



wwPDB EM Validation Summary Report ⓘ

Sep 22, 2026 – 10:14 pm BST

PDB ID : 29IW / pdb_000029iw
EMDB ID : EMD-57201
Title : Human monosomes with bound toxin NT-2, focus on 60S subunit. Cells treated with NT-2.
Authors : Rabl, J.; Karousis, E.D.
Deposited on : 2026-03-15
Resolution : 1.77 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:

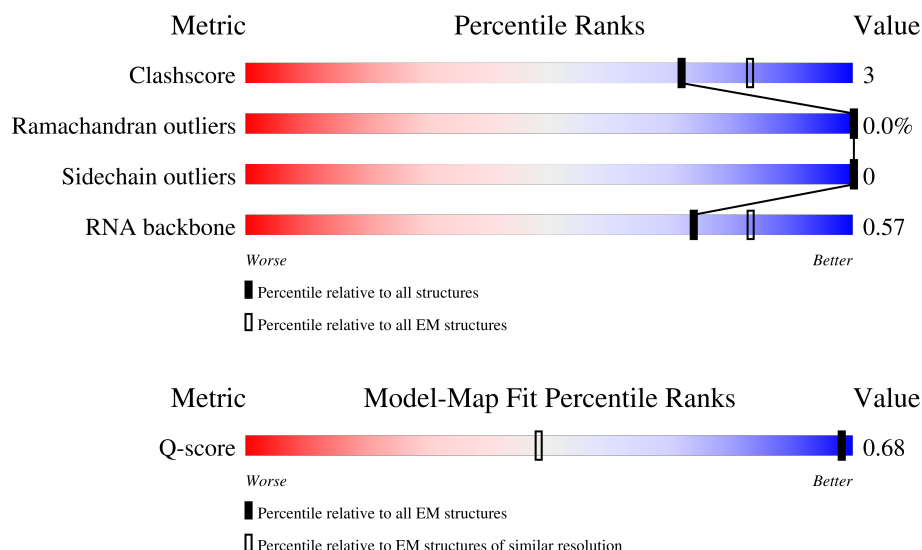
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 1.77 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	694 (1.27 - 2.27)

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	AA	248	
2	AB	266	
3	AC	192	

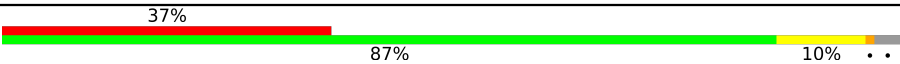
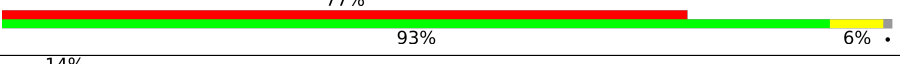
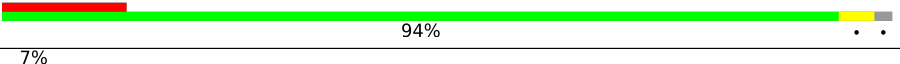
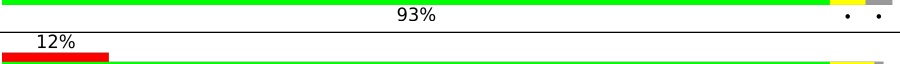
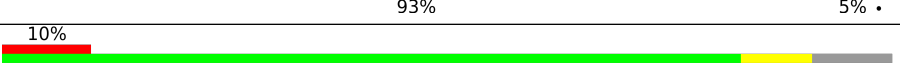
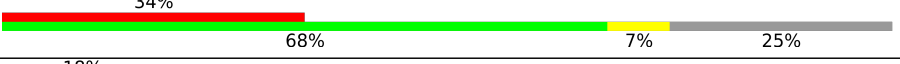
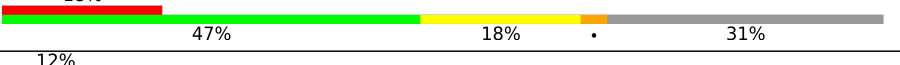
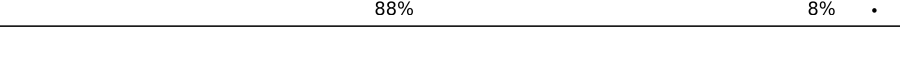
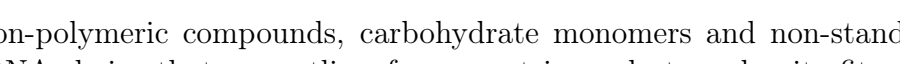
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Mol	Chain	Length	Quality of chain
4	AD	214	
5	AE	178	
6	AF	211	
7	AG	215	
8	AH	204	
9	AI	203	
10	AJ	184	
11	AK	188	
12	AL	196	
13	AM	176	
14	AN	160	
15	AO	128	
16	AP	140	
17	AQ	157	
18	AR	156	
19	AS	145	
20	AT	136	
21	AU	148	
22	AV	159	
23	AW	115	
24	AX	125	
25	AY	135	
26	AZ	110	
27	Aa	117	
28	Ab	123	

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Mol	Chain	Length	Quality of chain
29	Ac	105	
30	Ad	97	
31	Ae	70	
32	Af	51	
33	Ag	128	
34	Ah	106	
35	Ai	92	
36	Aj	137	
37	BA	403	
38	BB	427	
39	BC	297	
40	BD	288	
41	DA	5069	
42	DB	120	
43	DC	157	
44	DD	257	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	PUT	DA	5101	-	-	X	-
48	PUT	DA	5102	-	-	X	-
48	PUT	DA	5103	-	-	X	-
49	SPD	DA	5105	-	-	X	-
49	SPD	DA	5110	-	-	X	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 238693 atoms, of which 95192 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	AA	225	Total	C	H	N	O	S	0	0
			3866	1202	1996	358	301	9		

- Molecule 2 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AB	216	Total	C	H	N	O	S	0	0
			3640	1121	1884	339	292	4		

- Molecule 3 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	AC	190	Total	C	H	N	O	S	0	0
			3119	956	1601	284	272	6		

- Molecule 4 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AD	205	Total	C	H	N	O	S	0	0
			3362	1053	1701	321	274	13		

- Molecule 5 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	AE	171	Total	C	H	N	O	S	0	0
			2783	867	1412	256	242	6		

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	AF	207	Total	C	H	N	O	S	0	0
			3452	1046	1779	346	277	4		

- Molecule 7 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	AG	136	Total	C	H	N	O	S	0	0
			2307	719	1187	215	179	7		

- Molecule 8 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	AH	203	Total	C	H	N	O	S	0	0
			3450	1072	1749	359	266	4		

- Molecule 9 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AI	201	Total	C	H	N	O	S	0	0
			3445	1063	1795	321	261	5		

- Molecule 10 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AJ	151	Total	C	H	N	O	S	0	0
			2474	765	1250	238	212	9		

- Molecule 11 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AK	187	Total	C	H	N	O	S	0	0
			3141	944	1628	314	250	5		

- Molecule 12 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AL	156	Total	C	H	N	O	S	0	0
			2740	812	1438	279	202	9		

- Molecule 13 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AM	175	Total	C	H	N	O	S	0	0
			2943	925	1490	283	235	10		

- Molecule 14 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AN	159	Total	C	H	N	O	S	0	0
			2664	823	1366	252	217	6		

- Molecule 15 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AO	101	Total	C	H	N	O	S	0	0
			1675	529	850	144	150	2		

- Molecule 16 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AP	131	Total	C	H	N	O	S	0	0
			2018	618	1039	184	172	5		

- Molecule 17 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AQ	62	Total	C	H	N	O	S	0	0
			1053	332	534	101	83	3		

- Molecule 18 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AR	119	Total	C	H	N	O	S	0	0
			2029	624	1053	183	168	1		

- Molecule 19 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AS	134	Total	C	H	N	O	S	0	0
			2320	700	1205	226	186	3		

- Molecule 20 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AT	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 21 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AU	147	Total	C	H	N	O	S	0	0
			2373	736	1210	237	187	3		

- Molecule 22 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AV	100	Total	C	H	N	O	S	0	0
			1687	505	876	177	125	4		

- Molecule 23 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	93	Total	C	H	N	O	S	0	0
			1490	462	764	129	129	6		

- Molecule 24 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	109	Total	C	H	N	O	S	0	0
			1848	569	947	173	157	2		

- Molecule 25 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AY	130	Total	C	H	N	O	S	0	0
			2236	676	1166	221	168	5		

- Molecule 26 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AZ	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	144	3		

- Molecule 27 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Aa	106	Total	C	H	N	O	S	0	0
			1778	530	933	174	135	6		

- Molecule 28 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	Ab	122	Total	C	H	N	O	S	0	0
			2163	641	1148	205	168	1		

- Molecule 29 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Ac	102	Total	C	H	N	O	S	0	0
			1749	521	917	177	129	5		

- Molecule 30 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	Ad	86	Total	C	H	N	O	S	0	0
			1441	434	736	155	111	5		

- Molecule 31 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Ae	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 32 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	Af	50	Total	C	H	N	O	S	0	0
			927	281	483	98	64	1		

- Molecule 33 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Ag	52	Total	C	H	N	O	S	0	0
			896	267	466	90	67	6		

- Molecule 34 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Ah	103	Total	C	H	N	O	S	0	0
			1754	528	912	172	136	6		

- Molecule 35 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	Ai	91	Total	C	H	N	O	S	0	0
			1464	445	757	136	119	7		

- Molecule 36 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	Aj	125	Total	C	H	N	O	S	0	0
			2071	622	1069	207	168	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	BA	396	Total	C	H	N	O	S	0	0
			6538	2037	3340	601	546	14		

- Molecule 38 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	BB	359	Total	C	H	N	O	S	0	0
			5898	1802	3036	572	475	13		

- Molecule 39 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	BC	293	Total	C	H	N	O	S	0	0
			4807	1510	2421	435	427	14		

- Molecule 40 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	BD	216	Total	C	H	N	O	S	0	0
			3625	1119	1888	329	285	4		

- Molecule 41 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	DA	3483	Total	C	H	N	O	P	0	0
			112179	33315	37449	13662	24271	3482		

- Molecule 42 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	DB	119	Total	C	H	N	O	P	0	0
			3823	1132	1285	454	834	118		

- Molecule 43 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	DC	156	Total	C	H	N	O	P	0	0
			4989	1481	1674	585	1094	155		

- Molecule 44 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	DD	246	Total	C	H	N	O	S	0	0
			3867	1183	1979	387	312	6		

- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	AD	1	Total	Mg	0
			1	1	
45	AJ	1	Total	Mg	0
			1	1	
45	AP	1	Total	Mg	0
			1	1	
45	AY	1	Total	Mg	0
			1	1	
45	AZ	1	Total	Mg	0
			1	1	
45	Ad	1	Total	Mg	0
			1	1	
45	BA	1	Total	Mg	0
			1	1	
45	DA	169	Total	Mg	0
			169	169	
45	DB	2	Total	Mg	0
			2	2	
45	DC	3	Total	Mg	0
			3	3	

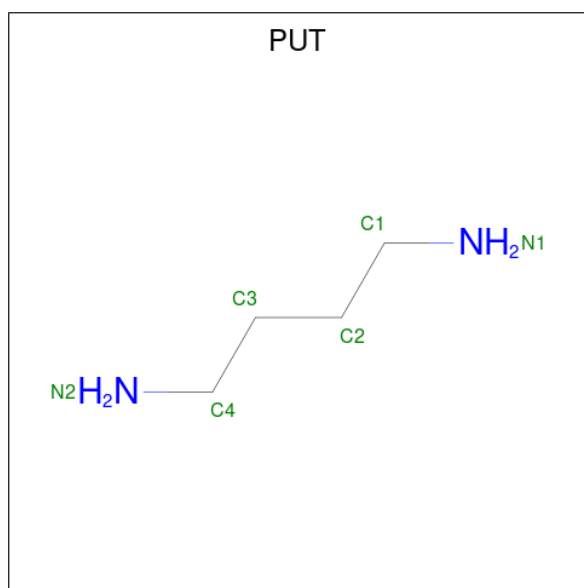
- Molecule 46 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
46	AM	1	Total K 1 1	0
46	AN	1	Total K 1 1	0
46	DA	41	Total K 41 41	0
46	DC	1	Total K 1 1	0
46	DD	2	Total K 2 2	0

- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

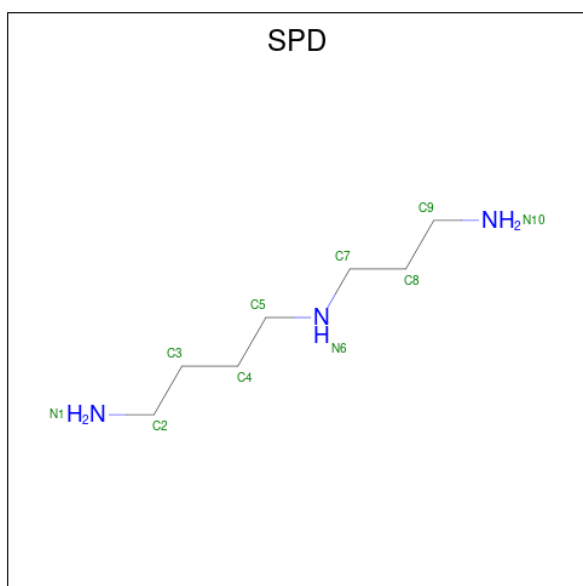
Mol	Chain	Residues	Atoms	AltConf
47	Aa	1	Total Zn 1 1	0
47	Ad	1	Total Zn 1 1	0
47	Ag	1	Total Zn 1 1	0
47	Ah	1	Total Zn 1 1	0
47	Ai	1	Total Zn 1 1	0

- Molecule 48 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



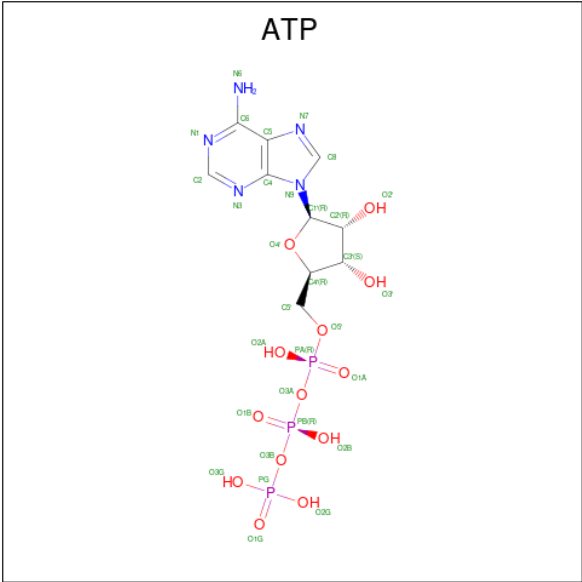
Mol	Chain	Residues	Atoms			AltConf
48	DA	1	Total	C	N	0
			6	4	2	
48	DA	1	Total	C	N	0
			6	4	2	
48	DA	1	Total	C	N	0
			6	4	2	
48	DA	1	Total	C	N	0
			6	4	2	
48	DB	1	Total	C	N	0
			6	4	2	

- Molecule 49 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



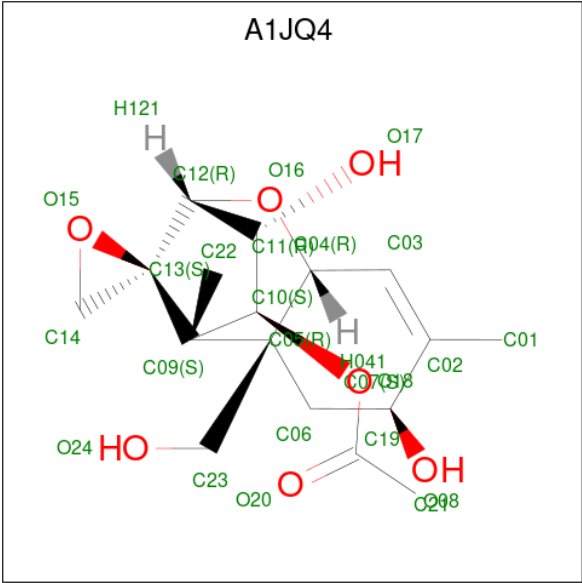
Mol	Chain	Residues	Atoms				AltConf
49	DA	1	Total	C	H	N	0
			12	7	2	3	
49	DA	1	Total	C	H	N	0
			12	7	2	3	
49	DA	1	Total	C	H	N	0
			12	7	2	3	
49	DA	1	Total	C	H	N	0
			12	7	2	3	
49	DA	1	Total	C	H	N	0
			12	7	2	3	
49	DA	1	Total	C	H	N	0
			12	7	2	3	

- Molecule 50 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
50	DA	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 51 is Toxin NT-2 (CCD ID: A1JQ4) (formula: C₁₇H₂₄O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
51	DA	1	Total	C	H	O	0
			48	17	24	7	

