



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 01:18 PM UTC

PDB ID : 8FKW / pdb_00008fkw
EMDB ID : EMD-29259
Title : Human nucleolar pre-60S ribosomal subunit (State D2)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

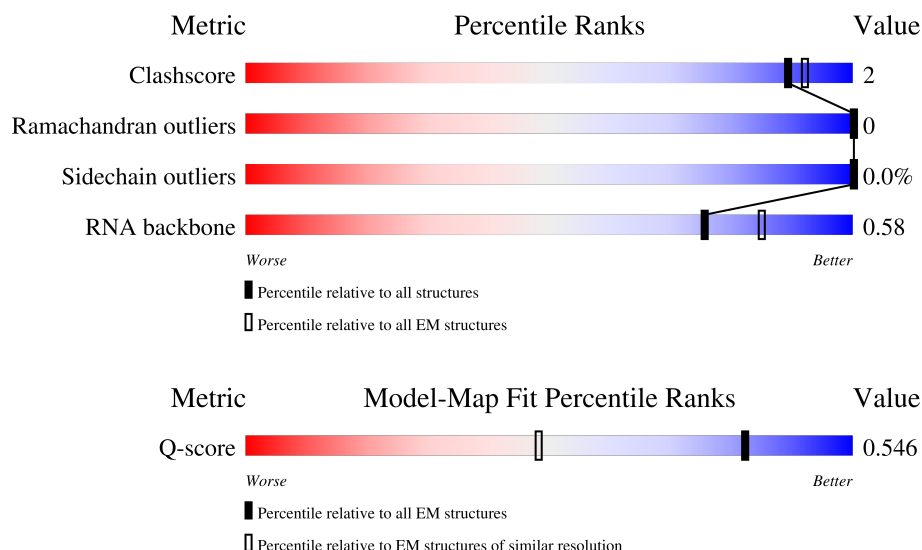
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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



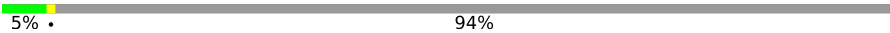
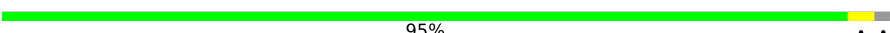
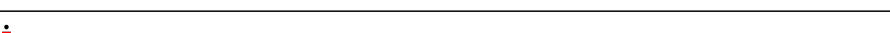
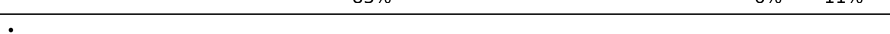
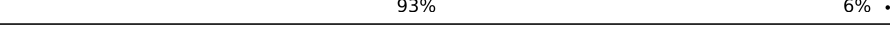
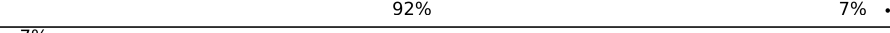
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	BA	165	42% 85% 12% .
2	BB	217	68% 98% .
3	L1	157	. 83% 11% . .

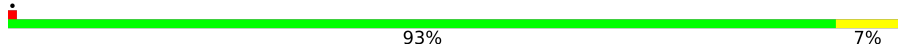
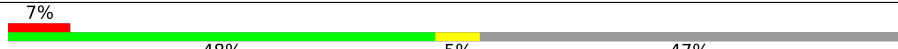
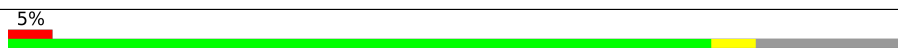
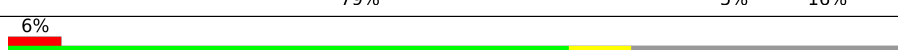
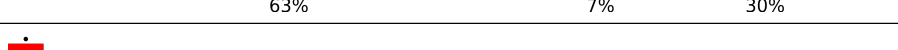
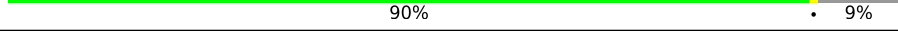
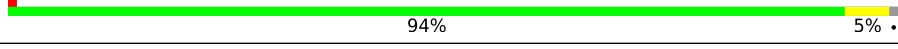
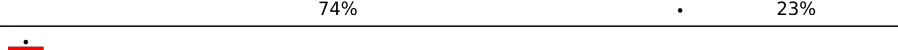
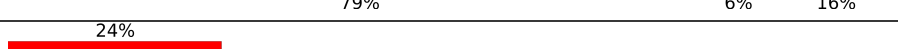
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Mol	Chain	Length	Quality of chain
4	L2	1167	
5	L3	5070	
6	L6	211	
7	L7	203	
8	L8	215	
9	L9	204	
10	LA	184	
11	LB	188	
12	LC	176	
13	LE	160	
14	LG	140	
15	LH	156	
16	LI	145	
17	LK	148	
18	LL	137	
19	LN	403	
20	LP	125	
21	LQ	135	
22	LS	123	
23	LT	110	
24	LU	105	
25	LW	97	
26	NA	749	
27	NB	549	
28	NF	260	

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Mol	Chain	Length	Quality of chain
29	NH	180	
30	NI	881	
31	NK	129	
32	SA	427	
33	SC	288	
34	SD	248	
35	SE	266	
36	SG	192	
37	SH	293	
38	SI	255	
39	SJ	847	
40	SK	245	
41	SL	490	
42	SM	588	
43	SN	306	
44	SO	353	
45	SQ	239	
46	SR	634	
47	SS	746	
48	ST	365	
49	SU	800	
50	SV	163	
51	SW	670	
52	SY	812	
53	SZ	178	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 139783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	160	Total	C	N	O	S	0	0
			1208	749	226	229	4		

- Molecule 2 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	BB	213	Total	C	N	O	0	0
			1057	631	213	213		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L1	152	Total	C	N	O	P	0	0
			3234	1443	571	1068	152		

- Molecule 4 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L2	69	Total	C	N	O	P	0	0
			1468	653	263	483	69		

- Molecule 5 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L3	2277	Total	C	N	O	P	0	0
			48813	21739	8937	15860	2277		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L6	120	Total	C	N	O	S	0	0
			998	625	218	154	1		

- Molecule 7 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 8 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L8	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 9 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L9	183	Total	C	N	O	S	0	0
			1546	974	325	243	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LA	138	Total	C	N	O	S	0	0
			1106	693	208	197	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LB	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 12 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LC	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 13 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	113	Total	C	N	O	S	0	0
			926	589	176	159	2		

- Molecule 14 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	134	Total	C	N	O	S	0	0
			993	625	187	176	5		

- Molecule 15 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LH	133	Total	C	N	O		0	0
			813	499	172	142			

- Molecule 16 is a protein called 60S ribosomal protein L26.

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

- Molecule 17 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LK	108	Total	C	N	O	S	0	0
			642	388	137	115	2		

- Molecule 18 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LL	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 19 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LN	358	Total	C	N	O	S	0	0
			2884	1834	531	506	13		

- Molecule 20 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LP	106	Total	C	N	O		0	0
			526	314	106	106			

- Molecule 21 is a protein called 60S ribosomal protein L32.

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

- Molecule 22 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LS	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 23 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LT	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 24 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	102	Total	C	N	O	S	1	0
			840	526	180	129	5		

- Molecule 25 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	74	Total	C	N	O	S	0	0
			612	379	134	94	5		

- Molecule 26 is a protein called Nucleolar complex protein 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	NA	484	Total	C	N	O	S	0	0
			3658	2355	644	638	21		

- Molecule 27 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	NB	67	Total	C	N	O	S	0	0
			569	355	119	92	3		

- Molecule 28 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	NF	218	Total	C	N	O	S	0	0
			1783	1136	337	301	9		

- Molecule 29 is a protein called 60S ribosome subunit biogenesis protein NIP7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	NH	180	Total	C	N	O	S	0	0
			1441	925	245	263	8		

- Molecule 30 is a protein called ATP-dependent RNA helicase DDX54.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	NI	647	Total	C	N	O	S	0	0
			5137	3254	934	934	15		

- Molecule 31 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	NK	69	Total	C	N	O	S	0	0
			594	371	131	90	2		

- Molecule 32 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SA	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 33 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SC	203	Total	C	N	O	S	0	0
			1627	1049	306	270	2		

- Molecule 34 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SD	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 35 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SE	185	Total	C	N	O	S	0	0
			1491	946	289	252	4		

- Molecule 36 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SG	190	Total	C	N	O	S	1	0
			1526	961	287	272	6		

- Molecule 37 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SH	150	Total	C	N	O	S	0	0
			1267	819	224	220	4		

- Molecule 38 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SI	223	Total	C	N	O	S	1	0
			1850	1197	347	302	4		

- Molecule 39 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SJ	313	Total	C	N	O	S	0	0
			2551	1634	461	450	6		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SK	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 41 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SL	243	Total	C	N	O	S	0	0
			1960	1254	344	356	6		

- Molecule 42 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SM	453	Total	C	N	O	S	0	0
			3735	2408	667	648	12		

- Molecule 43 is a protein called Probable rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SN	173	Total	C	N	O	S	0	0
			1350	849	251	243	7		

- Molecule 44 is a protein called Ribosome biogenesis protein BRX1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SO	296	Total	C	N	O	S	0	0
			2460	1583	446	416	15		

- Molecule 45 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SQ	217	Total	C	N	O	S	1	0
			1778	1134	313	320	11		

- Molecule 46 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SR	462	Total	C	N	O	S	0	0
			3808	2417	677	696	18		

- Molecule 47 is a protein called Ribosome biogenesis protein BOP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	SS	243	Total	C	N	O	P	S	0	0
			2011	1271	357	374	2	7		

- Molecule 48 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	ST	122	Total	C	N	O	S	0	0
			876	548	164	162	2		

- Molecule 49 is a protein called Nucleolar complex protein 3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SU	562	Total	C	N	O	S	0	0
			4442	2848	762	811	21		

- Molecule 50 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SV	137	Total	C	N	O	S	0	0
			1171	745	227	189	10		

- Molecule 51 is a protein called ATP-dependent RNA helicase DDX18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SW	444	Total	C	N	O	S	0	0
			3549	2282	605	645	17		

- Molecule 52 is a protein called Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SY	378	Total	C	N	O	S	0	0
			2985	1887	533	550	15		

- Molecule 53 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SZ	160	Total	C	N	O	S	0	0
			1338	835	260	238	5		

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	L1	5	Total	Mg	0
			5	5	
54	L2	1	Total	Mg	0
			1	1	
54	L3	46	Total	Mg	0
			46	46	
54	L9	1	Total	Mg	0
			1	1	
54	LQ	1	Total	Mg	0
			1	1	
54	LT	1	Total	Mg	0
			1	1	

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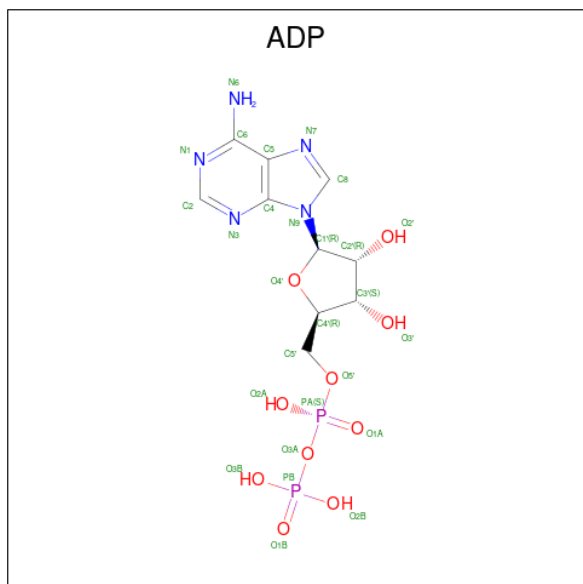
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Mol	Chain	Residues	Atoms		AltConf
54	NI	1	Total	Mg	0
			1	1	
54	SA	1	Total	Mg	0
			1	1	
54	SR	1	Total	Mg	0
			1	1	
54	SU	1	Total	Mg	0
			1	1	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

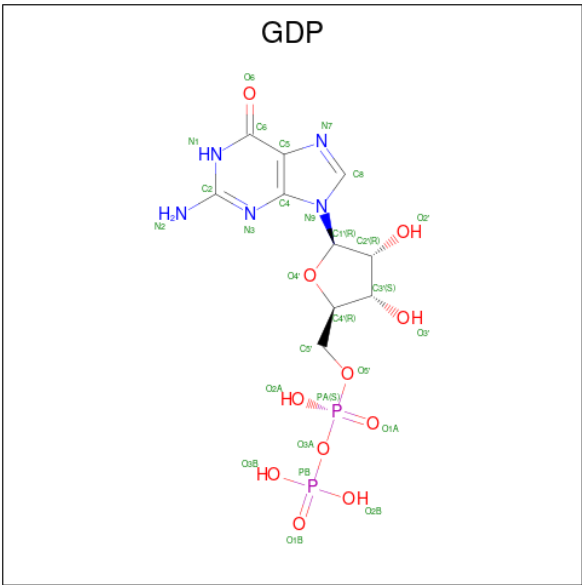
Mol	Chain	Residues	Atoms		AltConf
55	LW	1	Total	Zn	0
			1	1	
55	SV	1	Total	Zn	0
			1	1	

