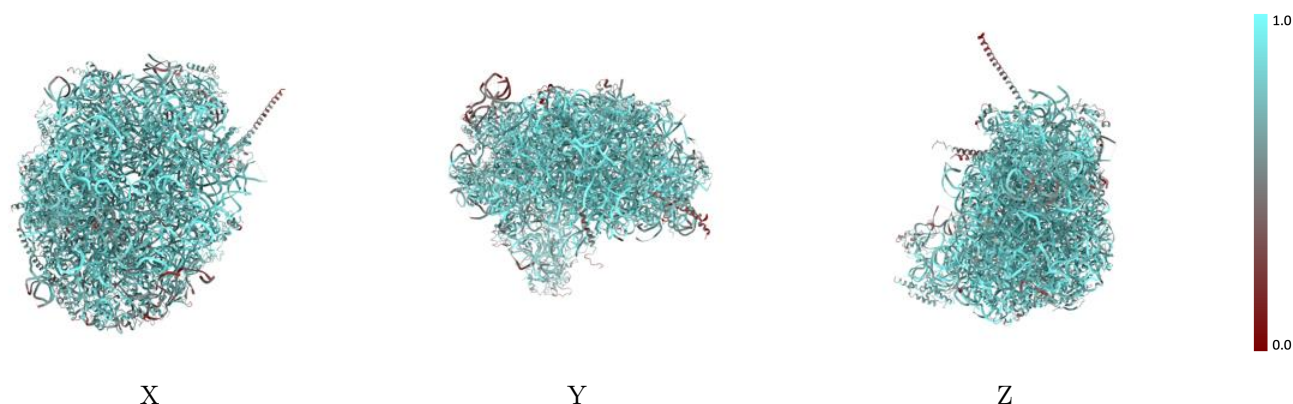
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



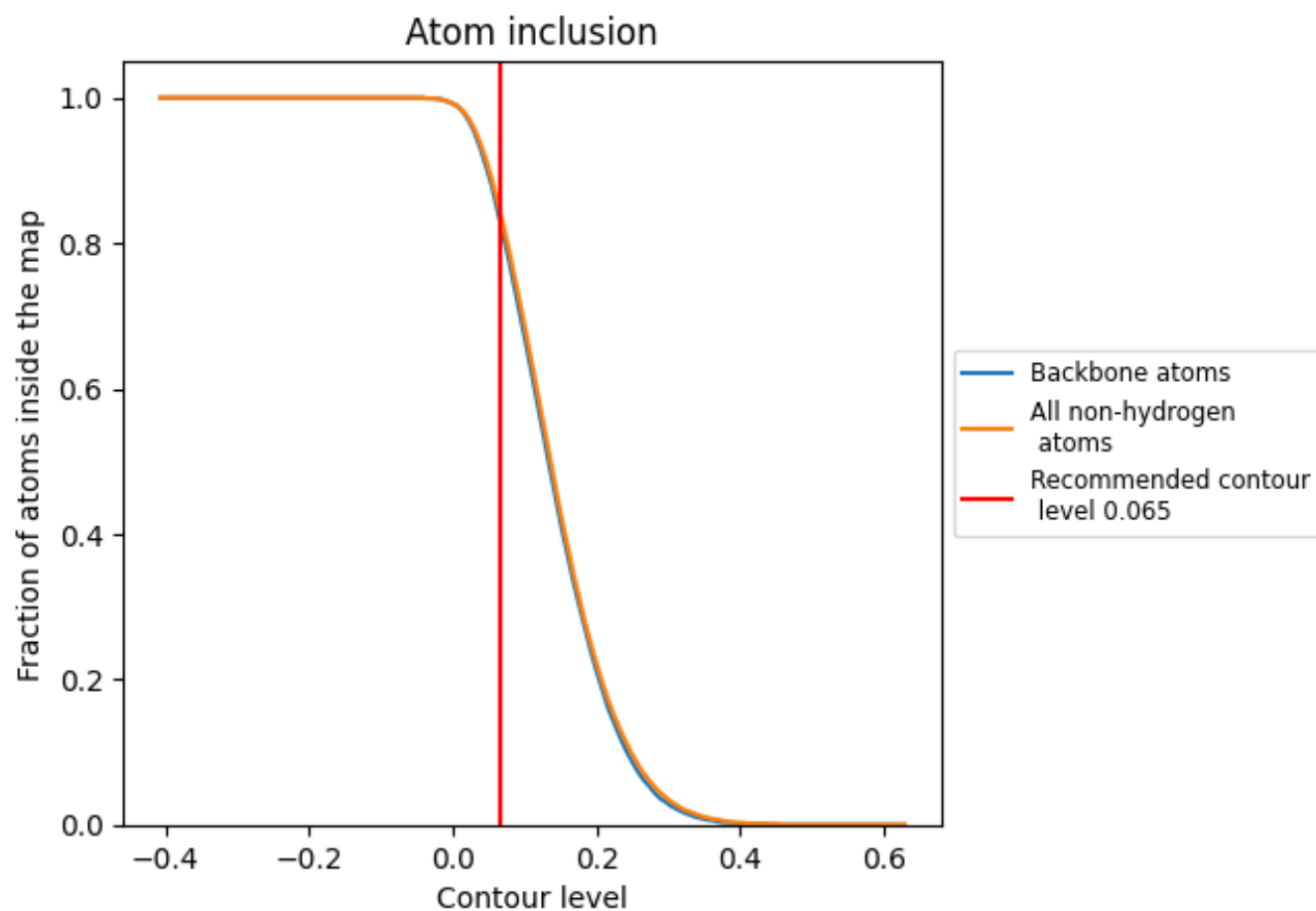
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

































The table lists the average atom inclusion at the recommended contour level (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.5990
1	 0.8890	 0.6060
2	 0.8720	 0.6030
3	 0.8770	 0.6030
4	 0.8940	 0.6070
5	 0.9040	 0.6110
6	 0.7850	 0.5640
7	 0.9180	 0.6160
8	 0.8880	 0.6020
A	 0.8650	 0.6180
B	 0.8470	 0.6060
C	 0.8130	 0.5930
D	 0.6280	 0.5280
E	 0.7480	 0.5770
F	 0.6960	 0.5560
G	 0.7880	 0.5850
H	 0.8080	 0.5990
I	 0.8120	 0.5880
J	 0.8240	 0.6040
K	 0.7180	 0.5670
L	 0.8690	 0.6140
M	 0.9130	 0.6250
N	 0.6680	 0.5660
O	 0.7540	 0.5720
P	 0.8610	 0.6080
Q	 0.7430	 0.5830
R	 0.7870	 0.5890
S	 0.7540	 0.5800
T	 0.8660	 0.6140
U	 0.6520	 0.5300
V	 0.7960	 0.5880
W	 0.8420	 0.6010
X	 0.8400	 0.5990
Y	 0.7640	 0.5850
Z	 0.7880	 0.5770



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Chain	Atom inclusion	Q-score
a	 0.7960	 0.5870
b	 0.8160	 0.6050
c	 0.8080	 0.5960
d	 0.7180	 0.5780
e	 0.7880	 0.5880
f	 0.8350	 0.5970
g	 0.8710	 0.6160
h	 0.7770	 0.5850
i	 0.7760	 0.5800
j	 0.9100	 0.6240
k	 0.7420	 0.5850
l	 0.8550	 0.6110
m	 0.7840	 0.5930
n	 0.4330	 0.4860
o	 0.8220	 0.6070
p	 0.8370	 0.6050