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	AA	111	Total 111	O 111	0
52	AB	169	Total 169	O 169	0
52	AC	128	Total 128	O 128	0
52	AD	118	Total 118	O 118	0
52	AE	113	Total 113	O 113	0
52	AF	116	Total 116	O 116	0
52	AG	85	Total 85	O 85	0
52	AH	127	Total 127	O 127	0
52	AI	105	Total 105	O 105	0
52	AJ	51	Total 51	O 51	0
52	AK	108	Total 108	O 108	0
52	AL	95	Total 95	O 95	0
52	AM	106	Total 106	O 106	0
52	AN	101	Total 101	O 101	0
52	AO	106	Total 106	O 106	0
52	AP	56	Total 56	O 56	0
52	AQ	30	Total 30	O 30	0
52	AR	69	Total 69	O 69	0
52	AS	54	Total 54	O 54	0
52	AT	105	Total 105	O 105	0
52	AU	77	Total 77	O 77	0
52	AV	51	Total 51	O 51	0

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Mol	Chain	Residues	Atoms		AltConf
52	AW	69	Total 69	O 69	0
52	AX	56	Total 56	O 56	0
52	AY	85	Total 85	O 85	0
52	AZ	54	Total 54	O 54	0
52	Aa	71	Total 71	O 71	0
52	Ab	55	Total 55	O 55	0
52	Ac	71	Total 71	O 71	0
52	Ad	42	Total 42	O 42	0
52	Ae	64	Total 64	O 64	0
52	Af	24	Total 24	O 24	0
52	Ag	30	Total 30	O 30	0
52	Ah	67	Total 67	O 67	0
52	Ai	45	Total 45	O 45	0
52	Aj	79	Total 79	O 79	0
52	BA	166	Total 166	O 166	0
52	BB	170	Total 170	O 170	0
52	BC	222	Total 222	O 222	0
52	BD	152	Total 152	O 152	0
52	DA	6755	Total 6755	O 6755	0
52	DB	199	Total 199	O 199	0
52	DC	240	Total 240	O 240	0

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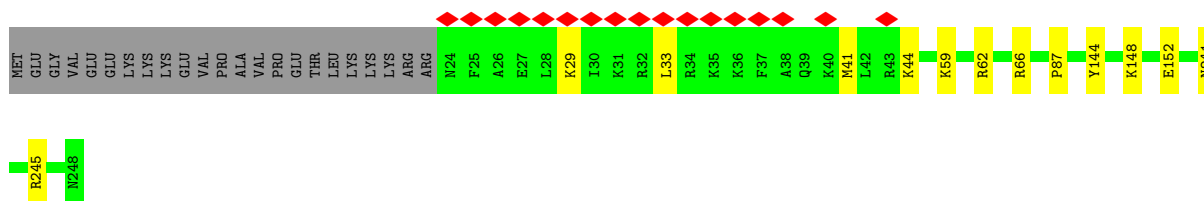
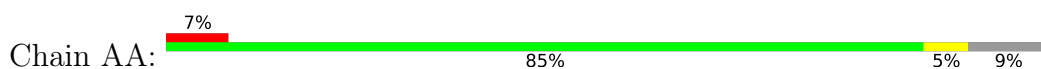
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Mol	Chain	Residues	Atoms		AltConf
52	DD	104	Total	O	0
			104	104	

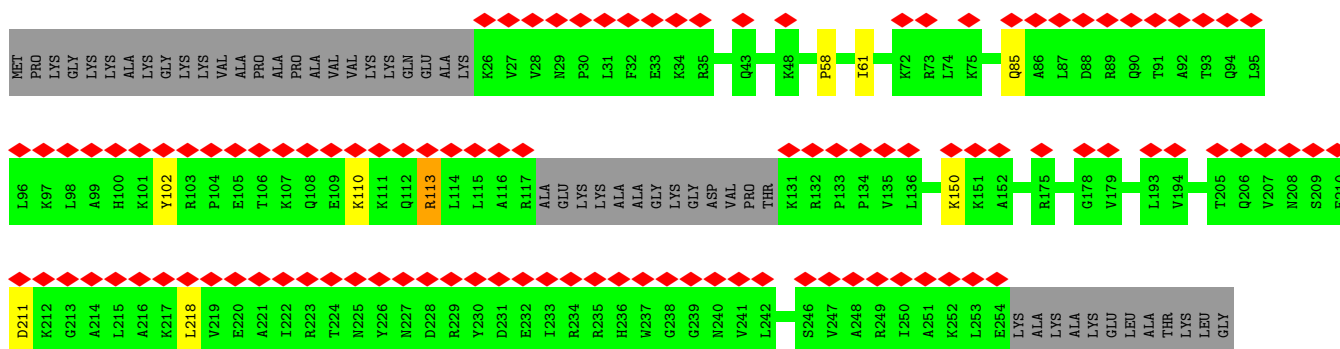
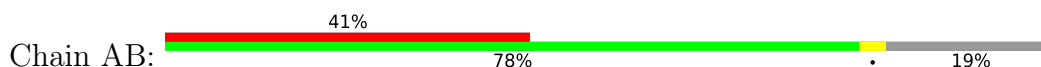
3 Residue-property plots

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.

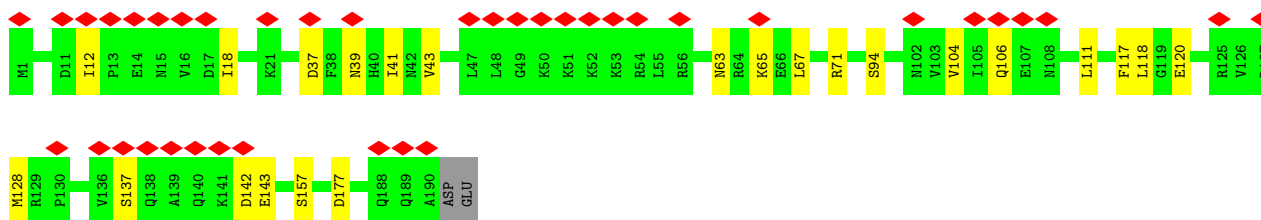
- Molecule 1: Large ribosomal subunit protein uL30



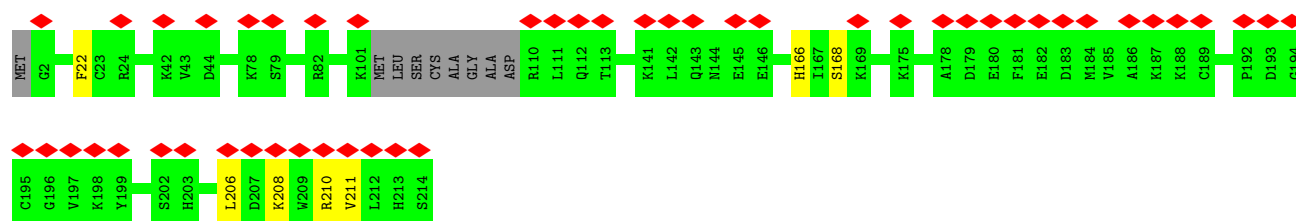
- Molecule 2: 60S ribosomal protein L7a



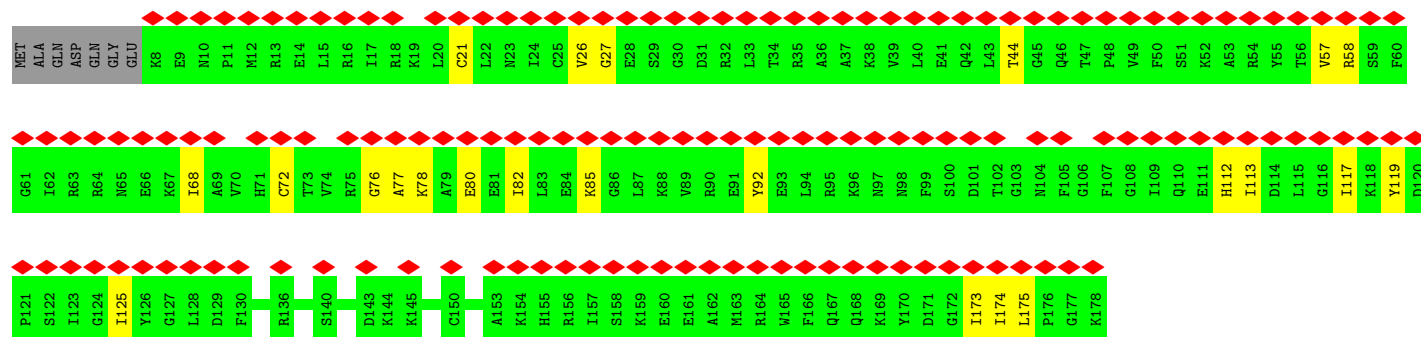
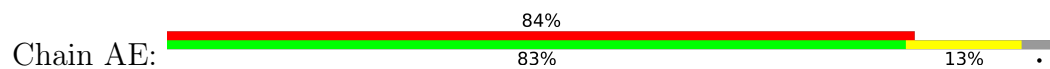
- Molecule 3: 60S ribosomal protein L9



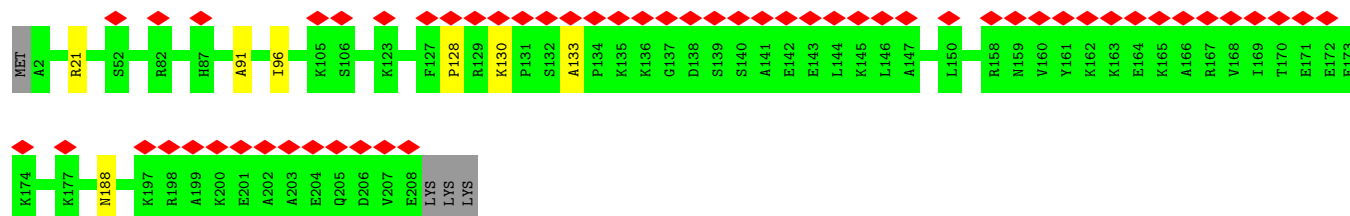
- Molecule 4: Ribosomal protein uL16-like



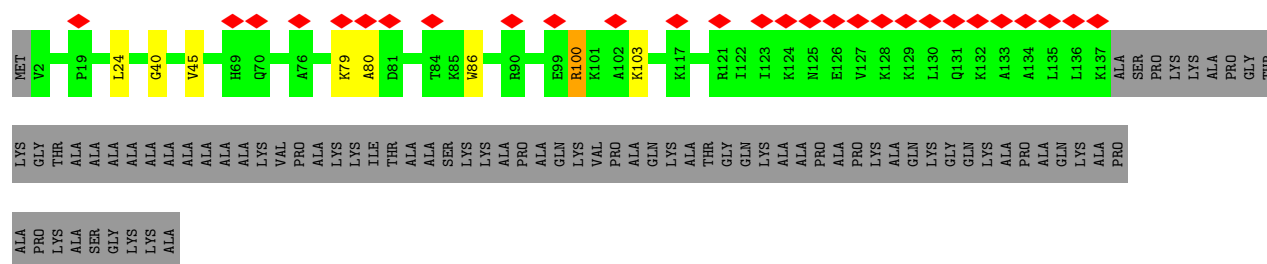
• Molecule 5: 60S ribosomal protein L11



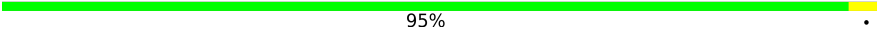
• Molecule 6: 60S ribosomal protein L13



• Molecule 7: 60S ribosomal protein L14



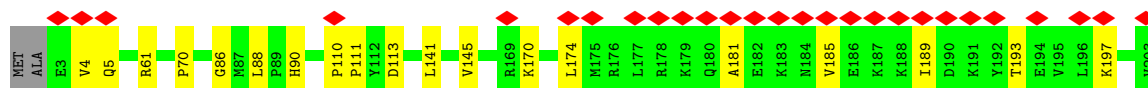
• Molecule 8: 60S ribosomal protein L15

Chain AH:  95% .



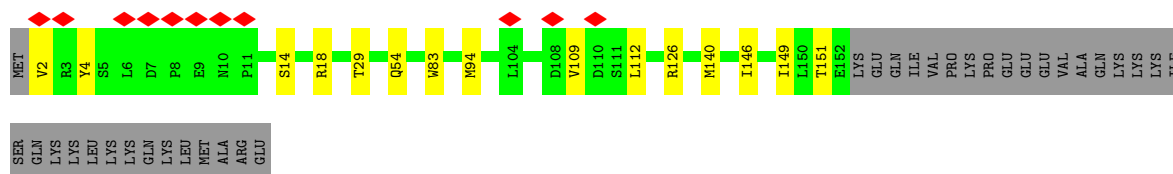
- Molecule 9: 60S ribosomal protein L13a

Chain AI:  13% 90% 9% .

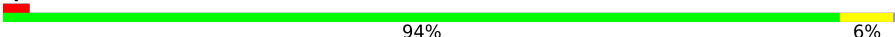


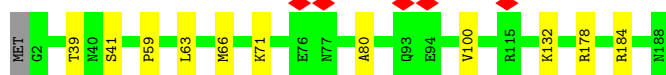
- Molecule 10: 60S ribosomal protein L17

Chain AJ:  6% 74% 8% 18%



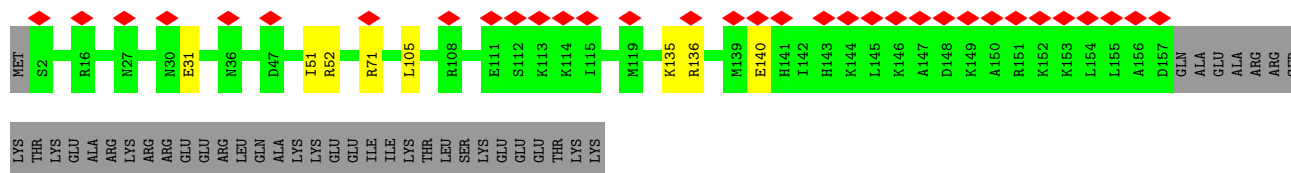
- Molecule 11: 60S ribosomal protein L18

Chain AK:  94% 6% .

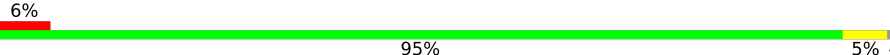


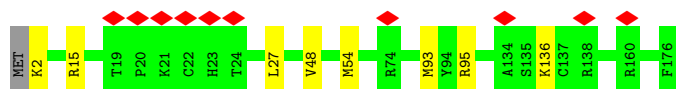
- Molecule 12: 60S ribosomal protein L19

Chain AL:  17% 76% 20%

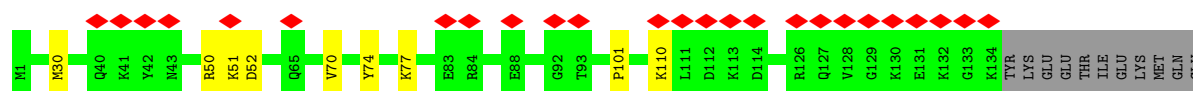
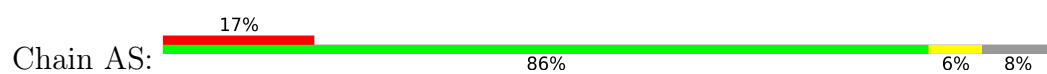


- Molecule 13: 60S ribosomal protein L18a

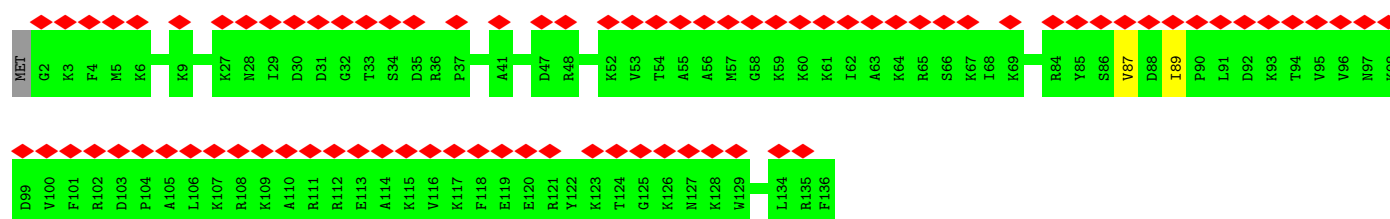
Chain AM:  6% 95% 5% .