- Molecule 56 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
56	NI	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 57 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
57	SR	1	Total	C	N	O	P	0
			28	10	5	11	2	

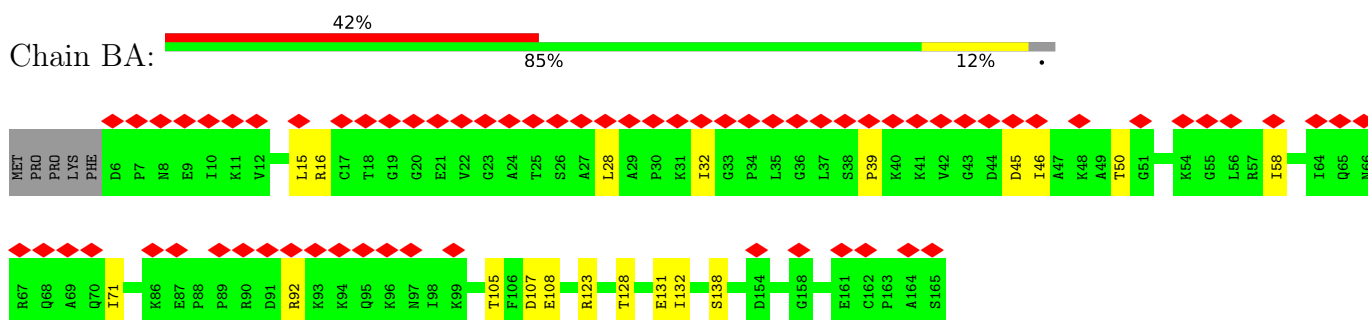
- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