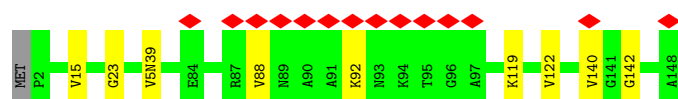
- Molecule 14: 60S ribosomal protein L21



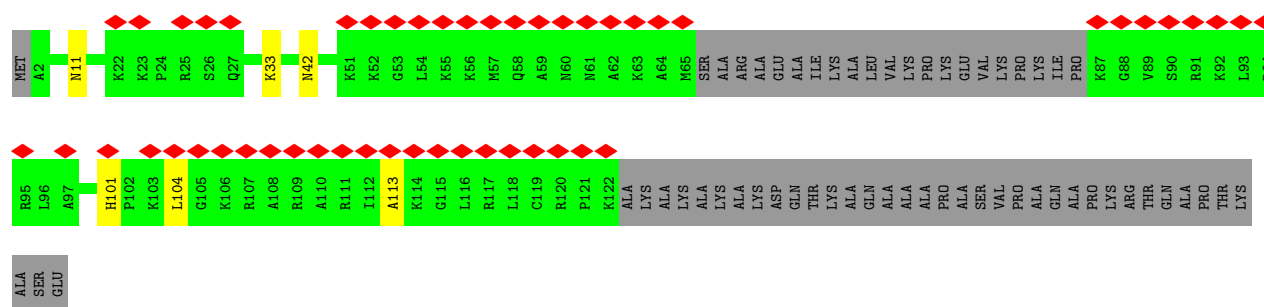
- Molecule 20: 60S ribosomal protein L27



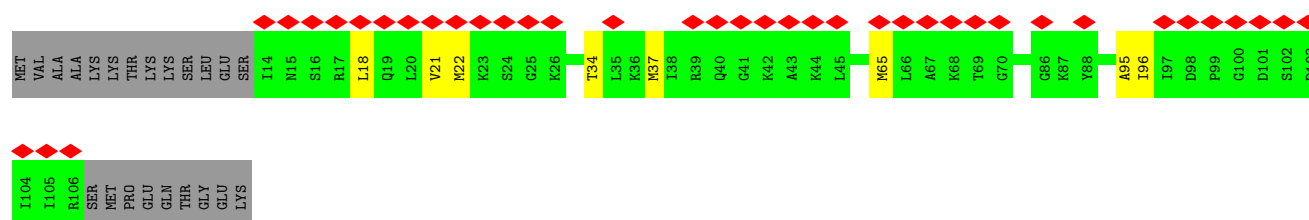
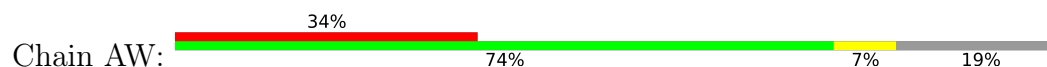
- Molecule 21: Large ribosomal subunit protein uL15



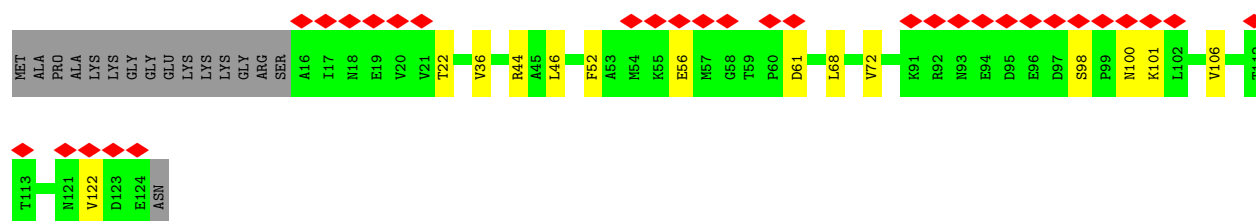
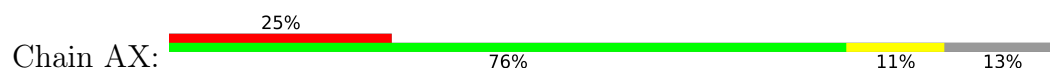
- Molecule 22: 60S ribosomal protein L29



- Molecule 23: 60S ribosomal protein L30



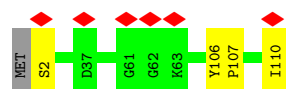
- Molecule 24: 60S ribosomal protein L31



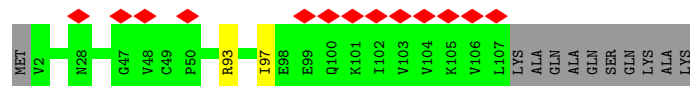
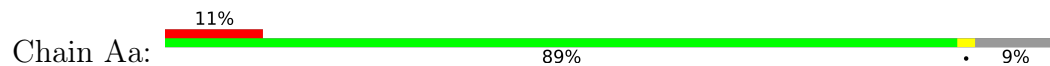
- Molecule 25: 60S ribosomal protein L32



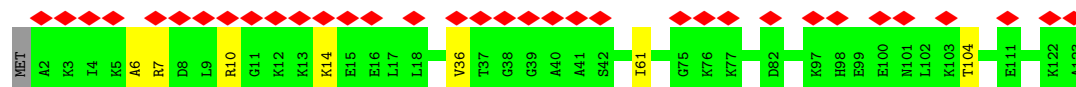
- Molecule 26: Large ribosomal subunit protein eL33



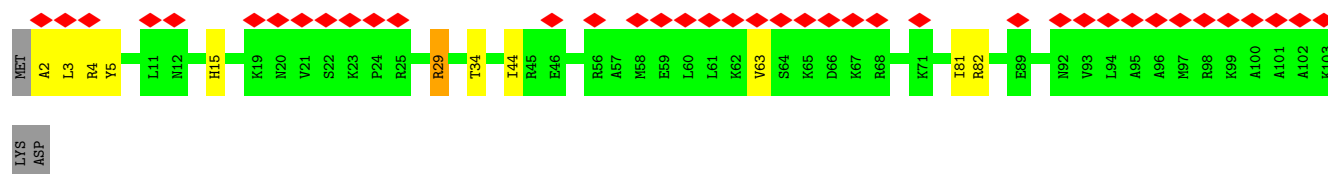
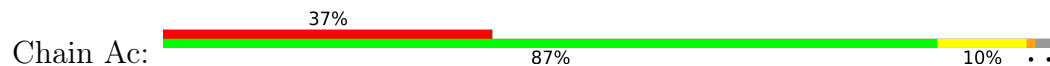
- Molecule 27: 60S ribosomal protein L34



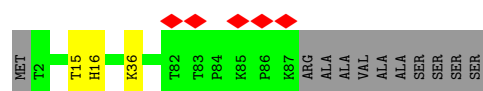
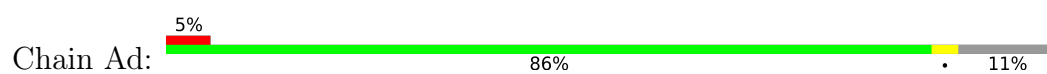
- Molecule 28: 60S ribosomal protein L35



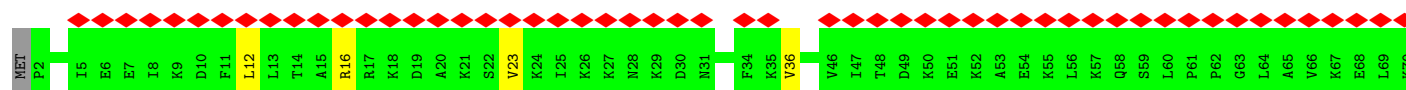
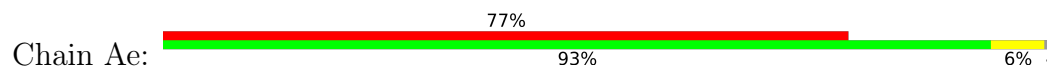
- Molecule 29: 60S ribosomal protein L36



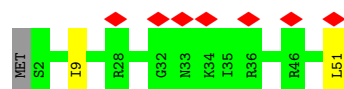
- Molecule 30: Large ribosomal subunit protein eL37



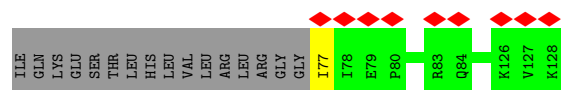
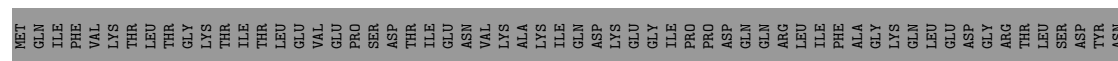
- Molecule 31: 60S ribosomal protein L38



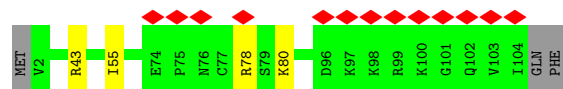
- Molecule 32: 60S ribosomal protein L39



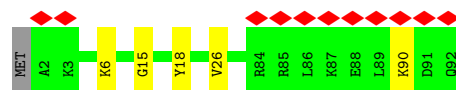
- Molecule 33: Large ribosomal subunit protein eL40



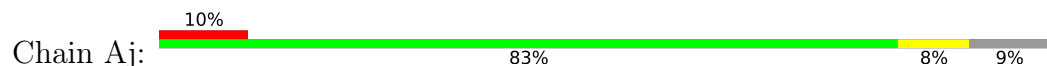
- Molecule 34: 60S ribosomal protein L36a

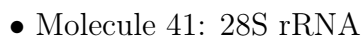


- Molecule 35: 60S ribosomal protein L37a



- Molecule 36: 60S ribosomal protein L28

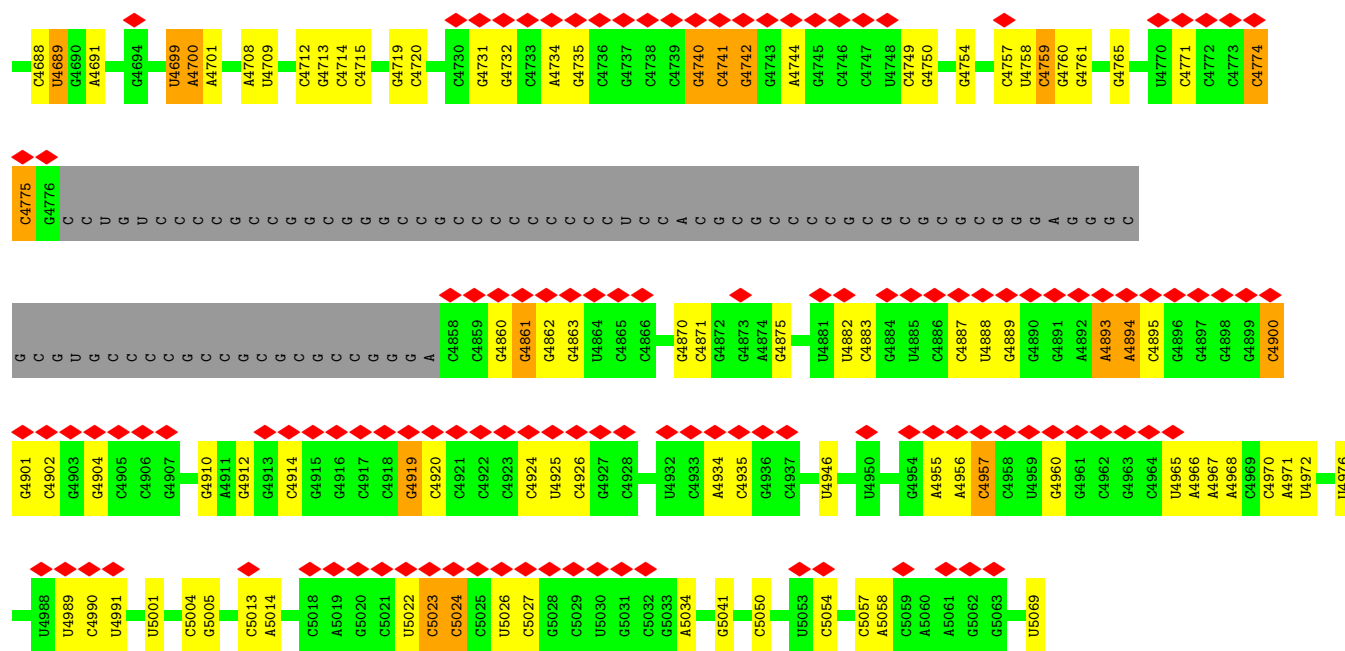




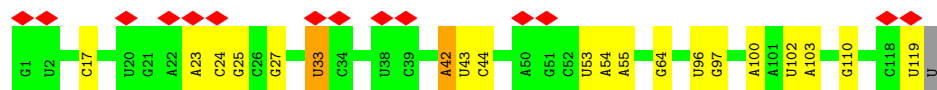
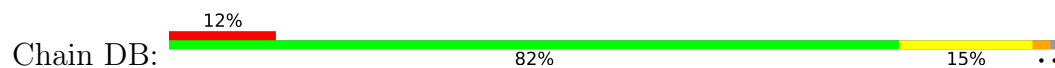




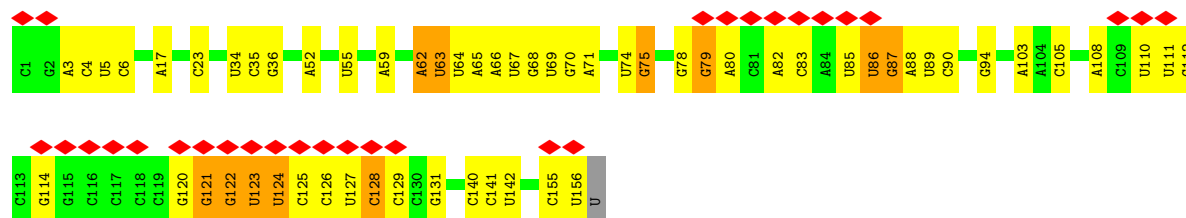




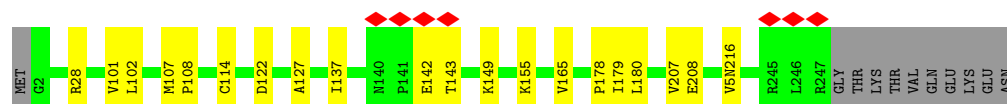
- Molecule 42: 5S rRNA



- Molecule 43: 5.8S rRNA



- Molecule 44: Large ribosomal subunit protein uL2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1587552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.822	Depositor
Minimum map value	-0.773	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.648, 0.648, 0.648	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MLZ, UR3, HIC, V5N, OMC, 5MC, PUT, UY1, SPD, MG, ATP, ZN, A2M, OMU, B8T, 1MA, PSU, A1JQ4, 6MZ, OMG

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	AA	0.19	0/1905	0.41	0/2539
2	AB	0.21	0/1787	0.40	0/2408
3	AC	0.18	0/1537	0.38	0/2066
4	AD	0.18	0/1700	0.36	0/2270
5	AE	0.24	0/1394	0.50	0/1863
6	AF	0.16	0/1704	0.35	0/2282
7	AG	0.17	0/1142	0.41	0/1527
8	AH	0.19	0/1746	0.41	0/2338
9	AI	0.18	0/1682	0.38	0/2250
10	AJ	0.22	0/1250	0.43	0/1678
11	AK	0.20	0/1537	0.37	1/2052 (0.0%)
12	AL	0.23	0/1318	0.41	0/1745
13	AM	0.16	0/1493	0.34	0/2003
14	AN	0.18	0/1326	0.39	0/1770
15	AO	0.23	0/839	0.47	0/1126
16	AP	0.15	0/993	0.37	0/1332
17	AQ	0.20	0/532	0.40	0/708
18	AR	0.14	0/993	0.31	0/1334
19	AS	0.26	0/1132	0.42	0/1504
20	AT	0.16	0/1130	0.32	0/1507
21	AU	0.17	0/1179	0.35	0/1573
22	AV	0.19	0/824	0.41	0/1086
23	AW	0.18	0/736	0.42	0/988
24	AX	0.18	0/916	0.39	0/1234
25	AY	0.14	0/1088	0.32	0/1451
26	AZ	0.14	0/895	0.35	0/1198
27	Aa	0.16	0/855	0.35	0/1140
28	Ab	0.17	0/1023	0.37	0/1351
29	Ac	0.25	0/843	0.44	0/1115
30	Ad	0.16	0/720	0.37	0/952
31	Ae	0.17	0/575	0.38	0/761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Af	0.16	0/454	0.39	0/599
33	Ag	0.12	0/425	0.35	0/561
34	Ah	0.17	0/855	0.36	0/1128
35	Ai	0.15	0/717	0.35	0/953
36	Aj	0.18	0/1017	0.36	0/1364
37	BA	0.19	0/3253	0.44	2/4352 (0.0%)
38	BB	0.18	0/2916	0.37	0/3917
39	BC	0.18	0/2432	0.41	2/3256 (0.1%)
40	BD	0.15	0/1771	0.35	0/2377
41	DA	0.15	14/80842 (0.0%)	0.31	0/126109
42	DB	0.11	0/2836	0.28	0/4421
43	DC	0.12	0/3631	0.28	0/5657
44	DD	0.19	0/1913	0.40	0/2563
All	All	0.16	14/139856 (0.0%)	0.34	5/206408 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	1
7	AG	0	1
12	AL	0	1
15	AO	0	1
29	Ac	0	1
44	DD	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	DA	4523	A2M	O3'-P	6.28	1.62	1.56
41	DA	3718	A2M	O3'-P	6.22	1.62	1.56
41	DA	3830	A2M	O3'-P	6.19	1.62	1.56
41	DA	1871	A2M	O3'-P	6.17	1.62	1.56
41	DA	2815	A2M	O3'-P	6.10	1.62	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BA	301	ASN	N-CA-C	-6.01	100.41	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BA	302	ASN	N-CA-CB	-5.96	107.37	114.17
11	AK	59	PRO	O-C-N	-5.36	118.63	121.15
39	BC	82	GLU	CA-C-N	5.06	126.08	120.06
39	BC	82	GLU	C-N-CA	5.06	126.08	120.06