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

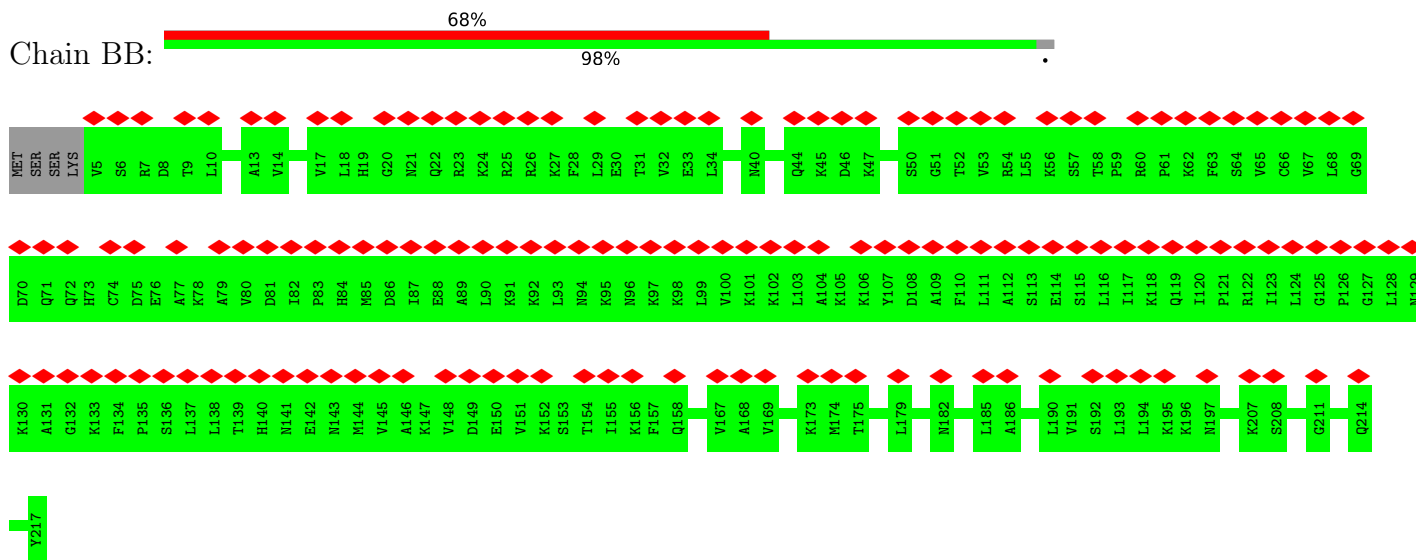
3 Residue-property plots

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

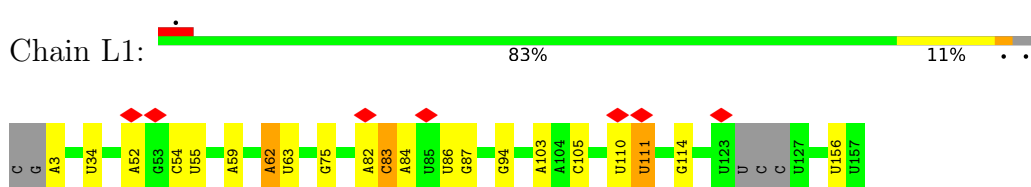
• Molecule 1: 60S ribosomal protein L12



• Molecule 2: 60S ribosomal protein L10a

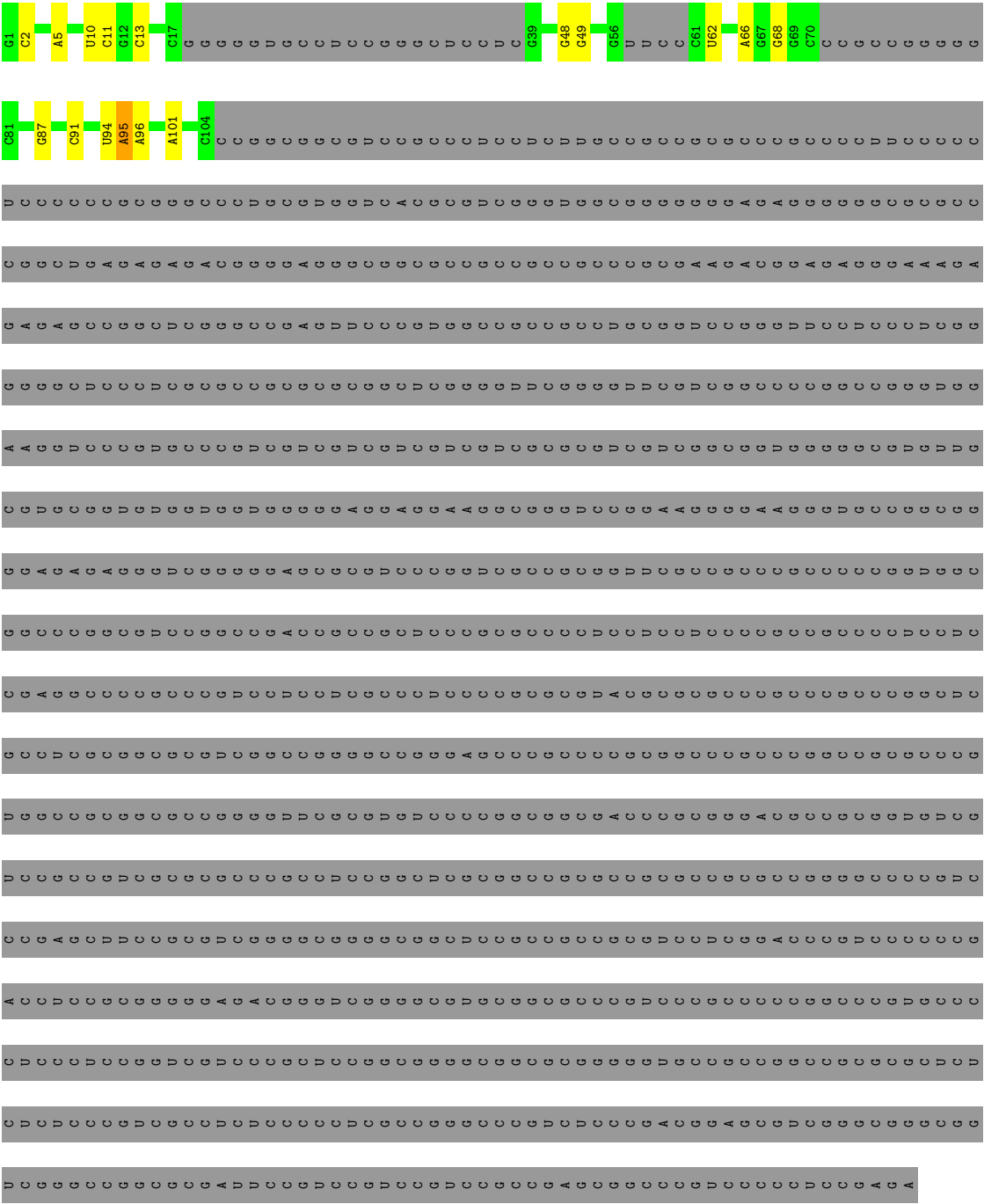


• Molecule 3: 5.8S rRNA



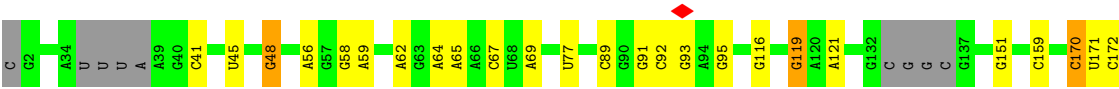
• Molecule 4: ITS2 rRNA

Chain L2: 5% . 94%



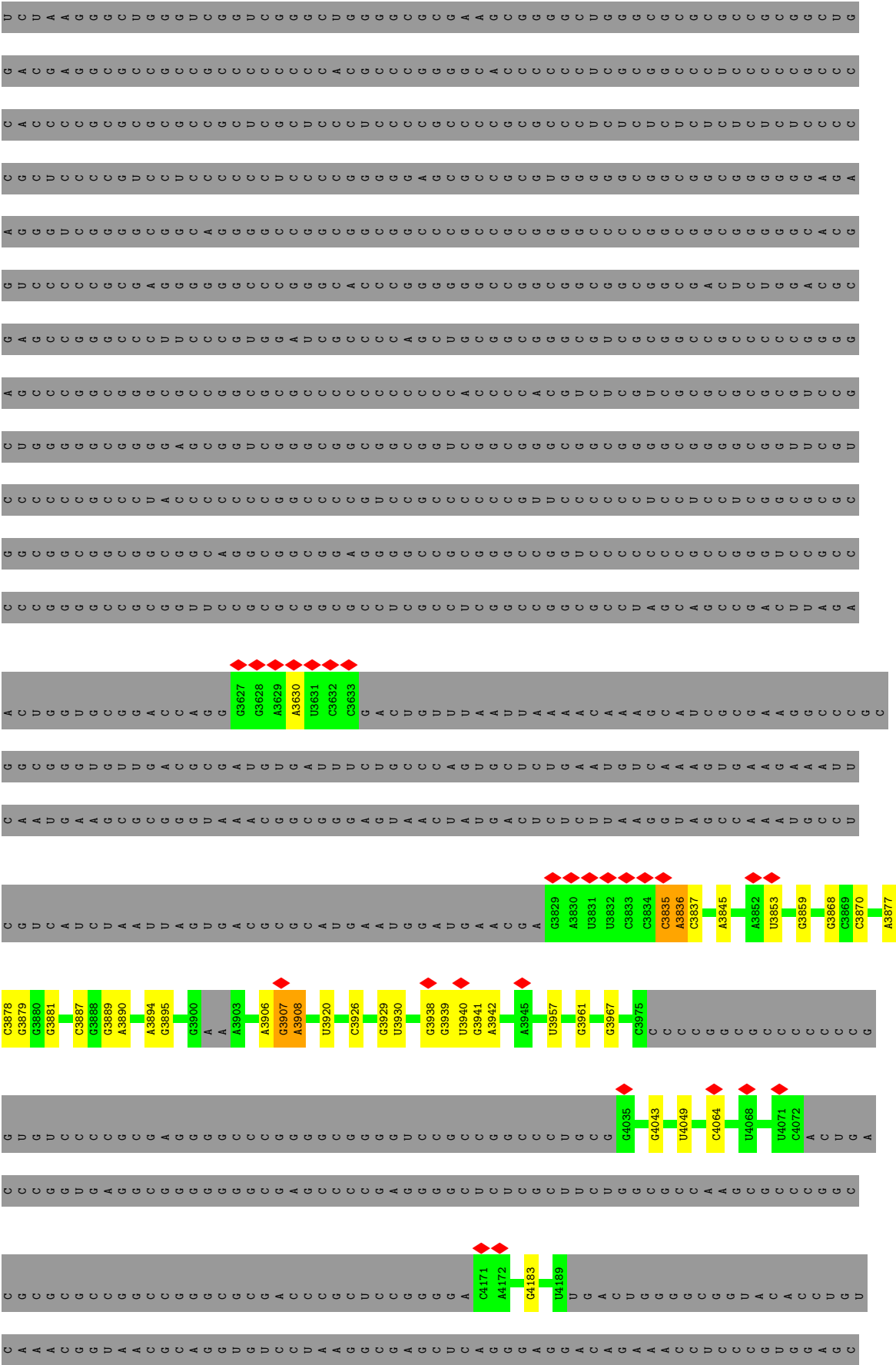
• Molecule 5: 28S rRNA

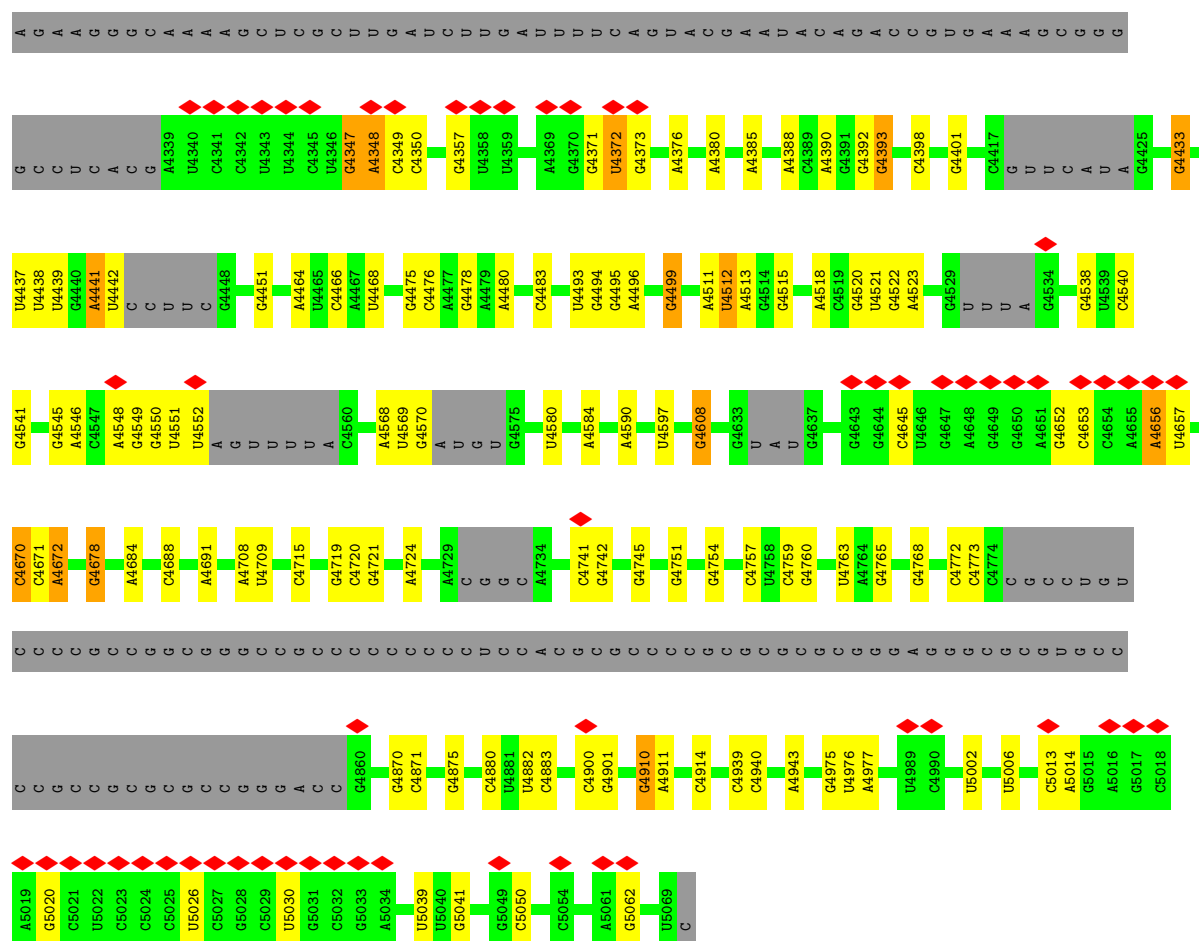
Chain L3: 37% 7% 55%





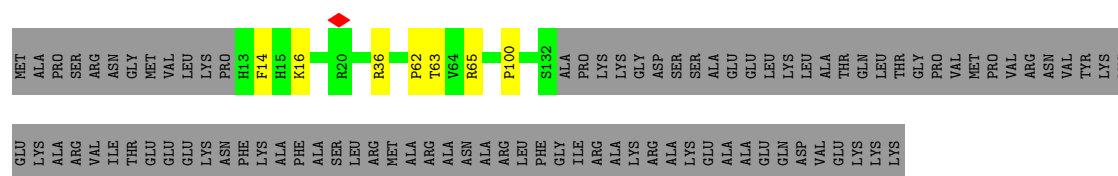






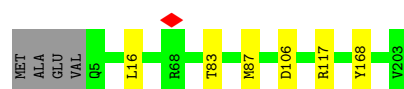
• Molecule 6: 60S ribosomal protein L13

Chain L6: 54% 43%



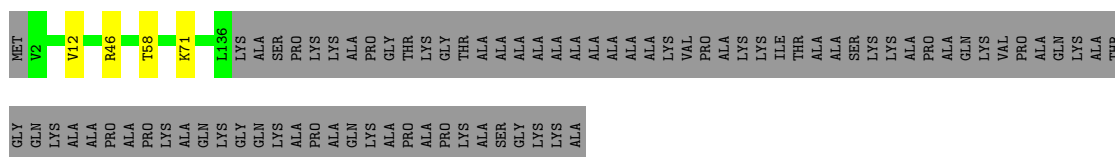
• Molecule 7: 60S ribosomal protein L13a

Chain L7: 95%



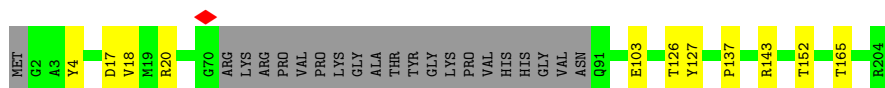
• Molecule 8: 60S ribosomal protein L14

Chain L8: 61% 37%



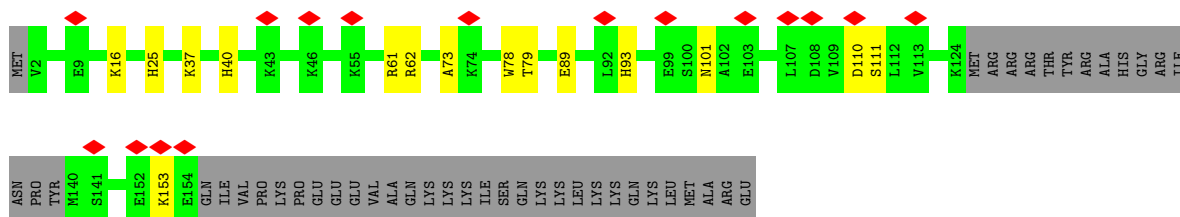
• Molecule 9: 60S ribosomal protein L15

Chain L9: 84% 5% 10%



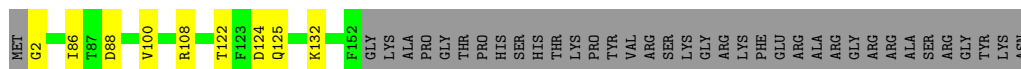
• Molecule 10: 60S ribosomal protein L17

Chain LA: 9% 67% 8% 25%



• Molecule 11: 60S ribosomal protein L18

Chain LB: 76% 5% 20%



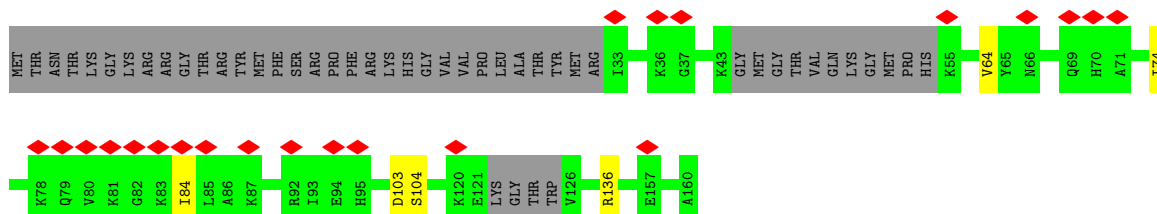
• Molecule 12: 60S ribosomal protein L18a

Chain LC: 94% 6%

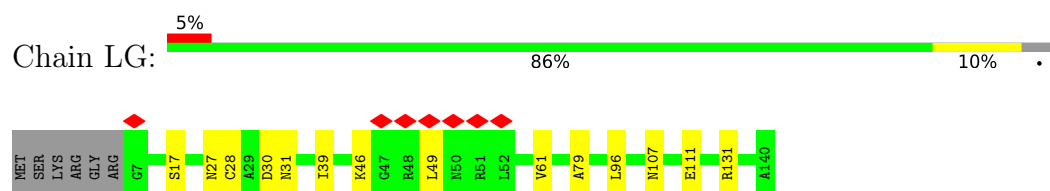


• Molecule 13: 60S ribosomal protein L21

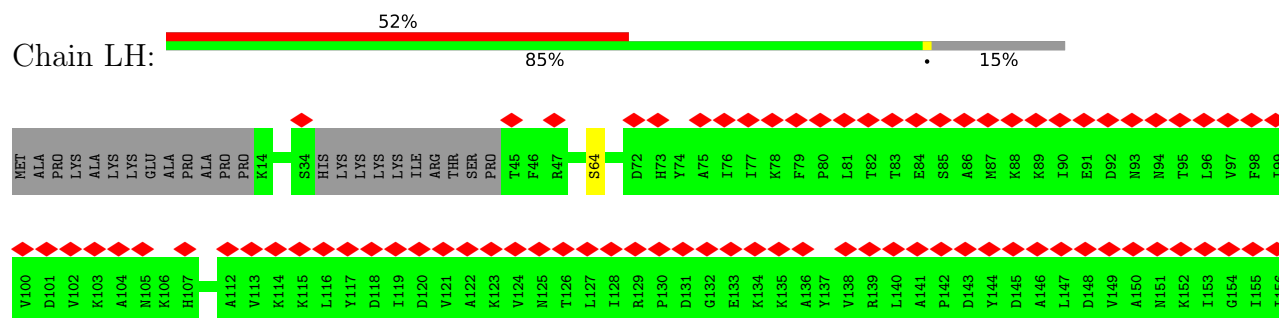
Chain LE: 14% 67% 29%



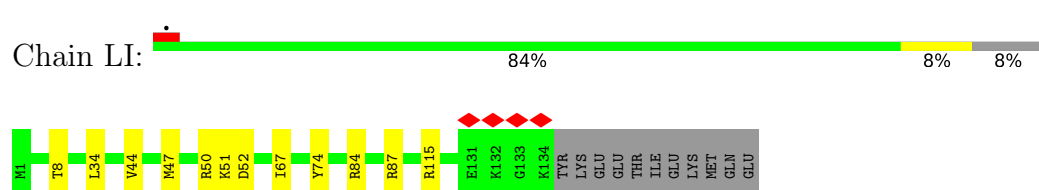
- Molecule 14: 60S ribosomal protein L23



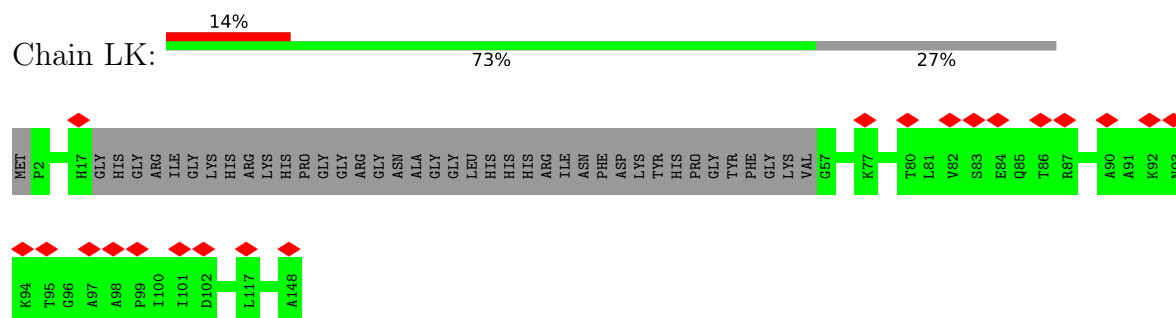
- Molecule 15: 60S ribosomal protein L23a



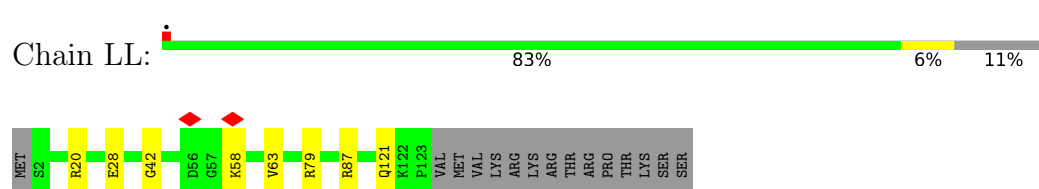
- Molecule 16: 60S ribosomal protein L26



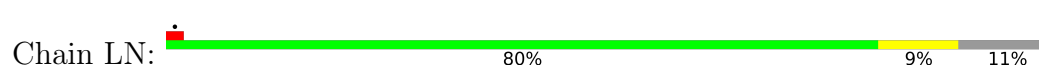
- Molecule 17: 60S ribosomal protein L27a

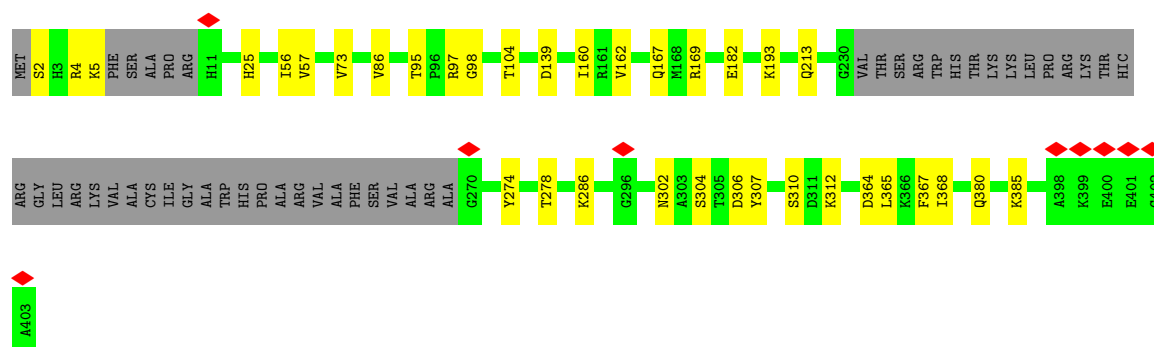


- Molecule 18: 60S ribosomal protein L28

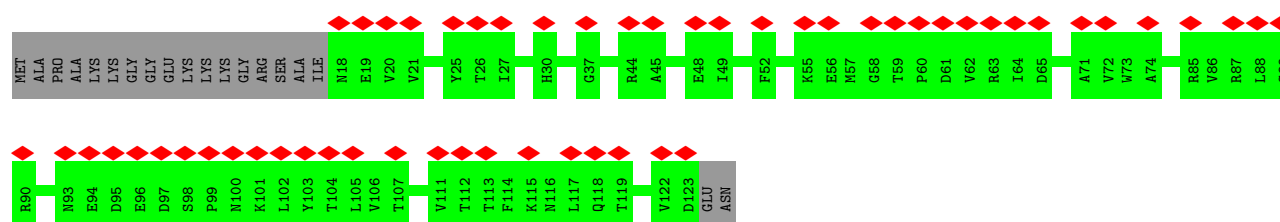
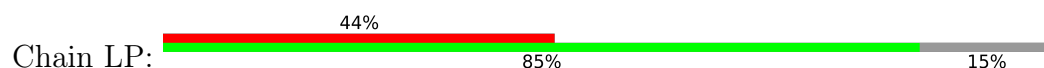


- Molecule 19: 60S ribosomal protein L3





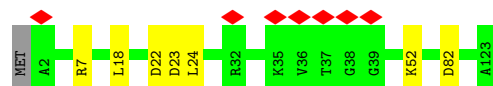
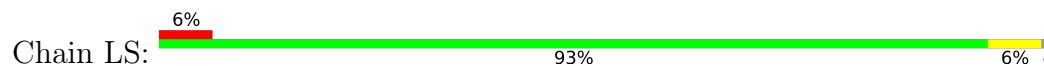
- Molecule 20: 60S ribosomal protein L31



- Molecule 21: 60S ribosomal protein L32



- Molecule 22: 60S ribosomal protein L35

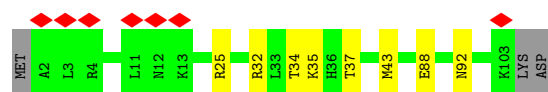


- Molecule 23: 60S ribosomal protein L35a



- Molecule 24: 60S ribosomal protein L36





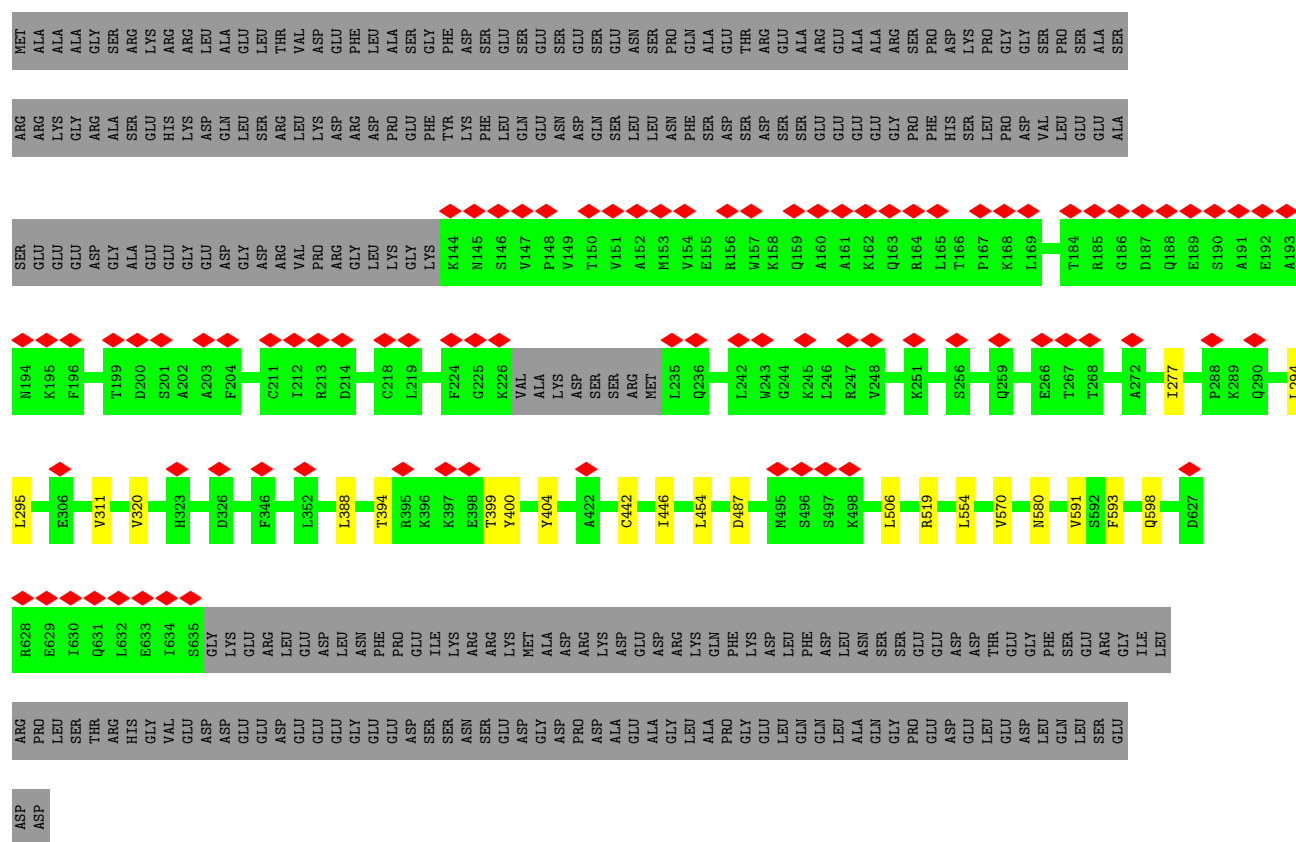
- Molecule 25: 60S ribosomal protein L37

Chain LW: 71% 5% 24%



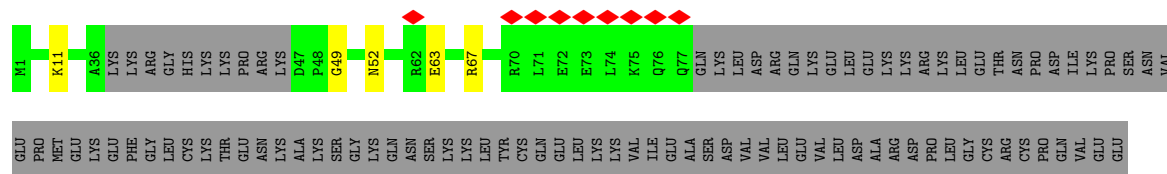
- Molecule 26: Nucleolar complex protein 2 homolog

Chain NA: 12% 62% 35%



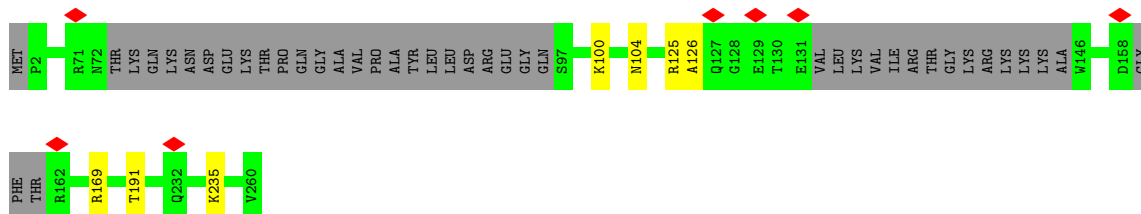
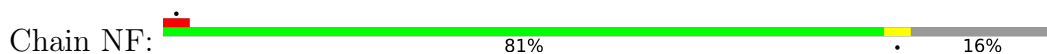
- Molecule 27: Guanine nucleotide-binding protein-like 3

Chain NB: 11% 88%

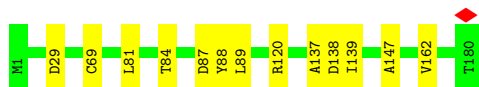




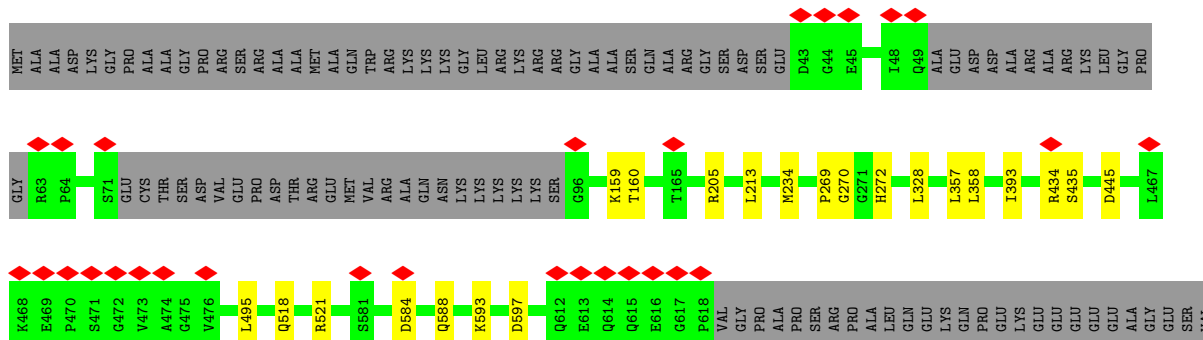
- Molecule 28: Ribosome biogenesis protein NSA2 homolog