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	113	ARG	Sidechain
7	AG	100	ARG	Sidechain
12	AL	71	ARG	Sidechain
15	AO	113	ARG	Sidechain
29	Ac	29	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1870	1996	1996	10	0
2	AB	1756	1884	1884	6	0
3	AC	1518	1601	1601	13	0
4	AD	1661	1701	1701	4	0
5	AE	1371	1412	1412	18	0
6	AF	1673	1779	1779	5	0
7	AG	1120	1187	1187	4	0
8	AH	1701	1749	1749	9	0
9	AI	1650	1795	1794	16	0
10	AJ	1224	1250	1250	10	0
11	AK	1513	1628	1628	7	0
12	AL	1302	1438	1438	4	0
13	AM	1453	1490	1490	5	0
14	AN	1298	1366	1366	6	0
15	AO	825	850	850	10	0
16	AP	979	1039	1039	3	0
17	AQ	519	534	533	4	0
18	AR	976	1053	1053	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AS	1115	1205	1205	11	0
20	AT	1107	1182	1182	1	0
21	AU	1163	1210	1206	5	0
22	AV	811	876	876	5	0
23	AW	726	764	764	5	0
24	AX	901	947	946	8	0
25	AY	1070	1166	1165	4	0
26	AZ	876	912	912	3	0
27	Aa	845	933	933	1	0
28	Ab	1015	1148	1148	8	0
29	Ac	832	917	917	9	0
30	Ad	705	736	736	2	0
31	Ae	569	637	637	2	0
32	Af	444	483	483	2	0
33	Ag	430	466	466	1	0
34	Ah	842	912	912	3	0
35	Ai	707	757	756	6	0
36	Aj	1002	1069	1068	6	0
37	BA	3198	3340	3339	27	0
38	BB	2862	3036	3036	15	0
39	BC	2386	2421	2421	18	0
40	BD	1737	1888	1888	14	0
41	DA	74730	37449	37836	461	0
42	DB	2538	1285	1286	11	0
43	DC	3315	1674	1685	41	0
44	DD	1888	1979	1976	14	0
45	AD	1	0	0	0	0
45	AJ	1	0	0	0	0
45	AP	1	0	0	0	0
45	AY	1	0	0	0	0
45	AZ	1	0	0	0	0
45	Ad	1	0	0	0	0
45	BA	1	0	0	0	0
45	DA	169	0	0	0	0
45	DB	2	0	0	0	0
45	DC	3	0	0	0	0
46	AM	1	0	0	0	0
46	AN	1	0	0	0	0
46	DA	41	0	0	0	0
46	DC	1	0	0	0	0
46	DD	2	0	0	0	0
47	Aa	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	Ad	1	0	0	0	0
47	Ag	1	0	0	0	0
47	Ah	1	0	0	0	0
47	Ai	1	0	0	0	0
48	DA	24	0	48	20	0
48	DB	6	0	0	0	0
49	DA	60	12	114	29	0
50	DA	31	12	12	3	0
51	DA	24	24	0	0	0
52	AA	111	0	0	1	0
52	AB	169	0	0	1	0
52	AC	128	0	0	1	0
52	AD	118	0	0	0	0
52	AE	113	0	0	2	0
52	AF	116	0	0	0	0
52	AG	85	0	0	0	0
52	AH	127	0	0	0	0
52	AI	105	0	0	1	0
52	AJ	51	0	0	0	0
52	AK	108	0	0	0	0
52	AL	95	0	0	0	0
52	AM	106	0	0	0	0
52	AN	101	0	0	0	0
52	AO	106	0	0	0	0
52	AP	56	0	0	0	0
52	AQ	30	0	0	0	0
52	AR	69	0	0	0	0
52	AS	54	0	0	0	0
52	AT	105	0	0	0	0
52	AU	77	0	0	1	0
52	AV	51	0	0	0	0
52	AW	69	0	0	0	0
52	AX	56	0	0	0	0
52	AY	85	0	0	0	0
52	AZ	54	0	0	0	0
52	Aa	71	0	0	0	0
52	Ab	55	0	0	1	0
52	Ac	71	0	0	1	0
52	Ad	42	0	0	0	0
52	Ae	64	0	0	0	0
52	Af	24	0	0	0	0
52	Ag	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	Ah	67	0	0	0	0
52	Ai	45	0	0	0	0
52	Aj	79	0	0	0	0
52	BA	166	0	0	0	0
52	BB	170	0	0	0	0
52	BC	222	0	0	0	0
52	BD	152	0	0	1	0
52	DA	6755	0	0	7	0
52	DB	199	0	0	0	0
52	DC	240	0	0	1	0
52	DD	104	0	0	0	0
All	All	143501	95192	95703	782	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 782 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DA:2050:G:H21	49:DA:5110:SPD:H72	1.50	0.77
9:AI:86:GLY:O	49:DA:5110:SPD:H92	1.85	0.77
38:BB:304:ALA:HB1	41:DA:2096:G:H21	1.50	0.76
37:BA:301:ASN:O	37:BA:302:ASN:HB3	1.86	0.74
41:DA:463:A:H61	41:DA:692:A:H61	1.34	0.74

There are no symmetry-related clashes.

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	AA	223/248 (90%)	219 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	212/266 (80%)	208 (98%)	4 (2%)	0	100	100
3	AC	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
4	AD	201/214 (94%)	199 (99%)	2 (1%)	0	100	100
5	AE	169/178 (95%)	165 (98%)	4 (2%)	0	100	100
6	AF	205/211 (97%)	196 (96%)	9 (4%)	0	100	100
7	AG	134/215 (62%)	130 (97%)	4 (3%)	0	100	100
8	AH	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
9	AI	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
10	AJ	149/184 (81%)	145 (97%)	4 (3%)	0	100	100
11	AK	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
12	AL	154/196 (79%)	153 (99%)	1 (1%)	0	100	100
13	AM	173/176 (98%)	171 (99%)	2 (1%)	0	100	100
14	AN	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
15	AO	99/128 (77%)	93 (94%)	6 (6%)	0	100	100
16	AP	129/140 (92%)	128 (99%)	1 (1%)	0	100	100
17	AQ	60/157 (38%)	58 (97%)	2 (3%)	0	100	100
18	AR	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
19	AS	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
20	AT	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
21	AU	144/148 (97%)	140 (97%)	3 (2%)	1 (1%)	18	8
22	AV	96/159 (60%)	92 (96%)	4 (4%)	0	100	100
23	AW	91/115 (79%)	89 (98%)	2 (2%)	0	100	100
24	AX	107/125 (86%)	103 (96%)	4 (4%)	0	100	100
25	AY	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
26	AZ	107/110 (97%)	107 (100%)	0	0	100	100
27	Aa	104/117 (89%)	104 (100%)	0	0	100	100
28	Ab	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
29	Ac	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
30	Ad	84/97 (87%)	84 (100%)	0	0	100	100
31	Ae	67/70 (96%)	67 (100%)	0	0	100	100
32	Af	48/51 (94%)	46 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Ag	49/128 (38%)	49 (100%)	0	0	100	100
34	Ah	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
35	Ai	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
36	Aj	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
37	BA	393/403 (98%)	381 (97%)	11 (3%)	1 (0%)	36	22
38	BB	357/427 (84%)	352 (99%)	5 (1%)	0	100	100
39	BC	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
40	BD	210/288 (73%)	203 (97%)	7 (3%)	0	100	100
44	DD	243/257 (95%)	230 (95%)	13 (5%)	0	100	100
All	All	6272/7187 (87%)	6130 (98%)	140 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	BA	303	ALA
21	AU	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	194/215 (90%)	194 (100%)	0	100	100
2	AB	189/223 (85%)	189 (100%)	0	100	100
3	AC	169/171 (99%)	169 (100%)	0	100	100
4	AD	175/181 (97%)	175 (100%)	0	100	100
5	AE	144/149 (97%)	144 (100%)	0	100	100
6	AF	173/177 (98%)	173 (100%)	0	100	100
7	AG	116/161 (72%)	116 (100%)	0	100	100
8	AH	171/172 (99%)	171 (100%)	0	100	100
9	AI	173/174 (99%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AJ	132/163 (81%)	132 (100%)	0	100	100
11	AK	164/165 (99%)	164 (100%)	0	100	100
12	AL	139/175 (79%)	139 (100%)	0	100	100
13	AM	156/157 (99%)	156 (100%)	0	100	100
14	AN	139/140 (99%)	139 (100%)	0	100	100
15	AO	91/115 (79%)	91 (100%)	0	100	100
16	AP	101/107 (94%)	101 (100%)	0	100	100
17	AQ	54/126 (43%)	54 (100%)	0	100	100
18	AR	107/133 (80%)	107 (100%)	0	100	100
19	AS	124/135 (92%)	124 (100%)	0	100	100
20	AT	117/118 (99%)	117 (100%)	0	100	100
21	AU	119/120 (99%)	119 (100%)	0	100	100
22	AV	82/126 (65%)	82 (100%)	0	100	100
23	AW	78/97 (80%)	78 (100%)	0	100	100
24	AX	99/110 (90%)	99 (100%)	0	100	100
25	AY	116/121 (96%)	116 (100%)	0	100	100
26	AZ	88/89 (99%)	88 (100%)	0	100	100
27	Aa	92/100 (92%)	92 (100%)	0	100	100
28	Ab	109/110 (99%)	109 (100%)	0	100	100
29	Ac	86/89 (97%)	86 (100%)	0	100	100
30	Ad	73/80 (91%)	73 (100%)	0	100	100
31	Ae	64/65 (98%)	64 (100%)	0	100	100
32	Af	47/48 (98%)	47 (100%)	0	100	100
33	Ag	47/115 (41%)	47 (100%)	0	100	100
34	Ah	91/94 (97%)	91 (100%)	0	100	100
35	Ai	74/75 (99%)	74 (100%)	0	100	100
36	Aj	109/121 (90%)	109 (100%)	0	100	100
37	BA	344/348 (99%)	344 (100%)	0	100	100
38	BB	299/348 (86%)	299 (100%)	0	100	100
39	BC	247/250 (99%)	247 (100%)	0	100	100
40	BD	192/252 (76%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DD	188/198 (95%)	188 (100%)	0	100	100
All	All	5472/6113 (90%)	5472 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
13	AM	50	GLN
38	BB	347	HIS
19	AS	65	GLN
38	BB	343	GLN
40	BD	101	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
41	DA	3467/5069 (68%)	523 (15%)	13 (0%)
42	DB	118/120 (98%)	8 (6%)	0
43	DC	155/157 (98%)	27 (17%)	0
All	All	3740/5346 (69%)	558 (14%)	13 (0%)

5 of 558 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
41	DA	15	A
41	DA	39	A
41	DA	42	A
41	DA	48	G
41	DA	58	G

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
41	DA	2252	G
41	DA	2562	G
41	DA	4893	A
41	DA	4378	A
41	DA	4699	U

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

122 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$
41	PSU	DA	1683	41,46	18,21,22	1.35	3 (16%)	22,30,33	1.55	3 (13%)
41	A2M	DA	1871	41,45	22,25,26	3.42	7 (31%)	31,36,39	2.78	12 (38%)
41	OMC	DA	2804	41	19,22,23	3.11	8 (42%)	26,31,34	0.60	0
41	PSU	DA	3920	41,45	18,21,22	1.33	3 (16%)	22,30,33	1.44	3 (13%)
41	PSU	DA	3695	41	18,21,22	1.36	3 (16%)	22,30,33	1.37	3 (13%)
41	OMU	DA	4227	41	19,22,23	0.77	0	26,31,34	1.23	4 (15%)
41	OMC	DA	3887	41	19,22,23	3.13	8 (42%)	26,31,34	0.62	0
41	OMU	DA	2415	41	19,22,23	0.79	1 (5%)	26,31,34	1.09	2 (7%)
41	UR3	DA	4530	41	19,22,23	3.04	8 (42%)	26,32,35	1.42	3 (11%)
41	PSU	DA	4500	41	18,21,22	1.32	4 (22%)	22,30,33	1.51	3 (13%)
41	PSU	DA	1781	41	18,21,22	1.30	2 (11%)	22,30,33	1.60	4 (18%)
41	OMG	DA	4392	41	23,26,27	2.54	7 (30%)	33,38,41	1.82	10 (30%)
41	PSU	DA	3639	41	18,21,22	1.32	2 (11%)	22,30,33	1.44	3 (13%)
41	OMC	DA	2824	41	19,22,23	3.16	8 (42%)	26,31,34	0.74	0
41	PSU	DA	3884	41	18,21,22	1.28	1 (5%)	22,30,33	1.60	4 (18%)
41	PSU	DA	3637	41,46	18,21,22	1.21	1 (5%)	22,30,33	1.59	5 (22%)
41	5MC	DA	4447	41,46	18,22,23	3.53	7 (38%)	26,32,35	1.12	1 (3%)
41	OMC	DA	2422	41,45	19,22,23	3.15	8 (42%)	26,31,34	0.66	0
41	A2M	DA	2815	41,45	22,25,26	3.36	7 (31%)	31,36,39	2.75	15 (48%)
41	OMG	DA	3669	41	23,26,27	2.54	7 (30%)	33,38,41	1.90	10 (30%)
41	OMG	DA	3744	41	23,26,27	2.52	7 (30%)	33,38,41	1.78	9 (27%)
41	A2M	DA	2401	41	22,25,26	3.41	7 (31%)	31,36,39	2.74	11 (35%)
41	A2M	DA	2787	41	22,25,26	3.35	8 (36%)	31,36,39	2.61	10 (32%)
41	OMG	DA	1522	41	23,26,27	2.53	7 (30%)	33,38,41	1.86	10 (30%)
41	OMG	DA	4370	41	23,26,27	2.53	7 (30%)	33,38,41	1.79	9 (27%)
41	PSU	DA	2508	41	18,21,22	1.28	2 (11%)	22,30,33	1.57	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	PSU	DA	2632	41	18,21,22	1.36	4 (22%)	22,30,33	1.46	3 (13%)
41	PSU	DA	3715	41	18,21,22	1.36	3 (16%)	22,30,33	1.47	4 (18%)
41	PSU	DA	1744	41	18,21,22	1.30	2 (11%)	22,30,33	1.58	4 (18%)
41	OMG	DA	4637	41	23,26,27	2.50	7 (30%)	33,38,41	1.84	10 (30%)
41	PSU	DA	4579	41	18,21,22	1.29	2 (11%)	22,30,33	1.49	3 (13%)
41	OMG	DA	4196	41	23,26,27	2.53	7 (30%)	33,38,41	1.84	7 (21%)
41	PSU	DA	4353	41	18,21,22	1.29	2 (11%)	22,30,33	1.61	4 (18%)
41	OMG	DA	3627	41	23,26,27	2.52	7 (30%)	33,38,41	1.86	10 (30%)
41	A2M	DA	4571	41	22,25,26	3.38	8 (36%)	31,36,39	3.04	18 (58%)
41	OMG	DA	2424	41	23,26,27	2.54	7 (30%)	33,38,41	1.85	10 (30%)
41	A2M	DA	3785	41	22,25,26	3.39	9 (40%)	31,36,39	2.78	12 (38%)
41	PSU	DA	3822	41	18,21,22	1.35	3 (16%)	22,30,33	1.28	4 (18%)
41	OMU	DA	3925	41	19,22,23	0.85	2 (10%)	26,31,34	1.22	2 (7%)
41	1MA	DA	1322	41,45	21,25,26	2.90	5 (23%)	31,37,40	2.05	8 (25%)
41	OMC	DA	3808	41	19,22,23	3.12	8 (42%)	26,31,34	0.74	0
41	A2M	DA	1524	41	22,25,26	3.40	9 (40%)	31,36,39	2.77	13 (41%)
41	OMG	DA	1316	41	23,26,27	2.53	7 (30%)	33,38,41	1.81	9 (27%)
41	A2M	DA	3830	41	22,25,26	3.40	8 (36%)	31,36,39	2.74	12 (38%)
41	PSU	DA	4689	41	18,21,22	1.23	1 (5%)	22,30,33	1.56	3 (13%)
41	PSU	DA	2839	41	18,21,22	1.31	1 (5%)	22,30,33	1.54	3 (13%)
41	OMG	DA	3899	41,45	23,26,27	2.53	7 (30%)	33,38,41	1.82	9 (27%)
41	A2M	DA	3825	41	22,25,26	3.41	7 (31%)	31,36,39	2.81	13 (41%)
41	PSU	DA	4420	41	18,21,22	1.28	3 (16%)	22,30,33	1.27	3 (13%)
41	A2M	DA	2363	41,45	22,25,26	3.38	7 (31%)	31,36,39	2.77	13 (41%)
41	PSU	DA	4457	41	18,21,22	1.34	3 (16%)	22,30,33	1.34	3 (13%)
41	OMG	DA	4623	41	23,26,27	2.53	7 (30%)	33,38,41	1.83	10 (30%)
41	PSU	DA	4972	41	18,21,22	1.35	3 (16%)	22,30,33	1.56	3 (13%)
41	PSU	DA	4576	41	18,21,22	1.29	2 (11%)	22,30,33	1.45	3 (13%)
41	PSU	DA	1779	41	18,21,22	1.32	2 (11%)	22,30,33	1.54	3 (13%)
37	HIC	BA	245	37	10,11,12	0.47	0	8,14,16	0.59	0
41	OMG	DA	4618	41	23,26,27	2.51	7 (30%)	33,38,41	1.83	9 (27%)
41	PSU	DA	4299	41	18,21,22	1.29	1 (5%)	22,30,33	1.54	3 (13%)
41	A2M	DA	3718	41	22,25,26	3.40	7 (31%)	31,36,39	2.81	14 (45%)
41	OMG	DA	2364	41,45	23,26,27	2.50	7 (30%)	33,38,41	1.81	10 (30%)
43	PSU	DC	69	43	18,21,22	1.29	2 (11%)	22,30,33	1.23	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	OMC	DA	3701	41,46	19,22,23	3.10	8 (42%)	26,31,34	0.73	0
41	PSU	DA	4361	41	18,21,22	1.30	2 (11%)	22,30,33	1.58	4 (18%)
41	PSU	DA	5001	41	18,21,22	1.36	3 (16%)	22,30,33	1.44	4 (18%)
41	OMG	DA	4499	41	23,26,27	2.53	7 (30%)	33,38,41	1.90	9 (27%)
41	PSU	DA	3844	41	18,21,22	1.31	2 (11%)	22,30,33	1.50	3 (13%)
41	PSU	DA	1862	41	18,21,22	1.27	2 (11%)	22,30,33	1.59	4 (18%)
41	PSU	DA	4312	41	18,21,22	1.34	3 (16%)	22,30,33	1.56	3 (13%)
41	5MC	DA	3782	41,45	18,22,23	3.56	7 (38%)	26,32,35	0.97	2 (7%)
41	PSU	DA	4521	41,45	18,21,22	1.33	3 (16%)	22,30,33	1.54	4 (18%)
41	OMC	DA	4456	41	19,22,23	3.12	8 (42%)	26,31,34	0.68	0
41	PSU	DA	4403	41	18,21,22	1.33	3 (16%)	22,30,33	1.56	3 (13%)
41	PSU	DA	4532	41	18,21,22	1.32	3 (16%)	22,30,33	1.58	4 (18%)
41	OMU	DA	4498	41	19,22,23	0.81	1 (5%)	26,31,34	1.16	3 (11%)
41	OMG	DA	2876	41	23,26,27	2.56	7 (30%)	33,38,41	1.89	9 (27%)
41	OMC	DA	4536	41	19,22,23	3.10	8 (42%)	26,31,34	0.68	0
41	OMC	DA	1881	41,45	19,22,23	3.13	8 (42%)	26,31,34	0.78	0
41	A2M	DA	1534	41,45	22,25,26	3.52	8 (36%)	31,36,39	2.74	11 (35%)
41	PSU	DA	1677	41	18,21,22	1.47	4 (22%)	22,30,33	1.61	3 (13%)
41	6MZ	DA	4220	41	22,25,26	3.78	8 (36%)	30,36,39	2.44	12 (40%)
41	OMC	DA	2861	41	19,22,23	3.17	8 (42%)	26,31,34	0.66	0
41	PSU	DA	4493	41,46	18,21,22	1.32	3 (16%)	22,30,33	1.58	4 (18%)
41	PSU	DA	4552	41	18,21,22	1.36	3 (16%)	22,30,33	1.52	2 (9%)
41	PSU	DA	224	41	18,21,22	1.37	4 (22%)	22,30,33	1.58	4 (18%)
41	PSU	DA	1792	41	18,21,22	1.29	1 (5%)	22,30,33	1.57	4 (18%)
41	OMG	DA	4228	41	23,26,27	2.50	7 (30%)	33,38,41	1.94	11 (33%)
41	OMC	DA	2351	41,45	19,22,23	3.10	8 (42%)	26,31,34	0.81	1 (3%)
41	PSU	DA	1782	41	18,21,22	1.27	2 (11%)	22,30,33	1.59	4 (18%)
41	PSU	DA	4431	41	18,21,22	1.29	3 (16%)	22,30,33	1.57	3 (13%)
33	MLZ	Ag	98	33	8,9,10	0.76	0	4,9,11	0.74	0
41	PSU	DA	3851	41	18,21,22	1.37	4 (22%)	22,30,33	1.49	4 (18%)
21	V5N	AU	39	21	9,11,12	1.59	2 (22%)	9,14,16	1.95	3 (33%)
41	OMC	DA	3869	41	19,22,23	3.14	8 (42%)	26,31,34	0.66	0
41	OMG	DA	3792	41	23,26,27	2.55	7 (30%)	33,38,41	1.83	7 (21%)
41	A2M	DA	3867	41	22,25,26	3.43	7 (31%)	31,36,39	2.83	13 (41%)
41	PSU	DA	4628	41	18,21,22	1.36	3 (16%)	22,30,33	1.51	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	OMU	DA	4306	41	19,22,23	0.75	0	26,31,34	1.26	2 (7%)
41	OMU	DA	4620	41	19,22,23	0.74	0	26,31,34	1.23	3 (11%)
41	PSU	DA	4293	41	18,21,22	1.28	1 (5%)	22,30,33	1.57	4 (18%)
41	PSU	DA	4471	41	18,21,22	1.34	4 (22%)	22,30,33	1.57	3 (13%)
41	PSU	DA	4423	41	18,21,22	1.31	1 (5%)	22,30,33	1.61	4 (18%)
41	PSU	DA	1536	41	18,21,22	1.32	2 (11%)	22,30,33	1.57	4 (18%)
41	OMG	DA	1625	41	23,26,27	2.55	7 (30%)	33,38,41	1.81	8 (24%)
41	PSU	DA	1860	41	18,21,22	1.26	1 (5%)	22,30,33	1.68	4 (18%)
41	A2M	DA	1326	41	22,25,26	3.44	7 (31%)	31,36,39	2.74	13 (41%)
41	PSU	DA	4296	41	18,21,22	1.34	3 (16%)	22,30,33	1.54	4 (18%)
41	PSU	DA	4442	41	18,21,22	1.28	2 (11%)	22,30,33	1.26	3 (13%)
41	PSU	DA	4673	41,45	18,21,22	1.35	2 (11%)	22,30,33	1.47	3 (13%)
41	OMU	DA	2837	41	19,22,23	0.83	1 (5%)	26,31,34	1.30	3 (11%)
41	OMC	DA	2365	41	19,22,23	3.11	8 (42%)	26,31,34	0.64	0
41	A2M	DA	4523	41,45	22,25,26	3.39	7 (31%)	31,36,39	2.89	13 (41%)
41	OMG	DA	4494	41	23,26,27	2.54	7 (30%)	33,38,41	1.82	9 (27%)
41	A2M	DA	1323	41	22,25,26	3.37	7 (31%)	31,36,39	2.78	14 (45%)
41	B8T	DA	1859	41	19,22,23	1.05	1 (5%)	26,31,34	0.78	1 (3%)
41	OMC	DA	3841	41	19,22,23	3.12	8 (42%)	26,31,34	0.57	0
41	A2M	DA	398	41	22,25,26	3.37	7 (31%)	31,36,39	2.92	14 (45%)
43	PSU	DC	55	43	18,21,22	1.31	2 (11%)	22,30,33	1.61	3 (13%)
41	OMC	DA	1340	41	19,22,23	3.11	8 (42%)	26,31,34	0.64	0
43	OMG	DC	75	43	23,26,27	2.53	7 (30%)	33,38,41	1.82	9 (27%)
41	A2M	DA	400	41	22,25,26	3.39	7 (31%)	31,36,39	2.88	13 (41%)
44	V5N	DD	216	44	9,11,12	1.61	2 (22%)	9,14,16	1.87	3 (33%)
41	UY1	DA	3818	41,46	19,22,23	4.30	6 (31%)	22,31,34	2.07	6 (27%)

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
41	PSU	DA	1683	41,46	-	0/7/25/26	0/2/2/2
41	A2M	DA	1871	41,45	-	0/9/27/28	0/3/3/3
41	OMC	DA	2804	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	3920	41,45	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PSU	DA	3695	41	-	0/7/25/26	0/2/2/2
41	OMU	DA	4227	41	-	0/9/27/28	0/2/2/2
41	OMC	DA	3887	41	-	0/9/27/28	0/2/2/2
41	OMU	DA	2415	41	-	0/9/27/28	0/2/2/2
41	UR3	DA	4530	41	-	2/7/25/26	0/2/2/2
41	PSU	DA	4500	41	-	3/7/25/26	0/2/2/2
41	PSU	DA	1781	41	-	1/7/25/26	0/2/2/2
41	OMG	DA	4392	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	3639	41	-	0/7/25/26	0/2/2/2
41	OMC	DA	2824	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	3884	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	3637	41,46	-	0/7/25/26	0/2/2/2
41	5MC	DA	4447	41,46	-	4/7/25/26	0/2/2/2
41	OMC	DA	2422	41,45	-	2/9/27/28	0/2/2/2
41	A2M	DA	2815	41,45	-	1/9/27/28	0/3/3/3
41	OMG	DA	3669	41	-	2/9/27/28	0/3/3/3
41	OMG	DA	3744	41	-	0/9/27/28	0/3/3/3
41	A2M	DA	2401	41	-	2/9/27/28	0/3/3/3
41	A2M	DA	2787	41	-	3/9/27/28	0/3/3/3
41	OMG	DA	1522	41	-	0/9/27/28	0/3/3/3
41	OMG	DA	4370	41	-	1/9/27/28	0/3/3/3
41	PSU	DA	2508	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	2632	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	3715	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	1744	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	4637	41	-	1/9/27/28	0/3/3/3
41	PSU	DA	4579	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	4196	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	4353	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	3627	41	-	0/9/27/28	0/3/3/3
41	A2M	DA	4571	41	-	2/9/27/28	0/3/3/3
41	OMG	DA	2424	41	-	0/9/27/28	0/3/3/3
41	A2M	DA	3785	41	-	2/9/27/28	0/3/3/3
41	PSU	DA	3822	41	-	0/7/25/26	0/2/2/2
41	OMU	DA	3925	41	-	0/9/27/28	0/2/2/2
41	1MA	DA	1322	41,45	-	1/7/25/26	0/3/3/3
41	OMC	DA	3808	41	-	0/9/27/28	0/2/2/2
41	A2M	DA	1524	41	-	0/9/27/28	0/3/3/3
41	OMG	DA	1316	41	-	0/9/27/28	0/3/3/3
41	A2M	DA	3830	41	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PSU	DA	4689	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	2839	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	3899	41,45	-	0/9/27/28	0/3/3/3
41	A2M	DA	3825	41	-	1/9/27/28	0/3/3/3
41	PSU	DA	4420	41	-	3/7/25/26	0/2/2/2
41	A2M	DA	2363	41,45	-	1/9/27/28	0/3/3/3
41	PSU	DA	4457	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	4623	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	4972	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4576	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	1779	41	-	0/7/25/26	0/2/2/2
37	HIC	BA	245	37	-	1/5/6/8	0/1/1/1
41	OMG	DA	4618	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	4299	41	-	0/7/25/26	0/2/2/2
41	A2M	DA	3718	41	-	1/9/27/28	0/3/3/3
41	OMG	DA	2364	41,45	-	0/9/27/28	0/3/3/3
43	PSU	DC	69	43	-	0/7/25/26	0/2/2/2
41	OMC	DA	3701	41,46	-	4/9/27/28	0/2/2/2
41	PSU	DA	4361	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	5001	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	4499	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	3844	41	-	1/7/25/26	0/2/2/2
41	PSU	DA	1862	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4312	41	-	0/7/25/26	0/2/2/2
41	5MC	DA	3782	41,45	-	0/7/25/26	0/2/2/2
41	PSU	DA	4521	41,45	-	1/7/25/26	0/2/2/2
41	OMC	DA	4456	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	4403	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4532	41	-	0/7/25/26	0/2/2/2
41	OMU	DA	4498	41	-	2/9/27/28	0/2/2/2
41	OMG	DA	2876	41	-	1/9/27/28	0/3/3/3
41	OMC	DA	4536	41	-	0/9/27/28	0/2/2/2
41	OMC	DA	1881	41,45	-	0/9/27/28	0/2/2/2
41	A2M	DA	1534	41,45	-	3/9/27/28	0/3/3/3
41	PSU	DA	1677	41	-	0/7/25/26	0/2/2/2
41	6MZ	DA	4220	41	-	0/9/27/28	0/3/3/3
41	OMC	DA	2861	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	4493	41,46	-	0/7/25/26	0/2/2/2
41	PSU	DA	4552	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	224	41	-	2/7/25/26	0/2/2/2
41	PSU	DA	1792	41	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	OMG	DA	4228	41	-	0/9/27/28	0/3/3/3
41	OMC	DA	2351	41,45	-	3/9/27/28	0/2/2/2
41	PSU	DA	1782	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4431	41	-	0/7/25/26	0/2/2/2
33	MLZ	Ag	98	33	-	1/7/8/10	-
41	PSU	DA	3851	41	-	0/7/25/26	0/2/2/2
21	V5N	AU	39	21	-	2/9/10/12	0/1/1/1
41	OMC	DA	3869	41	-	0/9/27/28	0/2/2/2
41	OMG	DA	3792	41	-	2/9/27/28	0/3/3/3
41	A2M	DA	3867	41	-	3/9/27/28	0/3/3/3
41	PSU	DA	4628	41	-	0/7/25/26	0/2/2/2
41	OMU	DA	4306	41	-	0/9/27/28	0/2/2/2
41	OMU	DA	4620	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	4293	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4471	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4423	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	1536	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	1625	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	1860	41	-	0/7/25/26	0/2/2/2
41	A2M	DA	1326	41	-	1/9/27/28	0/3/3/3
41	PSU	DA	4296	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4442	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4673	41,45	-	0/7/25/26	0/2/2/2
41	OMU	DA	2837	41	-	0/9/27/28	0/2/2/2
41	OMC	DA	2365	41	-	0/9/27/28	0/2/2/2
41	A2M	DA	4523	41,45	-	1/9/27/28	0/3/3/3
41	OMG	DA	4494	41	-	2/9/27/28	0/3/3/3
41	A2M	DA	1323	41	-	2/9/27/28	0/3/3/3
41	B8T	DA	1859	41	-	1/7/27/28	0/2/2/2
41	OMC	DA	3841	41	-	0/9/27/28	0/2/2/2
41	A2M	DA	398	41	-	1/9/27/28	0/3/3/3
43	PSU	DC	55	43	-	0/7/25/26	0/2/2/2
41	OMC	DA	1340	41	-	0/9/27/28	0/2/2/2
43	OMG	DC	75	43	-	0/9/27/28	0/3/3/3
41	A2M	DA	400	41	-	1/9/27/28	0/3/3/3
44	V5N	DD	216	44	-	1/9/10/12	0/1/1/1
41	UY1	DA	3818	41,46	-	2/9/27/28	0/2/2/2

The worst 5 of 573 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	DA	3818	UY1	C6-C5	12.23	1.49	1.35
41	DA	4220	6MZ	C6-N6	11.54	1.46	1.34
41	DA	3818	UY1	C2-N1	9.54	1.49	1.36
41	DA	4447	5MC	C6-C5	9.24	1.49	1.34
41	DA	3782	5MC	C6-C5	9.19	1.49	1.34

The worst 5 of 659 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	DA	3785	A2M	C5-C4-N3	-6.51	118.25	126.75
41	DA	1534	A2M	C5-C4-N3	-6.31	118.51	126.75
41	DA	3867	A2M	C5-C4-N3	-6.29	118.54	126.75
41	DA	4571	A2M	C5-C4-N3	-6.25	118.59	126.75
41	DA	3718	A2M	C5-C4-N3	-6.17	118.70	126.75

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	Ag	98	MLZ	O-C-CA-CB
37	BA	245	HIC	O-C-CA-CB
44	DD	216	V5N	O-C-CA-CB
41	DA	224	PSU	C2'-C1'-C5-C4
41	DA	398	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