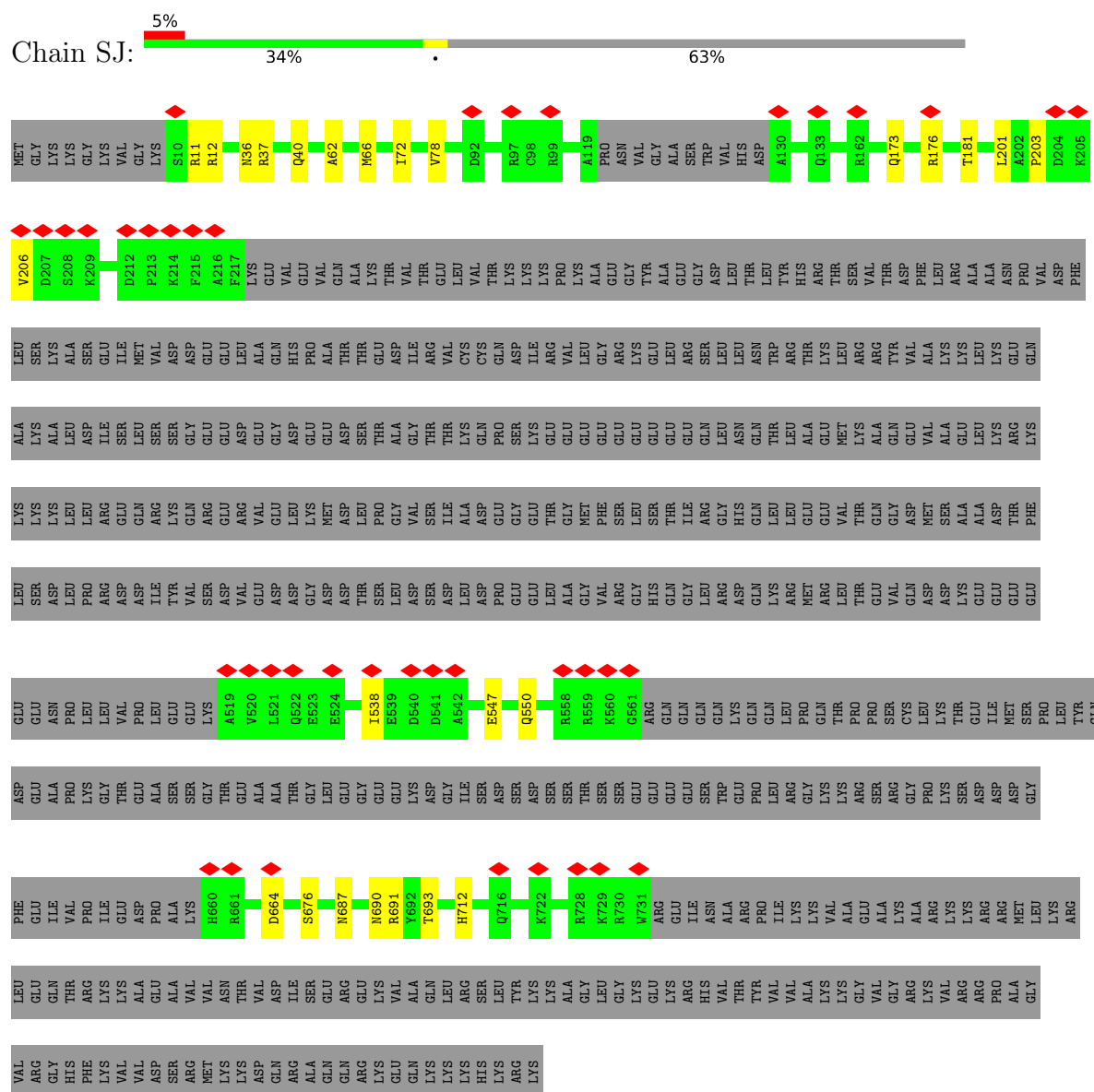


- Molecule 29: 60S ribosome subunit biogenesis protein NIP7 homolog

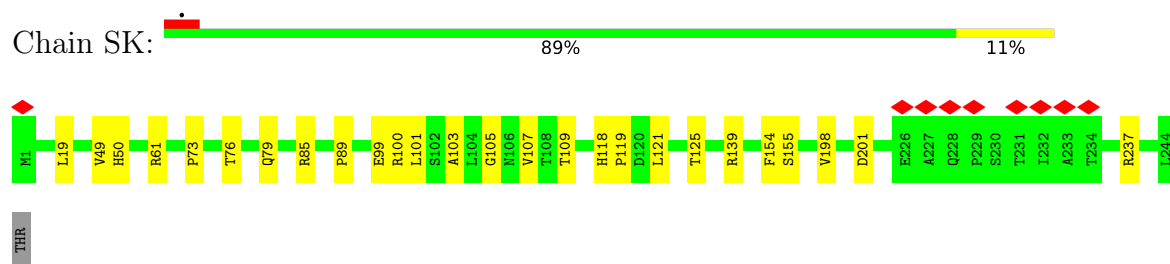


- Molecule 30: ATP-dependent RNA helicase DDX54





- Molecule 40: Eukaryotic translation initiation factor 6



- Molecule 41: Ribosomal L1 domain-containing protein 1



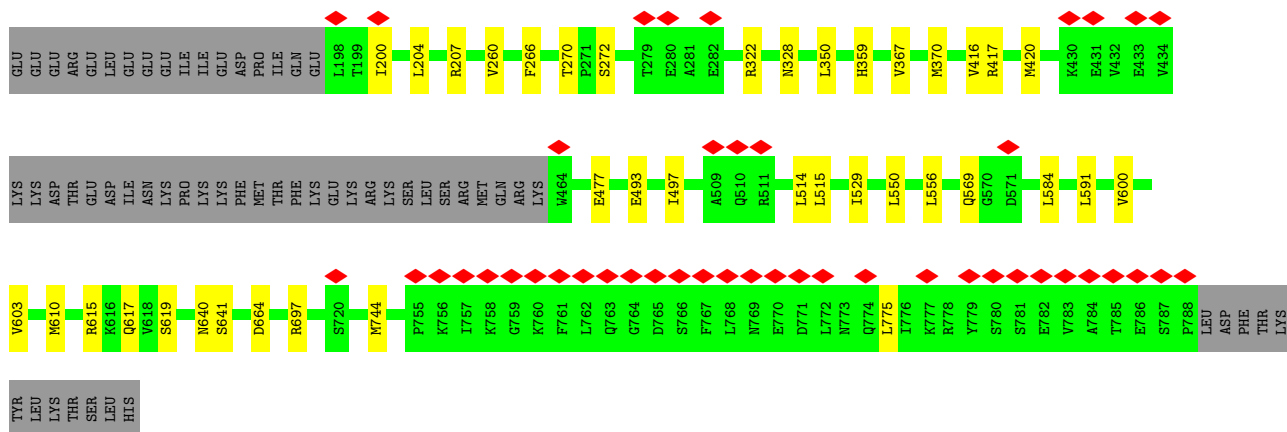
[illegible]

- Molecule 48: Ribosome biogenesis regulatory protein homolog

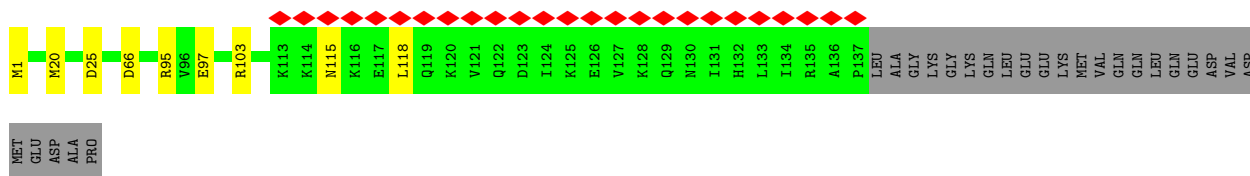
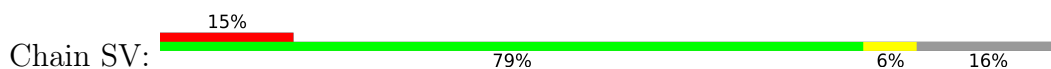
[illegible]

- Molecule 49: Nucleolar complex protein 3 homolog

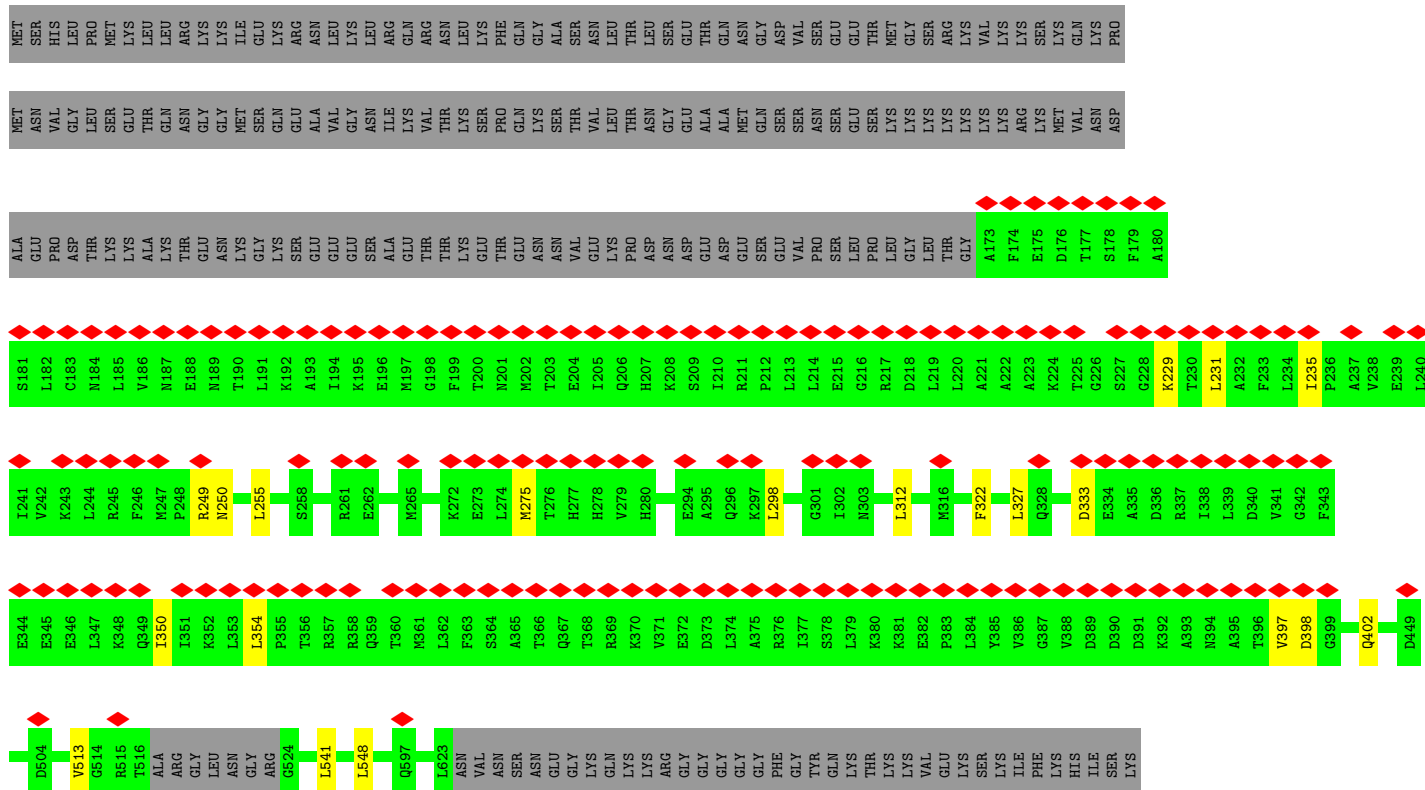
[illegible]



- Molecule 50: Probable ribosome biogenesis protein RLP24



- Molecule 51: ATP-dependent RNA helicase DDX18



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	214795	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.659	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.174	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	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, ZN, ADP, GDP, MG, SEP

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	BA	0.13	0/1224	0.30	0/1651
2	BB	0.13	0/1056	0.34	0/1472
3	L1	0.13	0/3611	0.24	0/5623
4	L2	0.14	0/1634	0.27	0/2538
5	L3	0.13	0/54570	0.27	0/85038
6	L6	0.14	0/1020	0.34	0/1367
7	L7	0.15	0/1666	0.32	0/2228
8	L8	0.15	0/1133	0.30	0/1516
9	L9	0.15	0/1584	0.34	0/2117
10	LA	0.11	0/1127	0.29	0/1511
11	LB	0.13	0/1239	0.27	0/1658
12	LC	0.16	0/1501	0.32	0/2013
13	LE	0.13	0/941	0.33	0/1254
14	LG	0.14	0/1007	0.32	0/1350
15	LH	0.10	0/818	0.25	0/1111
16	LI	0.16	0/1132	0.33	0/1504
17	LK	0.12	0/648	0.30	0/880
18	LL	0.13	0/995	0.28	0/1334
19	LN	0.14	0/2938	0.30	0/3923
20	LP	0.12	0/525	0.28	0/731
21	LQ	0.16	0/1071	0.33	0/1429
22	LS	0.11	0/1023	0.26	0/1351
23	LT	0.15	0/895	0.31	0/1198
24	LU	0.12	0/854	0.28	0/1129
25	LW	0.12	0/626	0.33	0/829
26	NA	0.12	0/3734	0.26	0/5079
27	NB	0.16	0/576	0.32	0/757
28	NF	0.15	0/1816	0.29	0/2420
29	NH	0.15	0/1473	0.30	0/1988
30	NI	0.12	0/5222	0.27	0/7025
31	NK	0.12	0/600	0.29	0/783
32	SA	0.14	0/2907	0.29	0/3905