33 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	DA	2415	OMU	1	0
41	DA	4500	PSU	1	0
41	DA	4447	5MC	1	0
41	DA	2815	A2M	2	0
41	DA	3669	OMG	1	0
41	DA	3744	OMG	1	0
41	DA	4637	OMG	1	0
41	DA	4579	PSU	1	0
41	DA	4196	OMG	1	0
41	DA	2424	OMG	1	0
41	DA	3785	A2M	1	0
41	DA	3830	A2M	1	0
41	DA	4689	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	DA	3825	A2M	3	0
41	DA	3718	A2M	4	0
41	DA	4499	OMG	3	0
41	DA	4456	OMC	1	0
41	DA	4498	OMU	4	0
41	DA	2876	OMG	1	0
41	DA	4536	OMC	3	0
41	DA	1881	OMC	1	0
41	DA	1534	A2M	1	0
41	DA	4220	6MZ	1	0
41	DA	2351	OMC	1	0
41	DA	3869	OMC	1	0
41	DA	3792	OMG	1	0
41	DA	4620	OMU	1	0
41	DA	1860	PSU	1	0
41	DA	1326	A2M	1	0
41	DA	1323	A2M	1	0
41	DA	1859	B8T	2	0
41	DA	1340	OMC	3	0
43	DC	75	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 245 ligands modelled in this entry, 232 are monoatomic - leaving 13 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	ATP	DA	5111	-	29,33,33	0.46	0	44,52,52	0.82	3 (6%)
48	PUT	DA	5101	-	5,5,5	0.18	0	4,4,4	0.39	0
49	SPD	DA	5106	-	9,9,9	0.97	0	8,8,8	1.45	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PUT	DA	5102	-	5,5,5	0.27	0	4,4,4	0.40	0
48	PUT	DA	5104	-	5,5,5	0.34	0	4,4,4	0.27	0
48	PUT	DA	5103	-	5,5,5	0.20	0	4,4,4	0.34	0
49	SPD	DA	5107	-	9,9,9	0.45	0	8,8,8	1.40	1 (12%)
49	SPD	DA	5109	-	9,9,9	0.60	0	8,8,8	1.36	1 (12%)
48	PUT	DB	10000	-	5,5,5	0.25	0	4,4,4	0.34	0
51	A1JQ4	DA	5322	46	27,27,27	2.69	9 (33%)	37,46,46	3.10	17 (45%)
49	SPD	DA	5108	-	9,9,9	0.68	0	8,8,8	1.54	1 (12%)
49	SPD	DA	5110	-	9,9,9	0.41	0	8,8,8	1.47	1 (12%)
49	SPD	DA	5105	-	9,9,9	0.30	0	8,8,8	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	ATP	DA	5111	-	-	4/22/38/38	0/3/3/3
48	PUT	DA	5101	-	-	1/3/3/3	-
49	SPD	DA	5106	-	-	2/7/7/7	-
48	PUT	DA	5102	-	-	1/3/3/3	-
48	PUT	DA	5104	-	-	1/3/3/3	-
48	PUT	DA	5103	-	-	0/3/3/3	-
49	SPD	DA	5107	-	-	4/7/7/7	-
49	SPD	DA	5109	-	-	4/7/7/7	-
48	PUT	DB	10000	-	-	1/3/3/3	-
51	A1JQ4	DA	5322	46	-	6/7/72/72	0/5/4/4
49	SPD	DA	5108	-	-	5/7/7/7	-
49	SPD	DA	5110	-	-	6/7/7/7	-
49	SPD	DA	5105	-	-	4/7/7/7	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	DA	5322	A1JQ4	C09-C10	10.64	1.69	1.55
51	DA	5322	A1JQ4	C07-C02	3.83	1.54	1.51
51	DA	5322	A1JQ4	C23-C05	3.49	1.59	1.54
51	DA	5322	A1JQ4	O16-C04	3.09	1.49	1.45
51	DA	5322	A1JQ4	O18-C19	2.95	1.41	1.35

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	DA	5322	A1JQ4	O15-C13-C09	10.26	131.79	118.00
51	DA	5322	A1JQ4	O15-C13-C12	-7.06	102.17	115.59
51	DA	5322	A1JQ4	C14-C13-C09	5.38	137.32	127.57
51	DA	5322	A1JQ4	C13-C09-C05	5.13	109.96	106.90
51	DA	5322	A1JQ4	C01-C02-C07	5.02	119.42	115.93

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

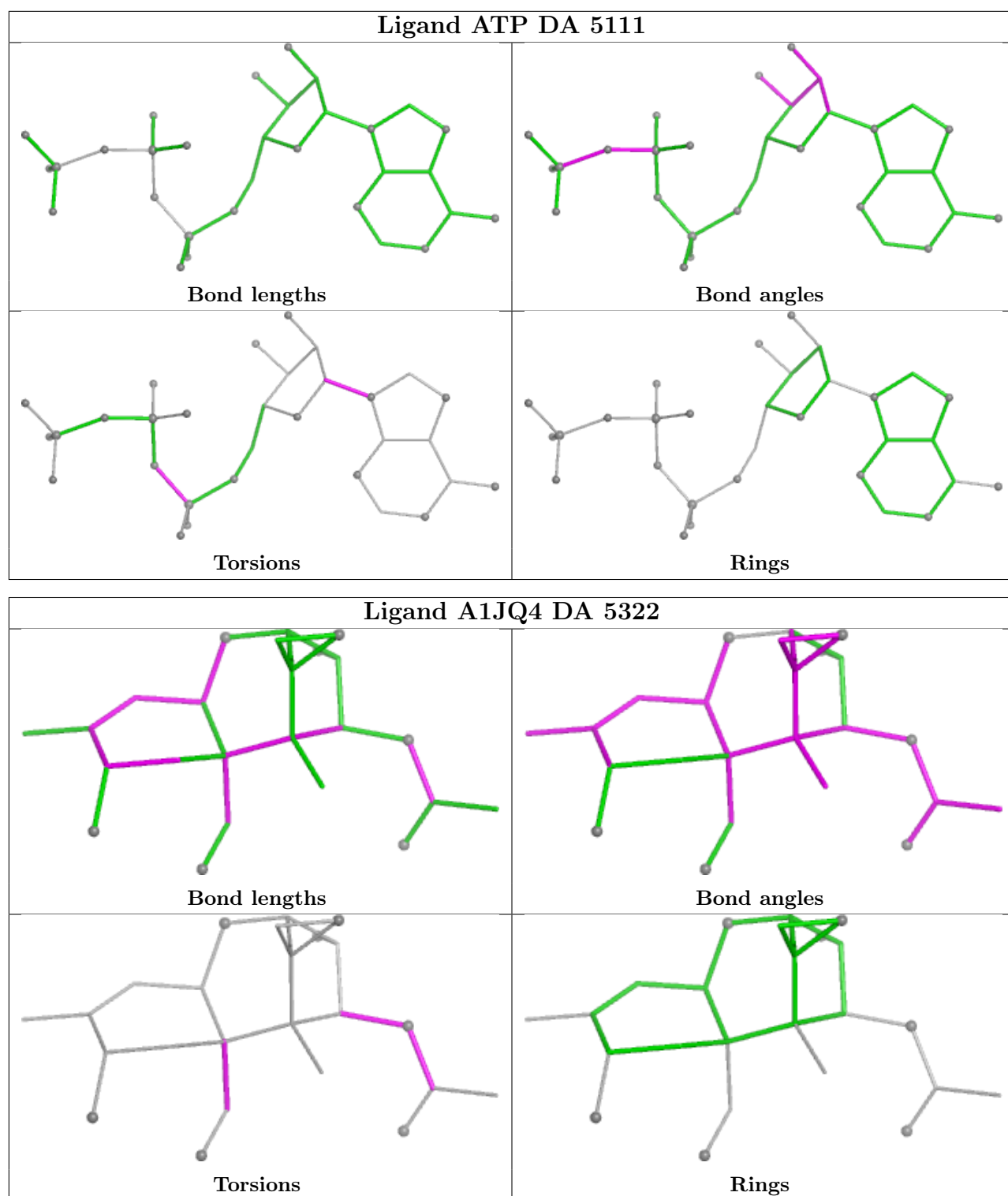
Mol	Chain	Res	Type	Atoms
49	DA	5105	SPD	C8-C7-N6-C5
49	DA	5107	SPD	C4-C5-N6-C7
49	DA	5110	SPD	C4-C5-N6-C7
50	DA	5111	ATP	O4'-C1'-N9-C8
50	DA	5111	ATP	O4'-C1'-N9-C4

There are no ring outliers.

8 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	DA	5111	ATP	3	0
48	DA	5101	PUT	6	0
48	DA	5102	PUT	7	0
48	DA	5104	PUT	3	0
48	DA	5103	PUT	4	0
49	DA	5108	SPD	5	0
49	DA	5110	SPD	18	0
49	DA	5105	SPD	6	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

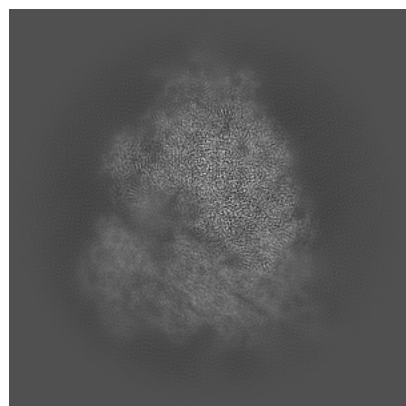
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57201. These allow visual inspection of the internal detail of the map and identification of artifacts.

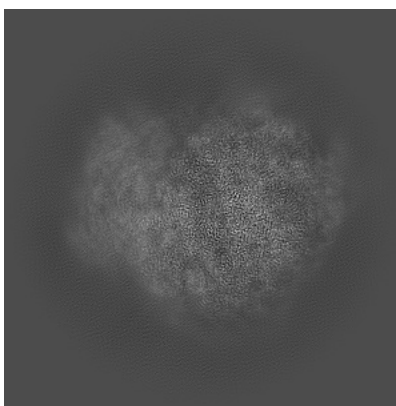
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

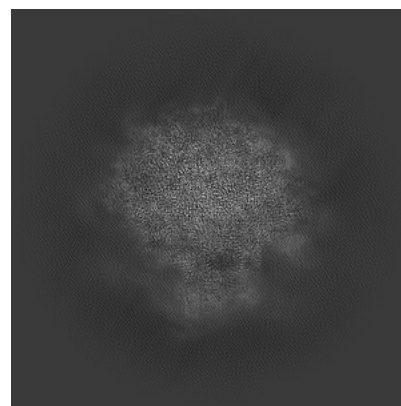
6.1.1 Primary map



X

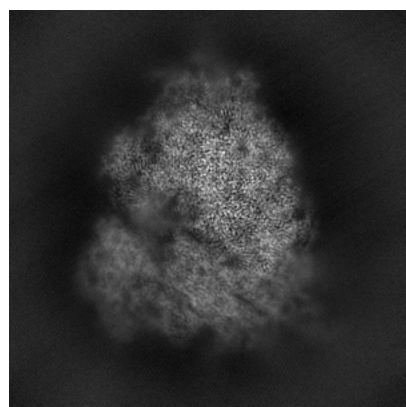


Y

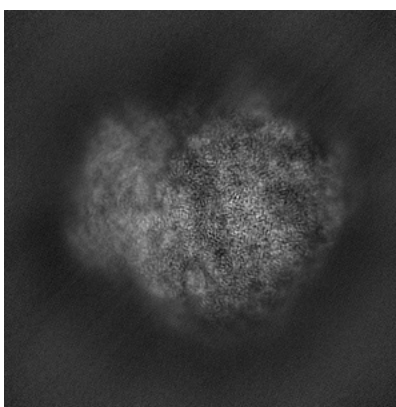


Z

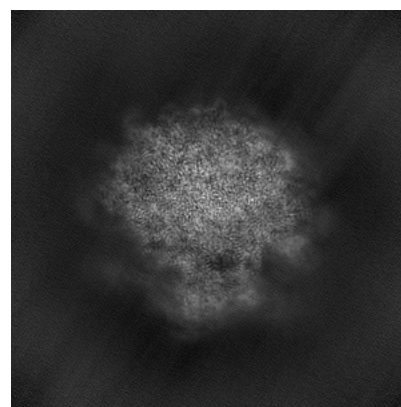
6.1.2 Raw map



X



Y

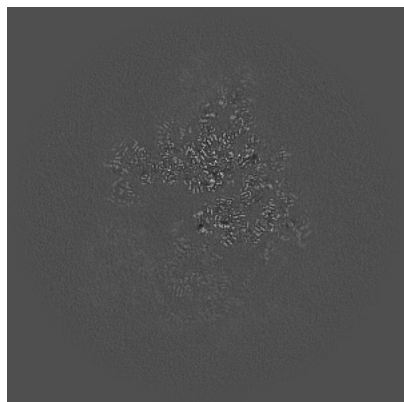


Z

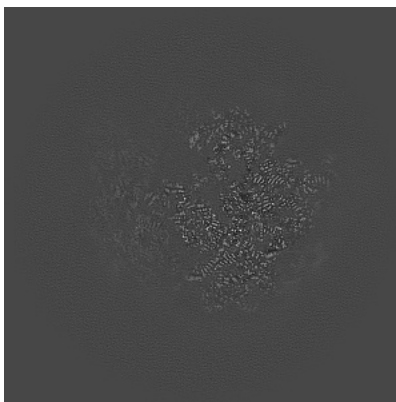
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

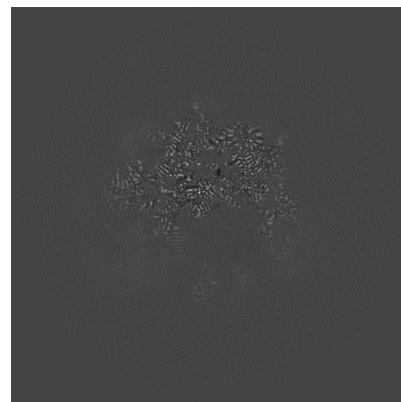
6.2.1 Primary map



X Index: 320

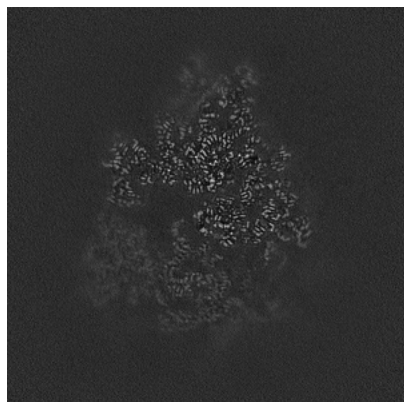


Y Index: 320

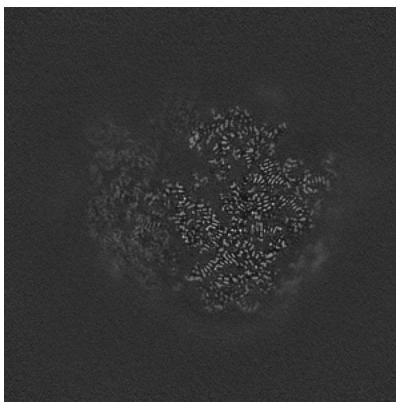


Z Index: 320

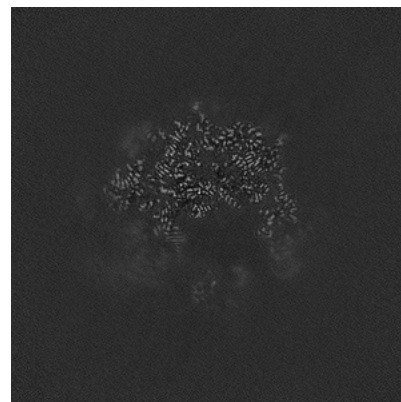
6.2.2 Raw map



X Index: 320



Y Index: 320

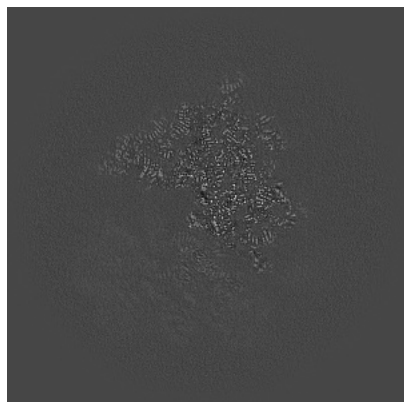


Z Index: 320

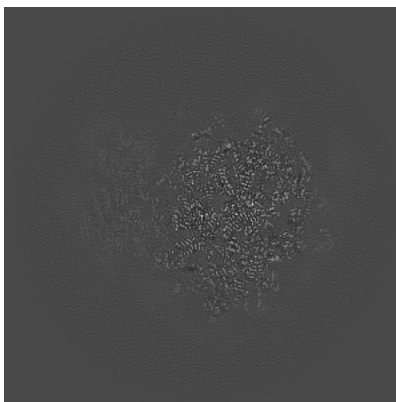
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