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SC	0.13	0/1657	0.30	0/2226
34	SD	0.14	0/1905	0.29	0/2539
35	SE	0.14	0/1517	0.30	0/2046
36	SG	0.14	0/1548	0.28	0/2081
37	SH	0.12	0/1298	0.26	0/1742
38	SI	0.13	0/1891	0.27	0/2539
39	SJ	0.13	0/2605	0.29	0/3506
40	SK	0.14	0/1877	0.32	0/2554
41	SL	0.12	0/1994	0.29	0/2684
42	SM	0.13	0/3819	0.26	0/5139
43	SN	0.10	0/1368	0.24	0/1830
44	SO	0.13	0/2521	0.30	0/3384
45	SQ	0.12	0/1817	0.28	0/2435
46	SR	0.14	0/3882	0.30	0/5237
47	SS	0.13	0/2052	0.29	0/2786
48	ST	0.11	0/891	0.25	0/1204
49	SU	0.13	0/4518	0.27	0/6093
50	SV	0.13	0/1194	0.30	0/1582
51	SW	0.12	0/3620	0.29	0/4886
52	SY	0.14	0/3046	0.29	0/4117
53	SZ	0.12	0/1364	0.25	0/1826
All	All	0.13	0/147550	0.28	0/211148

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
21	LQ	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	LQ	33	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	BA	1208	0	1257	15	0
2	BB	1057	0	464	0	0
3	L1	3234	0	1639	6	0
4	L2	1468	0	755	6	0
5	L3	48813	0	24704	120	0
6	L6	998	0	1067	6	0
7	L7	1634	0	1779	5	0
8	L8	1111	0	1174	3	0
9	L9	1546	0	1585	9	0
10	LA	1106	0	1130	10	0
11	LB	1223	0	1330	6	0
12	LC	1461	0	1502	9	0
13	LE	926	0	979	6	0
14	LG	993	0	1050	11	0
15	LH	813	0	640	1	0
16	LI	1115	0	1205	8	0
17	LK	642	0	455	0	0
18	LL	980	0	1041	5	0
19	LN	2884	0	3000	27	0
20	LP	526	0	225	0	0
21	LQ	1053	0	1147	8	0
22	LS	1015	0	1148	5	0
23	LT	876	0	912	6	0
24	LU	840	0	930	6	0
25	LW	612	0	640	4	0
26	NA	3658	0	3564	16	0
27	NB	569	0	625	4	0
28	NF	1783	0	1896	7	0
29	NH	1441	0	1448	9	0
30	NI	5137	0	5294	18	0
31	NK	594	0	672	7	0
32	SA	2853	0	3028	17	0
33	SC	1627	0	1771	16	0
34	SD	1870	0	1996	2	0
35	SE	1491	0	1592	7	0
36	SG	1526	0	1614	6	0
37	SH	1267	0	1291	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	SI	1850	0	1966	11	0
39	SJ	2551	0	2568	21	0
40	SK	1852	0	1828	18	0
41	SL	1960	0	2052	5	0
42	SM	3735	0	3830	12	0
43	SN	1350	0	1345	9	0
44	SO	2460	0	2551	16	0
45	SQ	1778	0	1817	9	0
46	SR	3808	0	3873	25	0
47	SS	2011	0	1919	12	0
48	ST	876	0	818	4	0
49	SU	4442	0	4562	33	0
50	SV	1171	0	1232	10	0
51	SW	3549	0	3628	12	0
52	SY	2985	0	3004	12	0
53	SZ	1338	0	1352	5	0
54	L1	5	0	0	0	0
54	L2	1	0	0	0	0
54	L3	46	0	0	0	0
54	L9	1	0	0	0	0
54	LQ	1	0	0	0	0
54	LT	1	0	0	0	0
54	NI	1	0	0	0	0
54	SA	1	0	0	0	0
54	SR	1	0	0	0	0
54	SU	1	0	0	0	0
55	LW	1	0	0	0	0
55	SV	1	0	0	0	0
56	NI	27	0	12	0	0
57	SR	28	0	12	0	0
58	SR	1	0	0	0	0
All	All	139783	0	114918	446	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 2.

All (446) 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)
30:NI:213:LEU:HD12	30:NI:234:MET:HE1	1.49	0.94
30:NI:328:LEU:HD11	30:NI:495:LEU:HD21	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:SA:340:ILE:HG21	33:SC:50:LEU:HD13	1.57	0.86
30:NI:434:ARG:NH1	30:NI:435:SER:O	2.09	0.85
1:BA:105:THR:OG1	1:BA:108:GLU:OE1	1.96	0.84
24:LU:35:LYS:NZ	47:SS:236:VAL:O	2.13	0.81
1:BA:16:ARG:NH2	5:L3:1975:G:O2'	2.15	0.80
5:L3:4678:G:OP1	31:NK:14:ARG:NH1	2.17	0.78
5:L3:184:U:O2'	5:L3:189:G:OP2	2.02	0.77
5:L3:1524:A:O2'	5:L3:1525:A:O5'	2.01	0.77
5:L3:5039:U:O3'	50:SV:115:ASN:ND2	2.17	0.77
44:SO:61:ARG:NH1	47:SS:128:ASP:OD2	2.18	0.77
16:LI:67:ILE:O	16:LI:84:ARG:NH2	2.18	0.77
3:L1:75:G:OP2	16:LI:74:TYR:OH	2.01	0.76
5:L3:4672:A:OP1	14:LG:17:SER:OG	2.04	0.76
21:LQ:20:PHE:O	21:LQ:33:ARG:NH2	2.20	0.75
52:SY:227:MET:SD	52:SY:269:ARG:NH1	2.60	0.75
5:L3:1280:C:O2'	32:SA:321:ASN:OD1	2.04	0.74
5:L3:739:G:OP2	8:L8:71:LYS:NZ	2.20	0.74
5:L3:1961:G:N7	45:SQ:71:LYS:NZ	2.31	0.74
5:L3:713:C:O2	33:SC:130:LYS:NZ	2.20	0.74
5:L3:48:G:OP1	6:L6:16:LYS:NZ	2.22	0.73
5:L3:254:G:OP2	44:SO:338:LYS:NZ	2.18	0.73
5:L3:3957:U:OP1	52:SY:564:ARG:NH2	2.21	0.73
36:SG:89:ARG:NH1	36:SG:147:GLU:OE1	2.21	0.73
5:L3:62:A:N3	5:L3:77:U:O2'	2.22	0.72
4:L2:10:U:OP2	41:SL:163:ARG:NH2	2.22	0.72
49:SU:266:PHE:O	49:SU:270:THR:OG1	2.07	0.72
5:L3:4493:U:O2	14:LG:46:LYS:NZ	2.19	0.72
5:L3:4468:U:HO2'	31:NK:2:ALA:N	1.88	0.72
5:L3:935:A:O2'	8:L8:46:ARG:NH1	2.22	0.72
49:SU:600:VAL:HG11	49:SU:641:SER:OG	1.90	0.71
6:L6:65:ARG:O	44:SO:278:ARG:NH2	2.24	0.70
46:SR:367:ARG:NH1	46:SR:369:ASP:O	2.25	0.70
30:NI:584:ASP:O	30:NI:588:GLN:NE2	2.24	0.70
33:SC:161:ARG:O	33:SC:182:ASN:ND2	2.24	0.70
5:L3:3835:C:O2'	5:L3:3836:A:OP1	2.09	0.69
45:SQ:47:ASN:ND2	45:SQ:129:ASN:OD1	2.25	0.69
11:LB:122:THR:OG1	11:LB:124:ASP:OD1	2.09	0.69
30:NI:719:GLU:OE1	30:NI:722:ASN:ND2	2.26	0.69
9:L9:137:PRO:O	9:L9:143:ARG:NE	2.26	0.69
18:LL:58:LYS:O	18:LL:121:GLN:NE2	2.25	0.69
5:L3:4940:C:OP1	33:SC:156:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LA:89:GLU:OE2	10:LA:93:HIS:NE2	2.21	0.68
5:L3:4768:G:OP1	7:L7:168:TYR:OH	2.12	0.68
38:SI:153:ASN:ND2	42:SM:263:GLY:O	2.27	0.68
51:SW:249:ARG:NH1	51:SW:250:ASN:OD1	2.25	0.68
5:L3:170:C:O2	53:SZ:109:ASN:ND2	2.27	0.68
5:L3:2300:A:N7	32:SA:143:ARG:NH1	2.42	0.67
5:L3:404:U:O3'	16:LI:87:ARG:NH2	2.27	0.67
18:LL:20:ARG:NH1	21:LQ:78:LEU:O	2.28	0.67
38:SI:143:VAL:O	38:SI:147:VAL:HG12	1.95	0.66
44:SO:53:LYS:NZ	47:SS:155:ASP:OD2	2.25	0.66
3:L1:87:G:OP2	22:LS:7:ARG:NH2	2.30	0.65
5:L3:3961:G:O2'	5:L3:4043:G:N2	2.29	0.65
39:SJ:37:ARG:NH2	49:SU:477:GLU:O	2.29	0.65
3:L1:111:U:OP2	25:LW:20:ARG:NH2	2.29	0.65
19:LN:57:VAL:HG12	19:LN:73:VAL:HG22	1.78	0.65
29:NH:138:ASP:OD1	49:SU:619:SER:OG	2.11	0.65
5:L3:4910:G:N2	7:L7:106:ASP:O	2.28	0.65
5:L3:458:C:O2'	33:SC:110:ARG:NH1	2.29	0.65
5:L3:1508:A:OP1	32:SA:110:ARG:NH2	2.30	0.64
5:L3:1238:A:OP2	33:SC:60:SER:OG	2.12	0.64
5:L3:4441:A:N6	30:NI:445:ASP:O	2.30	0.64
50:SV:66:ASP:OD2	50:SV:103:ARG:NH1	2.30	0.64
45:SQ:64:ARG:NH1	45:SQ:65:MET:O	2.30	0.64
18:LL:28:GLU:OE1	18:LL:42:GLY:N	2.30	0.63
29:NH:120:ARG:NH1	49:SU:617:GLN:O	2.31	0.63
19:LN:95:THR:OG1	19:LN:98:GLY:O	2.10	0.63
5:L3:4347:G:O2'	5:L3:4348:A:O5'	2.15	0.63
30:NI:270:GLY:O	49:SU:615:ARG:NH2	2.32	0.63
5:L3:1669:A:N3	5:L3:1852:U:O2'	2.32	0.63
42:SM:189:TYR:CZ	42:SM:202:ILE:HD12	2.34	0.63
39:SJ:550:GLN:NE2	49:SU:328:ASN:OD1	2.32	0.63
46:SR:441:TYR:OH	50:SV:97:GLU:OE2	2.13	0.62
46:SR:176:TYR:O	46:SR:181:LYS:NZ	2.32	0.62
30:NI:518:GLN:OE1	30:NI:521:ARG:NH1	2.32	0.62
38:SI:192:ILE:HD12	47:SS:351:ARG:HH11	1.65	0.62
4:L2:5:A:N6	4:L2:95:A:O2'	2.33	0.62
43:SN:140:MET:HE1	44:SO:159:LEU:HD23	1.81	0.62
5:L3:4670:C:O2'	19:LN:4:ARG:NH2	2.33	0.62
30:NI:269:PRO:O	30:NI:272:HIS:ND1	2.29	0.62
29:NH:87:ASP:OD2	29:NH:88:TYR:N	2.33	0.61
38:SI:29:ARG:NH2	47:SS:365:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LE:136:ARG:NH2	34:SD:86:GLU:OE2	2.33	0.61
1:BA:50:THR:HG22	1:BA:58:ILE:HD11	1.82	0.61
24:LU:88:GLU:OE2	24:LU:92:ASN:ND2	2.34	0.61
5:L3:1883:G:OP1	21:LQ:47:ARG:NH1	2.32	0.61
9:L9:126:THR:HG21	39:SJ:712:HIS:HD2	1.65	0.61
23:LT:54:LYS:O	23:LT:66:LYS:NZ	2.32	0.60
39:SJ:538:ILE:HD11	49:SU:260:VAL:HG21	1.83	0.60
51:SW:327:LEU:HD22	51:SW:354:LEU:HD23	1.83	0.60
5:L3:3907:G:O2'	5:L3:3908:A:OP1	2.14	0.60
21:LQ:26:ASP:OD1	21:LQ:27:ARG:N	2.35	0.60
42:SM:140:MET:HE1	42:SM:220:MET:HE2	1.84	0.60
5:L3:364:G:O6	25:LW:55:ARG:NH2	2.35	0.60
44:SO:223:ILE:HD11	44:SO:230:VAL:HG23	1.83	0.60
5:L3:4580:U:O2'	19:LN:182:GLU:OE2	2.19	0.59
1:BA:138:SER:OG	5:L3:2002:A:N6	2.36	0.59
5:L3:4483:C:H5''	46:SR:21:LEU:HD13	1.84	0.59
19:LN:213:GLN:O	31:NK:28:ARG:NH2	2.35	0.59
30:NI:358:LEU:HD12	30:NI:393:ILE:HD11	1.84	0.59
28:NF:100:LYS:O	28:NF:104:ASN:ND2	2.34	0.59
40:SK:100:ARG:NH1	50:SV:25:ASP:OD1	2.30	0.58
5:L3:309:C:O4'	24:LU:32:ARG:NH1	2.36	0.58
40:SK:107:VAL:HG13	40:SK:118:HIS:HB2	1.84	0.58
5:L3:2562:G:O2'	5:L3:2565:A:N6	2.35	0.58
49:SU:584:LEU:HD13	49:SU:610:MET:HE2	1.84	0.58
5:L3:67:C:OP2	5:L3:312:G:N2	2.37	0.58
5:L3:3890:A:OP2	5:L3:4570:G:N2	2.36	0.58
12:LC:17:LEU:HD21	13:LE:136:ARG:NH1	2.19	0.58
5:L3:2361:G:O6	10:LA:25:HIS:ND1	2.37	0.58
14:LG:30:ASP:OD1	14:LG:31:ASN:N	2.36	0.58
48:ST:163:ASN:OD1	48:ST:164:ALA:N	2.35	0.58
49:SU:529:ILE:O	49:SU:569:GLN:NE2	2.37	0.58
5:L3:423:G:OP1	10:LA:62:ARG:NH1	2.37	0.57
26:NA:487:ASP:O	26:NA:519:ARG:NH1	2.37	0.57
14:LG:96:LEU:HD13	50:SV:20:MET:HE3	1.87	0.57
5:L3:1952:G:OP1	12:LC:139:ARG:NE	2.37	0.57
5:L3:2361:G:O2'	5:L3:3859:G:O6	2.19	0.57
30:NI:593:LYS:NZ	30:NI:597:ASP:OD2	2.24	0.57
26:NA:400:TYR:CE2	26:NA:446:ILE:HD12	2.39	0.56
3:L1:3:A:O2'	10:LA:61:ARG:NH1	2.38	0.56
10:LA:40:HIS:NE2	10:LA:110:ASP:O	2.39	0.56
28:NF:125:ARG:HE	28:NF:126:ALA:H	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:NA:388:LEU:HD23	49:SU:744:MET:HE3	1.87	0.56
19:LN:86:VAL:HG13	19:LN:162:VAL:HG13	1.87	0.56
1:BA:128:THR:O	1:BA:132:ILE:HD12	2.06	0.56
29:NH:81:LEU:HD21	29:NH:89:LEU:CD2	2.36	0.56
19:LN:312:LYS:NZ	19:LN:380:GLN:OE1	2.38	0.56
5:L3:4691:A:OP1	36:SG:75:SER:OG	2.20	0.55
32:SA:101:MET:HE3	32:SA:104:PRO:HA	1.88	0.55
5:L3:4499:G:O3'	30:NI:750:LYS:NZ	2.39	0.55
5:L3:1524:A:HO2'	5:L3:1525:A:P	2.29	0.55
5:L3:369:G:N2	5:L3:372:A:OP2	2.33	0.55
19:LN:160:ILE:HD11	19:LN:193:LYS:HB3	1.87	0.55
5:L3:4678:G:N7	31:NK:11:ARG:NH2	2.55	0.55
9:L9:126:THR:HG21	39:SJ:712:HIS:CD2	2.42	0.55
51:SW:350:ILE:O	51:SW:354:LEU:HD12	2.07	0.55
21:LQ:84:GLU:O	21:LQ:87:VAL:HG22	2.07	0.55
39:SJ:676:SER:O	47:SS:133:ARG:NH2	2.40	0.55
49:SU:493:GLU:O	49:SU:497:ILE:HD12	2.07	0.55
43:SN:210:LEU:HD22	43:SN:212:PHE:CZ	2.42	0.55
44:SO:205:VAL:CG2	44:SO:222:ILE:HD11	2.37	0.55
32:SA:204:ARG:NH1	32:SA:205:ARG:O	2.40	0.54
5:L3:244:G:O6	53:SZ:20:LYS:NZ	2.40	0.54
5:L3:4393:G:OP1	43:SN:174:ARG:NH1	2.39	0.54
12:LC:17:LEU:HD21	13:LE:136:ARG:HH11	1.73	0.54
16:LI:47:MET:HE2	16:LI:115:ARG:HE	1.71	0.54
38:SI:101:ARG:NH1	38:SI:122:LYS:O	2.41	0.54
1:BA:105:THR:OG1	1:BA:107:ASP:OD2	2.26	0.54
32:SA:13:GLU:N	32:SA:155:GLU:OE1	2.38	0.54
49:SU:350:LEU:HD12	49:SU:359:HIS:CE1	2.43	0.54
5:L3:1833:G:N2	5:L3:1835:G:O4'	2.40	0.53
45:SQ:49:ARG:NH1	45:SQ:125:ALA:O	2.41	0.53
5:L3:4569:U:H5''	10:LA:79:THR:HG21	1.90	0.53
19:LN:364:ASP:OD1	46:SR:428:LYS:NZ	2.33	0.53
30:NI:328:LEU:CD1	30:NI:495:LEU:HD21	2.35	0.53
23:LT:59:THR:OG1	23:LT:65:ASN:ND2	2.41	0.53
32:SA:54:VAL:HG21	32:SA:101:MET:HE2	1.90	0.53
51:SW:402:GLN:NE2	51:SW:513:VAL:HG11	2.23	0.53
33:SC:50:LEU:HD12	33:SC:51:VAL:N	2.23	0.53
35:SE:101:LYS:NZ	35:SE:211:ASP:OD2	2.25	0.53
39:SJ:181:THR:OG1	49:SU:272:SER:OG	2.23	0.53
46:SR:454:GLU:OE1	50:SV:95:ARG:NH2	2.41	0.53
14:LG:39:ILE:HG23	14:LG:61:VAL:CG1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L9:17:ASP:OD1	9:L9:18:VAL:N	2.42	0.53
13:LE:64:VAL:HG22	13:LE:74:ILE:CD1	2.39	0.53
5:L3:307:A:N3	5:L3:310:G:O2'	2.42	0.53
16:LI:34:LEU:HD22	16:LI:44:VAL:HG13	1.90	0.53
9:L9:143:ARG:HD3	9:L9:152:THR:HG21	1.91	0.52
10:LA:111:SER:OG	10:LA:153:LYS:O	2.27	0.52
40:SK:99:GLU:OE1	40:SK:125:THR:OG1	2.25	0.52
46:SR:287:VAL:HG11	46:SR:331:VAL:HG21	1.91	0.52
46:SR:174:CYS:SG	46:SR:244:LEU:HD21	2.49	0.52
26:NA:404:TYR:CD2	26:NA:454:LEU:HD13	2.45	0.52
14:LG:49:LEU:HD11	19:LN:5:LYS:HA	1.91	0.52
49:SU:664:ASP:OD2	52:SY:320:ARG:NH1	2.43	0.52
15:LH:64:SER:OG	22:LS:82:ASP:OD2	2.25	0.52
6:L6:100:PRO:O	24:LU:25[A]:ARG:NH2	2.36	0.52
26:NA:388:LEU:CD2	49:SU:744:MET:HE3	2.40	0.52
5:L3:5039:U:O2'	50:SV:115:ASN:ND2	2.43	0.52
42:SM:268:ASP:OD1	42:SM:269:SER:N	2.43	0.52
45:SQ:80:SER:OG	45:SQ:83:ASP:OD2	2.13	0.52
53:SZ:162:GLU:OE2	53:SZ:162:GLU:N	2.40	0.52
5:L3:346:G:OP1	16:LI:8:THR:HG23	2.10	0.52
5:L3:2043:A:N1	5:L3:4515:G:O2'	2.41	0.52
49:SU:477:GLU:N	49:SU:477:GLU:OE1	2.40	0.52
46:SR:188:VAL:HG23	46:SR:189:THR:HG23	1.93	0.51
52:SY:388:ILE:HD12	52:SY:406:MET:HE2	1.91	0.51