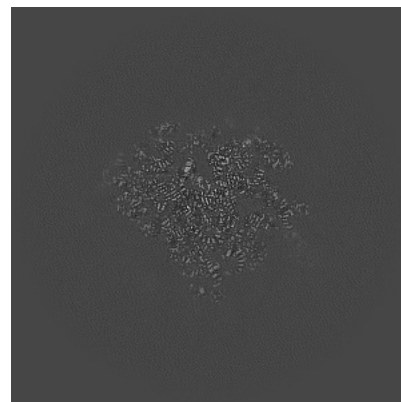
6.3.1 Primary map



X Index: 285

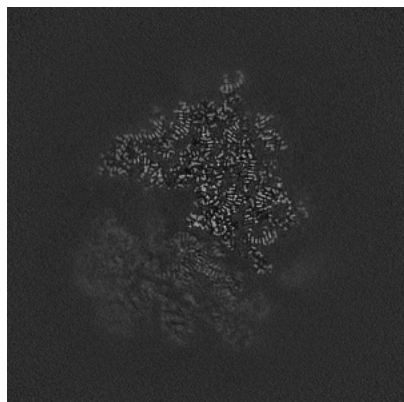


Y Index: 339

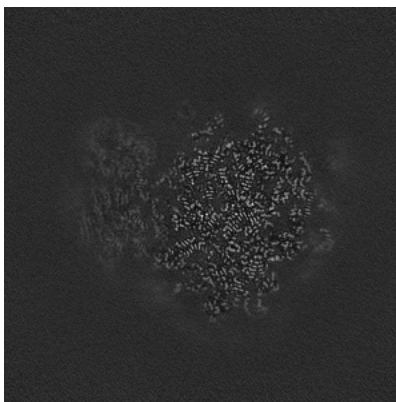


Z Index: 365

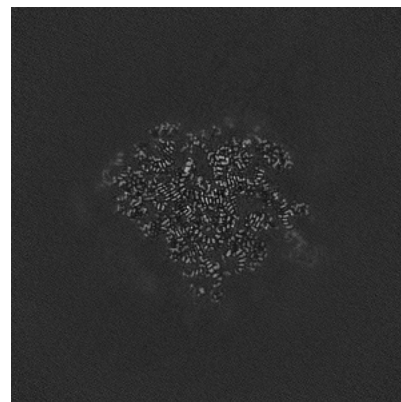
6.3.2 Raw map



X Index: 286



Y Index: 339

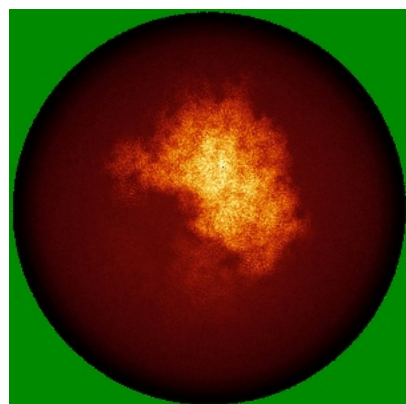


Z Index: 365

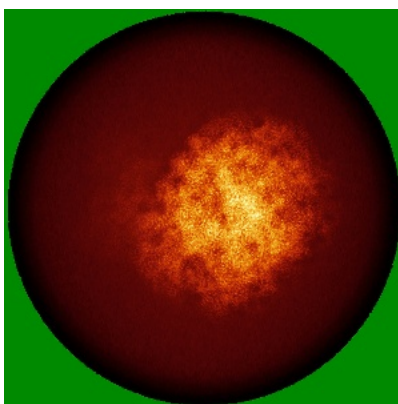
The images above show the largest variance slices of the map in three orthogonal directions.

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

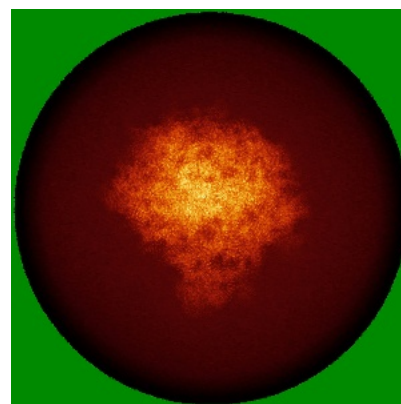
6.4.1 Primary map



X

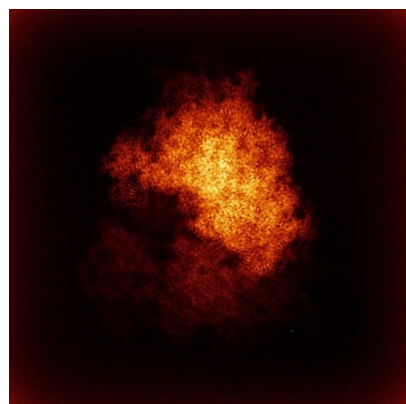


Y

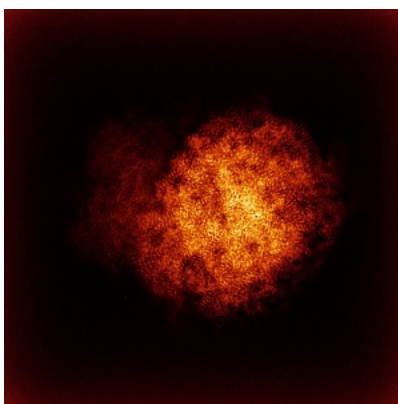


Z

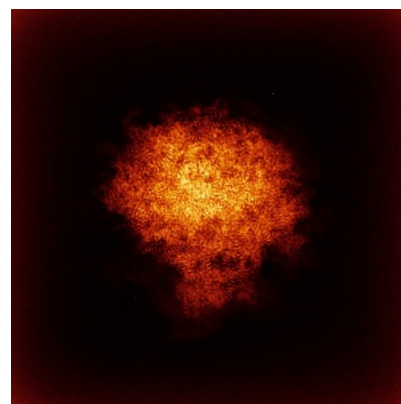
6.4.2 Raw map



X



Y

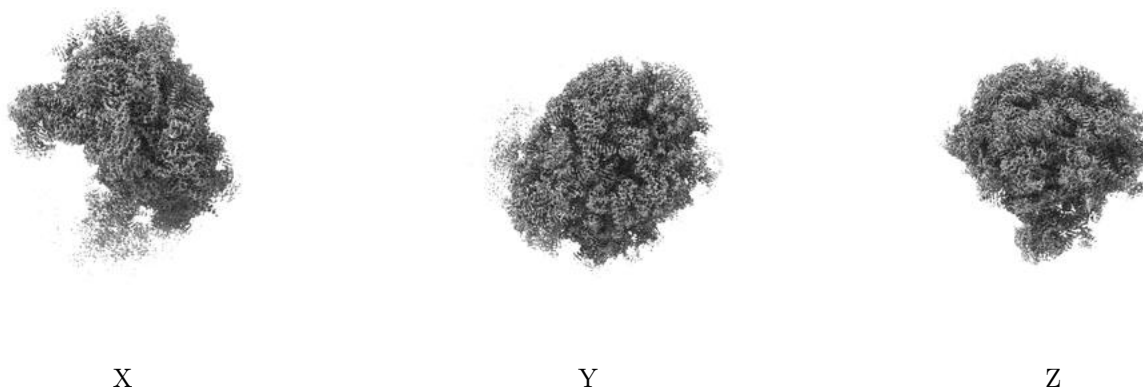


Z

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.

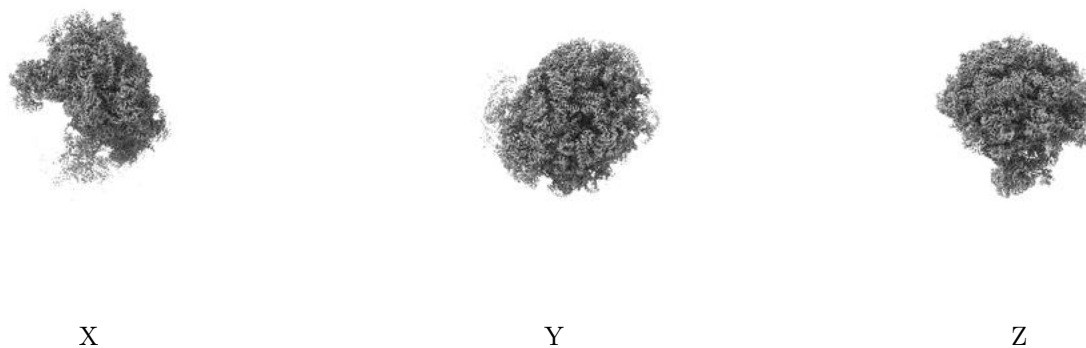
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

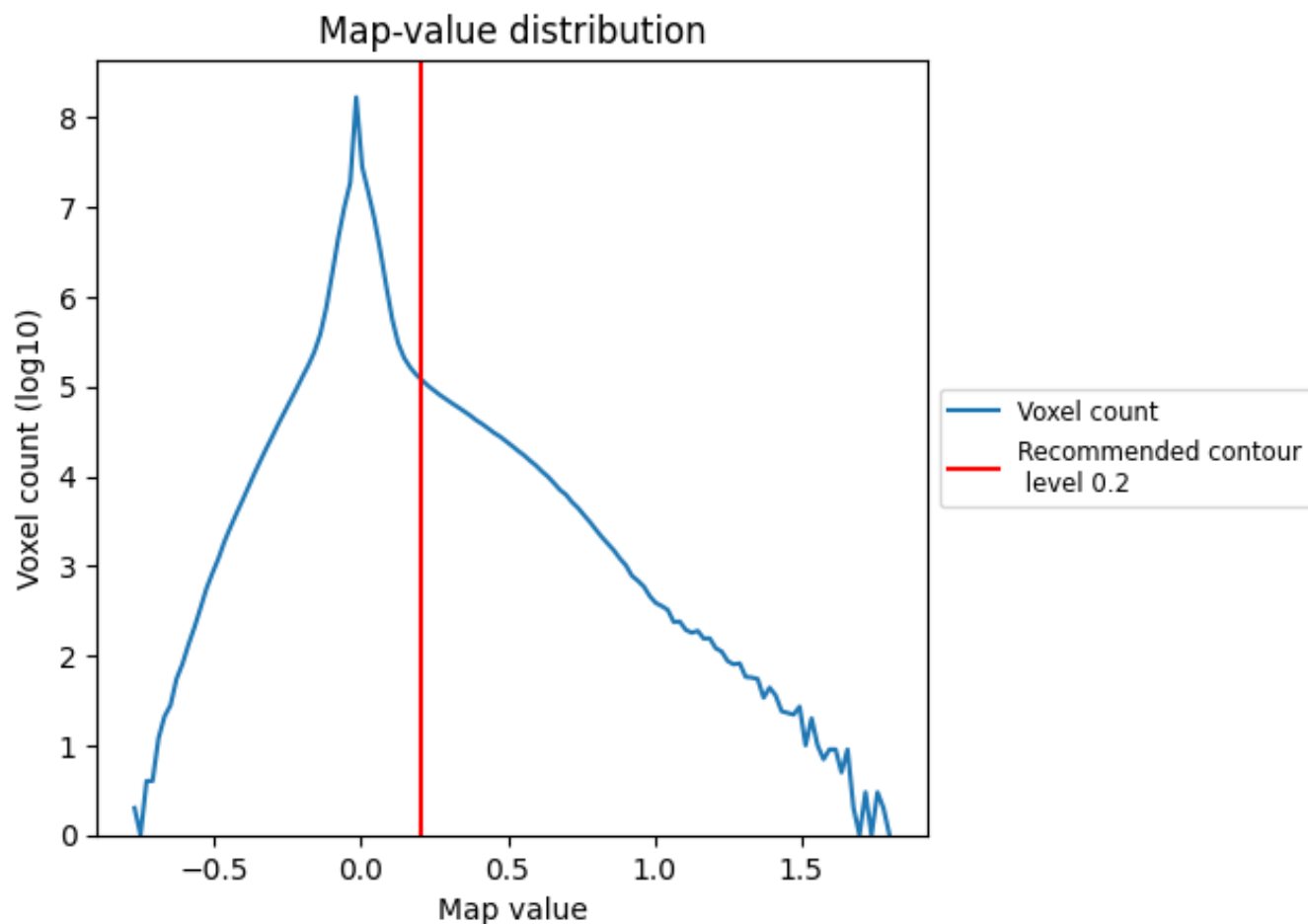
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

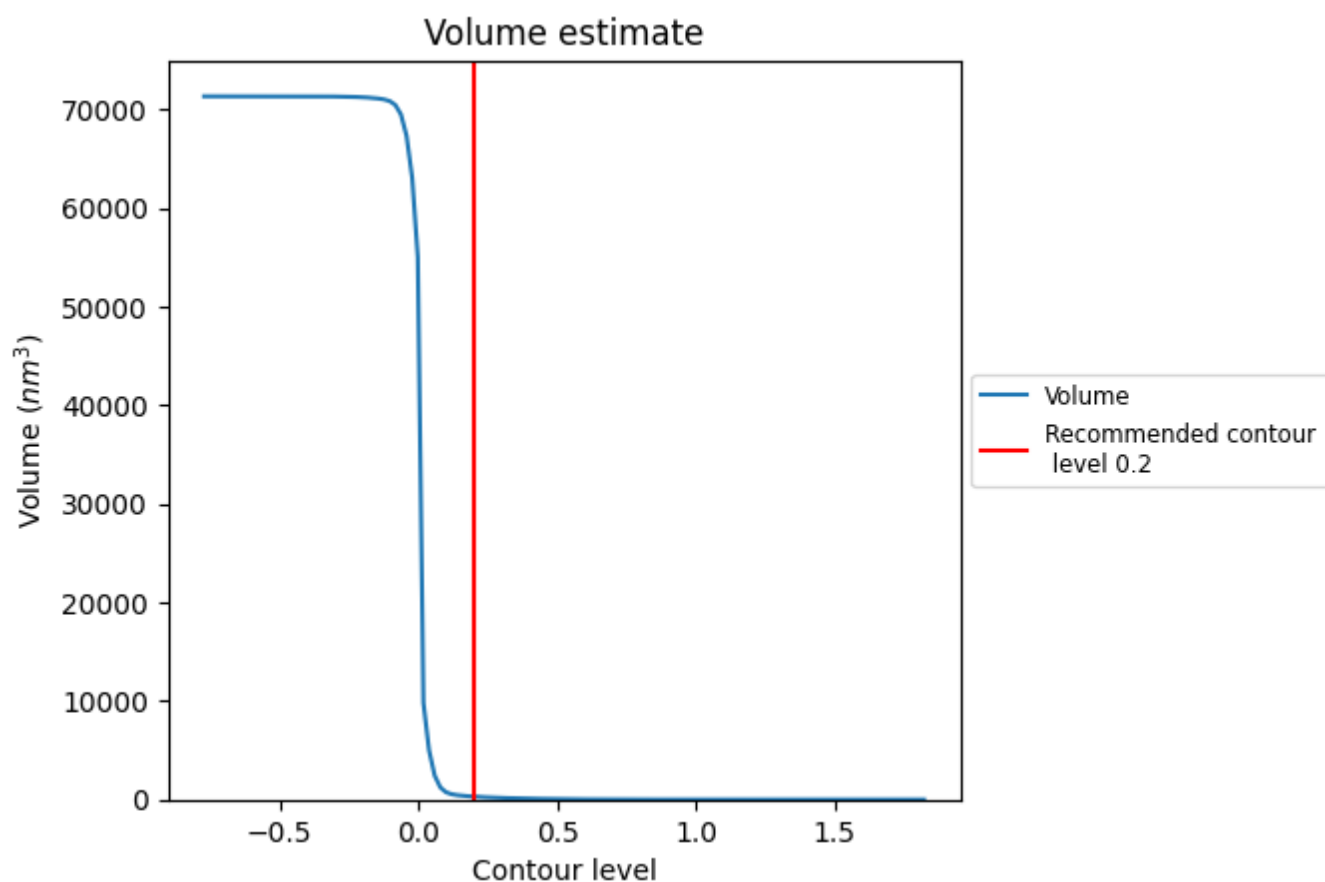
This section contains the results of statistical analysis of the map.

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.

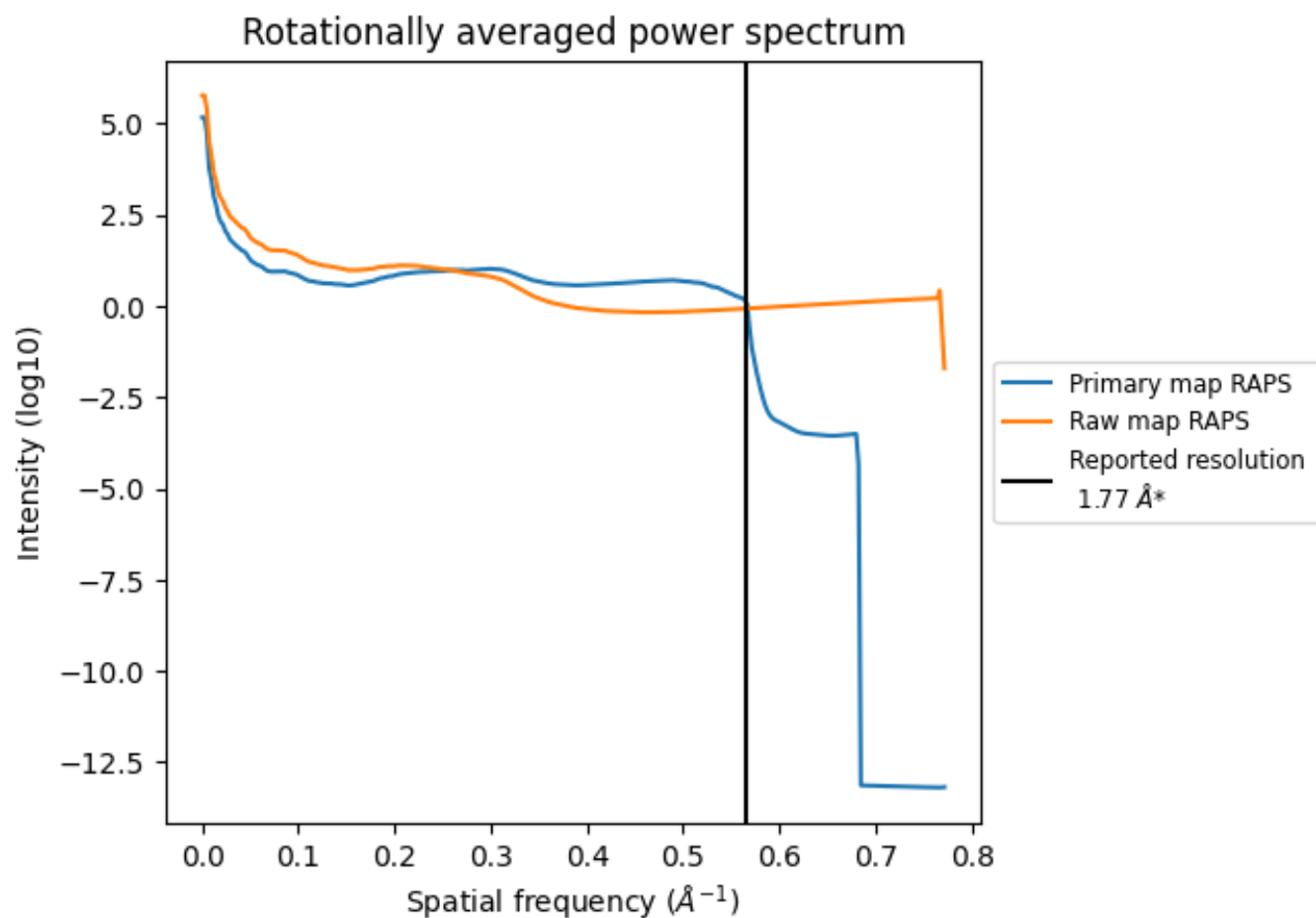
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 298 nm³; this corresponds to an approximate mass of 269 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 ⓘ

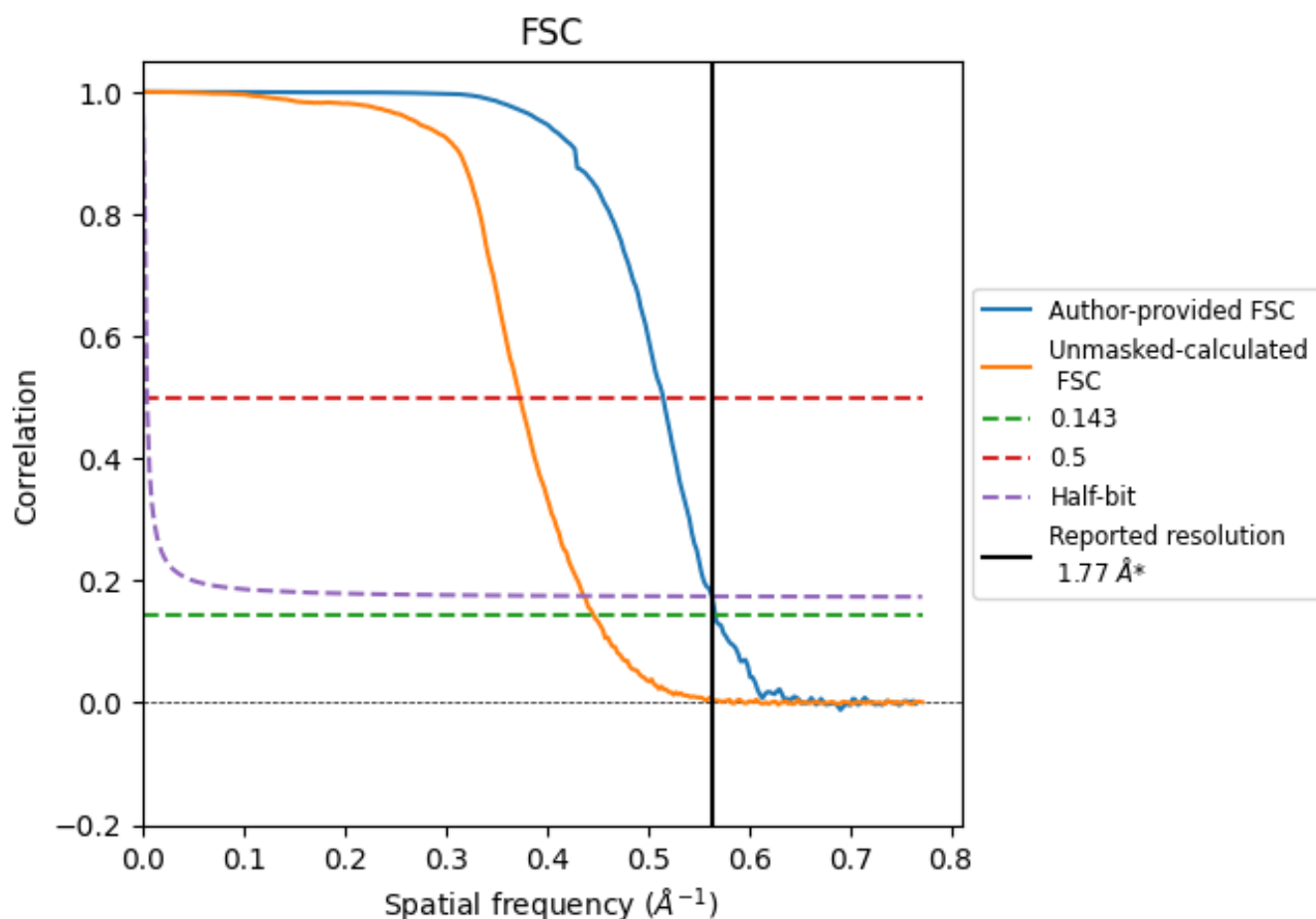


*Reported resolution corresponds to spatial frequency of 0.565 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.565 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

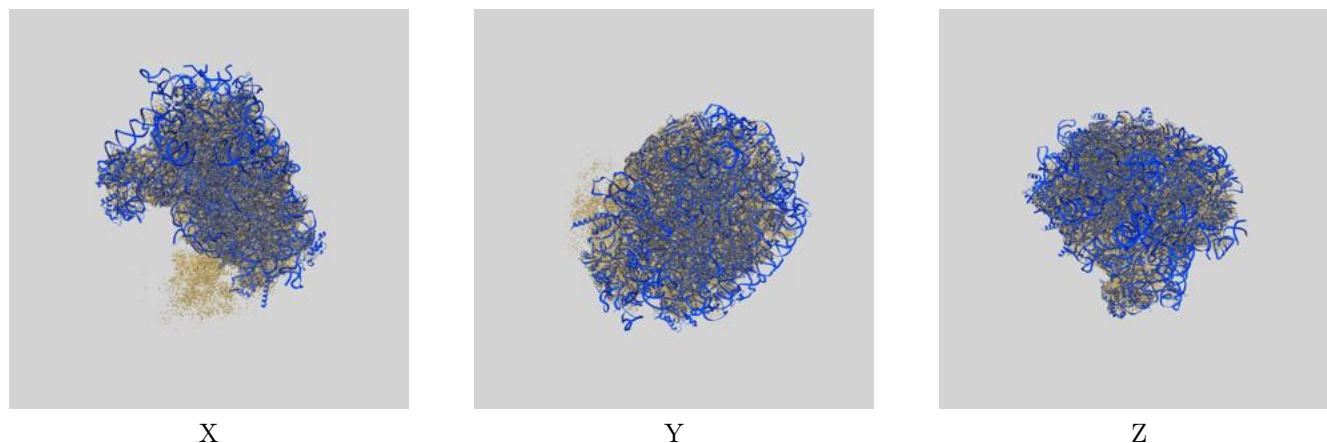
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.77	-	-
Author-provided FSC curve	1.76	1.94	1.77
Unmasked-calculated*	2.24	2.68	2.29

*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 2.24 differs from the reported value 1.77 by more than 10 %

9 Map-model fit [i](#)

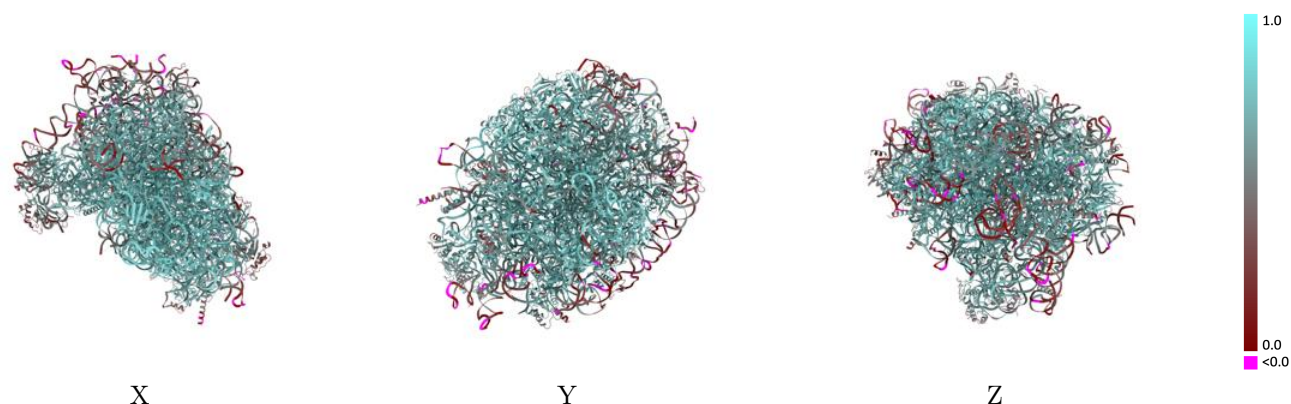
This section contains information regarding the fit between EMDB map EMD-57201 and PDB model 29IW. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



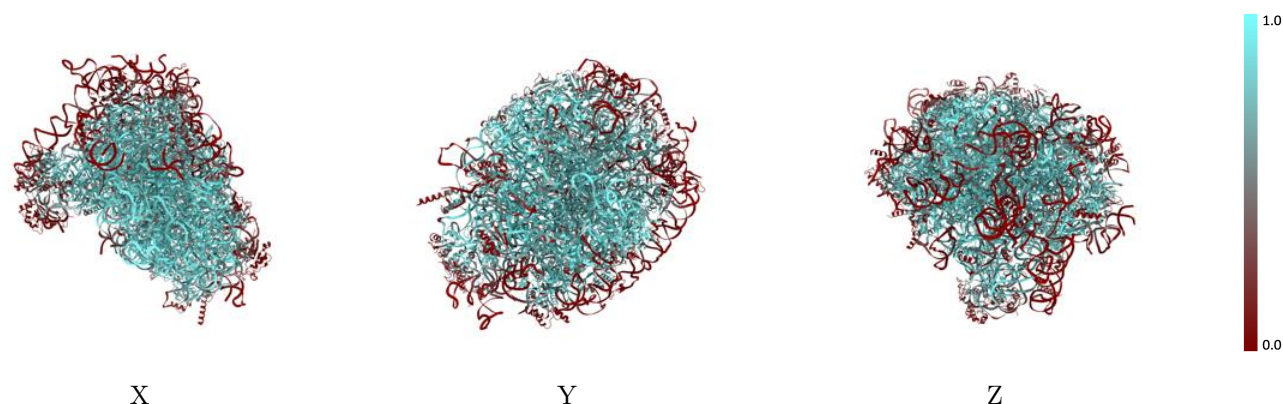
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



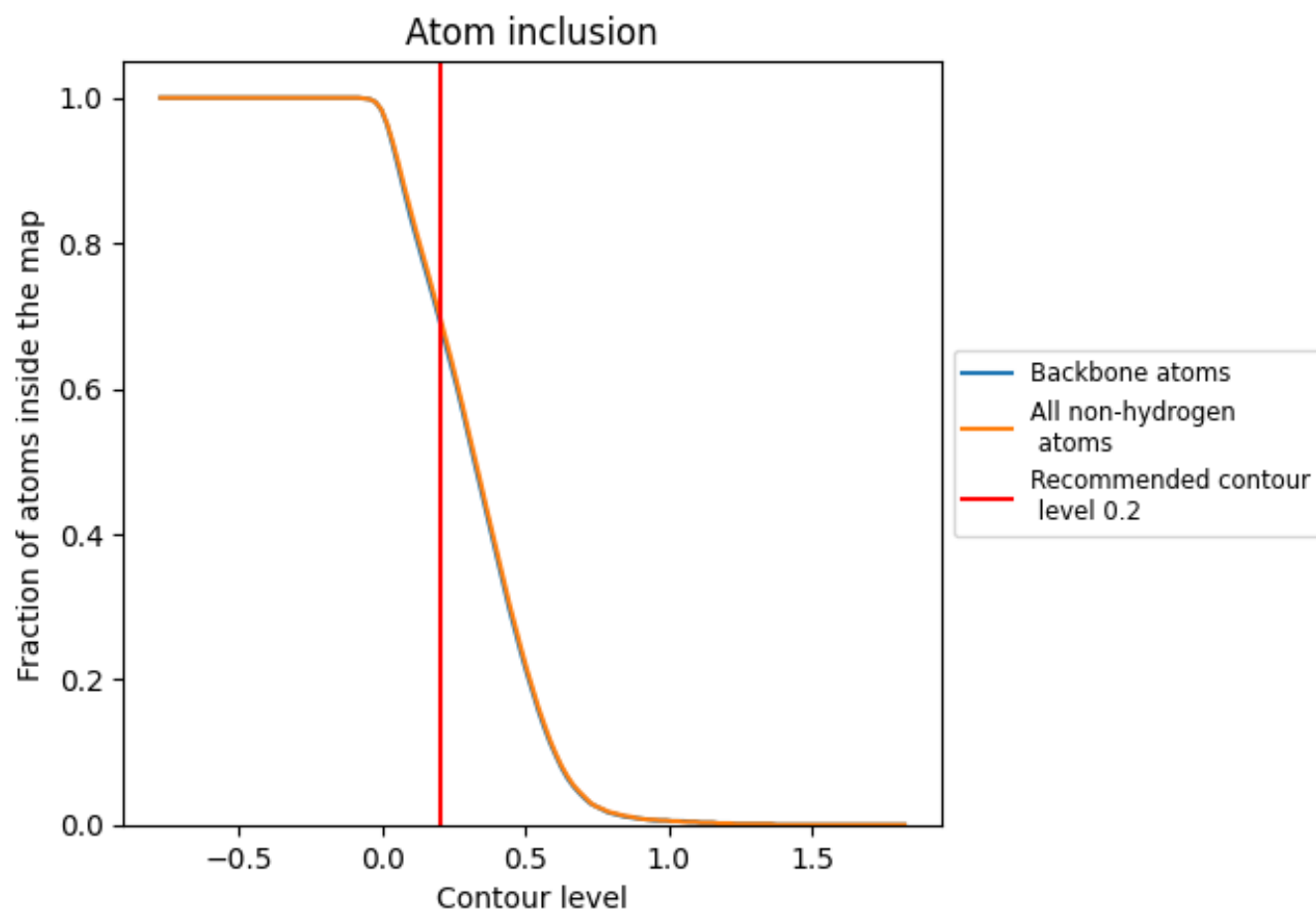
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 70% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7020	 0.6800
AA	 0.8400	 0.7560
AB	 0.4320	 0.5960
AC	 0.6720	 0.7080
AD	 0.6800	 0.7150
AE	 0.1520	 0.4430
AF	 0.6570	 0.6890
AG	 0.6750	 0.6770
AH	 0.9310	 0.7950
AI	 0.7990	 0.7580
AJ	 0.8290	 0.7710
AK	 0.8810	 0.7890
AL	 0.6970	 0.6670
AM	 0.8470	 0.7600
AN	 0.6860	 0.6920
AO	 0.0980	 0.4130
AP	 0.8360	 0.7810
AQ	 0.7500	 0.7270
AR	 0.6800	 0.7100
AS	 0.7170	 0.7190
AT	 0.3840	 0.5860
AU	 0.8460	 0.7720
AV	 0.4610	 0.6110
AW	 0.4720	 0.5820
AX	 0.6390	 0.6530
AY	 0.8370	 0.7760
AZ	 0.8940	 0.7930
Aa	 0.7750	 0.7220
Ab	 0.6190	 0.7010
Ac	 0.5060	 0.6240
Ad	 0.8750	 0.7880
Ae	 0.2060	 0.4720
Af	 0.7680	 0.7370
Ag	 0.7340	 0.7380
Ah	 0.7600	 0.7480



Continued on next page...

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Chain	Atom inclusion	Q-score
Ai	 0.7750	 0.7240
Aj	 0.7890	 0.7410
BA	 0.7920	 0.7520
BB	 0.8220	 0.7590
BC	 0.4300	 0.5800
BD	 0.4740	 0.6300
DA	 0.7060	 0.6670
DB	 0.7540	 0.6950
DC	 0.7520	 0.6670
DD	 0.8900	 0.7820