39:SJ:62:ALA:HB1	39:SJ:66:MET:HE2	1.92	0.51
5:L3:4875:G:H2'	12:LC:169:THR:HG22	1.93	0.51
24:LU:34:THR:HB	24:LU:37:THR:HG22	1.91	0.51
46:SR:285:ILE:HG21	46:SR:331:VAL:HG23	1.91	0.51
4:L2:13:C:OP1	38:SI:86:HIS:NE2	2.35	0.51
5:L3:264:C:OP2	53:SZ:112:SER:OG	2.29	0.51
14:LG:111:GLU:OE2	14:LG:131:ARG:NH1	2.44	0.51
26:NA:311:VAL:CG2	49:SU:775:LEU:HD21	2.41	0.51
38:SI:192:ILE:HD12	47:SS:351:ARG:NH1	2.26	0.51
9:L9:126:THR:HG23	9:L9:127:TYR:CD2	2.46	0.50
51:SW:275:MET:HE3	51:SW:275:MET:HA	1.92	0.50
19:LN:139:ASP:OD2	31:NK:96:TRP:NE1	2.41	0.50
21:LQ:19:LYS:HB3	21:LQ:33:ARG:NH2	2.25	0.50
5:L3:2296:G:O2'	32:SA:242:PRO:O	2.29	0.50
5:L3:4975:G:O2'	5:L3:4977:A:N6	2.44	0.50
12:LC:99:ASP:OD2	12:LC:100:LEU:N	2.43	0.50
14:LG:27:ASN:OD1	14:LG:28:CYS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:119:G:N2	35:SE:133:PRO:O	2.36	0.50
28:NF:125:ARG:HE	28:NF:126:ALA:N	2.10	0.50
30:NI:682:ILE:O	52:SY:575:ASN:ND2	2.43	0.50
49:SU:367:VAL:HA	49:SU:370:MET:HE2	1.94	0.50
5:L3:4388:A:OP1	28:NF:169:ARG:NH1	2.45	0.49
32:SA:140:LYS:O	32:SA:204:ARG:NH2	2.43	0.49
1:BA:123:ARG:NH2	45:SQ:61:LYS:O	2.45	0.49
9:L9:20:ARG:NH2	39:SJ:693:THR:O	2.42	0.49
5:L3:121:A:OP1	35:SE:110:LYS:NZ	2.42	0.49
52:SY:230:ASP:OD2	52:SY:269:ARG:NH2	2.45	0.49
5:L3:4910:G:H4'	19:LN:95:THR:HG22	1.93	0.49
39:SJ:66:MET:HE1	39:SJ:72:ILE:HG12	1.94	0.49
39:SJ:664:ASP:OD1	47:SS:208:GLN:NE2	2.42	0.49
49:SU:640:ASN:OD1	49:SU:641:SER:N	2.45	0.49
39:SJ:11:ARG:O	39:SJ:12:ARG:HD3	2.12	0.49
48:ST:232:VAL:O	48:ST:232:VAL:HG12	2.13	0.49
26:NA:404:TYR:OH	26:NA:442:CYS:O	2.25	0.49
14:LG:107:ASN:OD1	14:LG:111:GLU:N	2.45	0.49
23:LT:33:VAL:HG23	23:LT:38:GLU:HB2	1.95	0.49
10:LA:16:LYS:O	10:LA:101:ASN:ND2	2.46	0.48
5:L3:2045:G:O6	5:L3:3870:C:O2'	2.28	0.48
27:NB:63:GLU:OE1	27:NB:67:ARG:NE	2.46	0.48
33:SC:203:ILE:O	33:SC:203:ILE:HG22	2.13	0.48
5:L3:4724:A:O2'	19:LN:104:THR:HG22	2.13	0.48
12:LC:99:ASP:OD1	12:LC:108:GLN:NE2	2.46	0.48
46:SR:457:GLU:OE2	50:SV:103:ARG:NE	2.44	0.48
29:NH:69:CYS:O	29:NH:84:THR:OG1	2.26	0.48
46:SR:73:ASP:OD1	46:SR:74:ASP:N	2.47	0.48
46:SR:325:GLU:OE2	46:SR:325:GLU:N	2.46	0.48
46:SR:171:LEU:HD23	46:SR:252:LEU:HD11	1.96	0.48
19:LN:167:GLN:OE1	19:LN:169:ARG:NH2	2.47	0.48
40:SK:99:GLU:OE2	40:SK:100:ARG:N	2.46	0.48
46:SR:225:ILE:HG13	46:SR:271:LEU:HD21	1.96	0.48
29:NH:29:ASP:OD1	48:ST:269:LEU:HD21	2.14	0.47
37:SH:42:LEU:HD21	37:SH:95:SER:OG	2.14	0.47
49:SU:416:VAL:HG12	49:SU:514:LEU:HD11	1.96	0.47
5:L3:45:U:O2'	6:L6:14:PHE:O	2.31	0.47
46:SR:88:ASP:O	46:SR:91:HIS:N	2.48	0.47
5:L3:2812:A:N6	39:SJ:78:VAL:HG11	2.29	0.47
5:L3:4760:G:OP1	7:L7:117:ARG:NH2	2.47	0.47
5:L3:1358:G:O2'	5:L3:1360:G:O6	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L6:62:PRO:O	6:L6:63:THR:OG1	2.26	0.47
47:SS:150:VAL:HG23	47:SS:150:VAL:O	2.14	0.47
11:LB:124:ASP:OD1	11:LB:125:GLN:N	2.47	0.47
12:LC:19:THR:HG23	12:LC:22:CYS:H	1.80	0.47
21:LQ:33:ARG:HD3	21:LQ:33:ARG:C	2.40	0.47
26:NA:591:VAL:HG21	26:NA:593:PHE:CE2	2.49	0.47
33:SC:131:LYS:O	33:SC:136:HIS:NE2	2.48	0.47
42:SM:555:LYS:O	42:SM:559:ILE:HD12	2.14	0.47
5:L3:315:G:N7	44:SO:96:ARG:NH2	2.61	0.47
40:SK:73:PRO:O	40:SK:76:THR:HG22	2.14	0.47
5:L3:1364:U:OP2	6:L6:36:ARG:NH2	2.47	0.47
5:L3:1934:A:OP2	27:NB:11:LYS:NZ	2.43	0.47
36:SG:12:ILE:HG12	36:SG:18:ILE:HD12	1.97	0.47
29:NH:147:ALA:N	29:NH:162:VAL:O	2.48	0.46
19:LN:304:SER:OG	19:LN:310:SER:O	2.27	0.46
40:SK:237:ARG:HE	46:SR:360:LEU:HD13	1.80	0.46
49:SU:515:LEU:CD2	49:SU:550:LEU:HD22	2.46	0.46
33:SC:49:VAL:O	33:SC:49:VAL:HG23	2.15	0.46
33:SC:153:LEU:HD11	33:SC:195:ILE:HG13	1.97	0.46
5:L3:1912:G:N2	7:L7:87:MET:HE2	2.31	0.46
5:L3:1955:G:OP2	27:NB:52:ASN:ND2	2.48	0.46
5:L3:2562:G:N2	5:L3:2565:A:OP2	2.47	0.46
18:LL:63:VAL:HG22	18:LL:79:ARG:HG2	1.97	0.46
39:SJ:36:ASN:O	39:SJ:40:GLN:N	2.46	0.46
1:BA:50:THR:CG2	1:BA:58:ILE:HD11	2.45	0.46
5:L3:977:C:O5'	32:SA:333:LYS:NZ	2.48	0.46
5:L3:2334:C:OP2	32:SA:195:LYS:NZ	2.45	0.46
32:SA:339:THR:HG22	32:SA:342:ARG:HH22	1.80	0.46
40:SK:155:SER:OG	40:SK:201:ASP:OD1	2.34	0.46
5:L3:4511:A:H62	19:LN:2:SER:HB3	1.80	0.46
10:LA:73:ALA:HB1	10:LA:78:TRP:O	2.16	0.46
44:SO:226:ASP:OD1	44:SO:227:ALA:N	2.49	0.45
3:L1:62:A:OP1	22:LS:52:LYS:NZ	2.49	0.45
26:NA:277:ILE:HG21	26:NA:294:LEU:HD11	1.98	0.45
46:SR:446:ILE:HG23	46:SR:447:MET:HE2	1.97	0.45
50:SV:115:ASN:O	50:SV:118:LEU:N	2.50	0.45
51:SW:541:LEU:HD12	51:SW:548:LEU:HD11	1.98	0.45
5:L3:2485:U:O2'	42:SM:216:ASP:OD2	2.31	0.45
5:L3:4911:A:OP1	19:LN:97:ARG:NH2	2.49	0.45
5:L3:4939:C:OP1	33:SC:187:ARG:NH1	2.48	0.45
14:LG:61:VAL:O	14:LG:79:ALA:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SN:119:VAL:HG11	44:SO:165:LEU:HD22	1.99	0.45
5:L3:2340:C:H4'	32:SA:42:THR:HG23	1.99	0.45
9:L9:103:GLU:OE1	9:L9:165:THR:HG21	2.16	0.45
7:L7:16:LEU:HD21	7:L7:83:THR:HG21	1.99	0.45
19:LN:306:ASP:OD1	19:LN:307:TYR:N	2.50	0.45
45:SQ:207:MET:SD	45:SQ:216:GLN:NE2	2.90	0.45
46:SR:324:THR:O	46:SR:324:THR:HG23	2.17	0.45
33:SC:133:PHE:O	33:SC:138:ARG:NH2	2.50	0.45
5:L3:2816:G:N2	5:L3:4645:C:O3'	2.49	0.45
16:LI:51:LYS:NZ	16:LI:52:ASP:OD2	2.45	0.45
19:LN:160:ILE:HD11	19:LN:193:LYS:CB	2.47	0.45
40:SK:119:PRO:O	40:SK:139:ARG:NH1	2.47	0.45
44:SO:223:ILE:HD11	44:SO:230:VAL:CG2	2.47	0.45
5:L3:458:C:OP1	18:LL:87:ARG:NH2	2.50	0.45
8:L8:12:VAL:O	8:L8:58:THR:OG1	2.19	0.45
26:NA:311:VAL:HG21	49:SU:775:LEU:HD21	1.99	0.45
47:SS:197:THR:HG22	47:SS:198:ASP:N	2.31	0.45
5:L3:3835:C:HO2'	5:L3:3836:A:P	2.35	0.45
23:LT:33:VAL:HG23	23:LT:38:GLU:CB	2.46	0.45
26:NA:454:LEU:HD12	26:NA:506:LEU:HD22	1.99	0.44
39:SJ:173:GLN:O	39:SJ:201:LEU:HD22	2.18	0.44
3:L1:83:C:H42	16:LI:50:ARG:CZ	2.31	0.44
5:L3:2796:G:H21	49:SU:477:GLU:HG3	1.83	0.44
25:LW:15:THR:HG23	25:LW:16:HIS:ND1	2.33	0.44
35:SE:207:VAL:HG21	35:SE:215:LEU:HD22	1.99	0.44
46:SR:170:THR:HG23	46:SR:249:ALA:HB2	1.98	0.44
5:L3:419:A:N3	5:L3:1332:C:O2'	2.43	0.44
5:L3:5002:U:OP2	19:LN:385:LYS:NZ	2.48	0.44
35:SE:164:ILE:O	35:SE:168:VAL:HG13	2.17	0.44
38:SI:177:THR:HB	47:SS:355:ALA:HB3	1.99	0.44
42:SM:185:ILE:HD11	47:SS:342:PHE:CD2	2.52	0.44
5:L3:425:U:P	10:LA:37:LYS:HZ1	2.41	0.44
19:LN:57:VAL:HG22	19:LN:367:PHE:HB3	1.99	0.44
30:NI:357:LEU:HD11	30:NI:495:LEU:HD22	2.00	0.44
51:SW:231:LEU:HD22	51:SW:235:ILE:HD11	2.00	0.44
51:SW:255:LEU:HD11	51:SW:312:LEU:HD21	1.98	0.44
51:SW:397:VAL:HG22	51:SW:398:ASP:H	1.82	0.44
22:LS:23:ASP:OD1	22:LS:24:LEU:N	2.51	0.44
39:SJ:547:GLU:OE1	49:SU:207:ARG:NH2	2.51	0.44
43:SN:140:MET:CE	44:SO:159:LEU:HD23	2.48	0.44
43:SN:146:GLN:NE2	44:SO:149:LEU:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:SJ:687:ASN:O	39:SJ:690:ASN:ND2	2.51	0.44
39:SJ:690:ASN:O	39:SJ:691:ARG:HG2	2.18	0.44
49:SU:416:VAL:HG21	49:SU:420:MET:CE	2.47	0.44
37:SH:50:ARG:NH2	37:SH:117:GLU:OE1	2.49	0.43
49:SU:591:LEU:HD11	49:SU:603:VAL:HG21	1.98	0.43
4:L2:66:A:OP2	37:SH:168:LYS:NZ	2.45	0.43
5:L3:2814:C:H41	39:SJ:11:ARG:HG2	1.82	0.43
40:SK:103:ALA:O	40:SK:107:VAL:HG23	2.18	0.43
43:SN:62:ARG:NH1	44:SO:58:ASN:OD1	2.51	0.43
46:SR:176:TYR:O	46:SR:179:VAL:HG12	2.18	0.43
1:BA:28:LEU:HB3	1:BA:32:ILE:HD12	2.01	0.43
40:SK:121:LEU:O	40:SK:139:ARG:NH1	2.46	0.43
46:SR:170:THR:C	46:SR:171:LEU:HD12	2.44	0.43
5:L3:3929:G:H21	48:ST:258:PHE:HD2	1.67	0.43
38:SI:237:MET:HE1	38:SI:254:LEU:HD11	2.00	0.43
5:L3:151:G:OP2	9:L9:4:TYR:OH	2.27	0.43
5:L3:709:C:OP1	23:LT:89:ARG:NH2	2.52	0.43
13:LE:103:ASP:OD2	13:LE:104:SER:N	2.51	0.43
30:NI:159:LYS:O	30:NI:160:THR:HG23	2.18	0.43
1:BA:46:ILE:O	1:BA:50:THR:HG23	2.19	0.42
5:L3:4371:G:H1'	5:L3:4372:U:O4'	2.19	0.42
53:SZ:47:LYS:NZ	53:SZ:55:GLU:OE2	2.28	0.42
22:LS:18:LEU:O	22:LS:22:ASP:N	2.49	0.42
49:SU:200:ILE:O	49:SU:204:LEU:HD23	2.20	0.42
19:LN:286:LYS:NZ	19:LN:302:ASN:O	2.36	0.42
29:NH:137:ALA:O	29:NH:139:ILE:N	2.51	0.42
36:SG:85:THR:O	36:SG:86:LEU:HD23	2.20	0.42
39:SJ:203:PRO:HG2	39:SJ:206:VAL:HG22	2.01	0.42
26:NA:394:THR:HG21	26:NA:399:THR:HG21	2.01	0.42
49:SU:322:ARG:HG3	49:SU:322:ARG:O	2.20	0.42
51:SW:298:LEU:HD22	51:SW:322:PHE:CD1	2.54	0.42
26:NA:554:LEU:HD22	26:NA:570:VAL:HG13	2.02	0.42
28:NF:126:ALA:HB3	52:SY:357:ALA:HB2	2.02	0.42
28:NF:235:LYS:HZ1	52:SY:478:ASN:HA	1.84	0.42
40:SK:109:THR:HG22	40:SK:154:PHE:CE1	2.54	0.42
41:SL:255:THR:HG22	41:SL:256:GLU:N	2.35	0.42
5:L3:2836:A:O5'	5:L3:4656:A:N6	2.53	0.42
14:LG:61:VAL:N	14:LG:79:ALA:O	2.46	0.42
32:SA:67:TRP:CE3	32:SA:73:VAL:HG21	2.55	0.42
41:SL:149:LEU:HD21	41:SL:176:ARG:HG3	2.01	0.42
42:SM:170:HIS:HB3	42:SM:283:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L2:68:G:OP2	37:SH:164:ARG:NH2	2.49	0.42
33:SC:278:THR:HG22	33:SC:279:ASN:N	2.35	0.42
49:SU:617:GLN:OE1	49:SU:617:GLN:N	2.52	0.42
51:SW:327:LEU:CD2	51:SW:354:LEU:HD23	2.50	0.42
26:NA:598:GLN:OE1	49:SU:697:ARG:NH1	2.52	0.42
38:SI:98:PHE:HB2	38:SI:152:PRO:HG3	2.02	0.42
5:L3:2481:G:OP1	42:SM:19:THR:HG21	2.20	0.41
24:LU:43:MET:HE2	35:SE:173:LEU:HA	2.02	0.41
42:SM:242:LEU:HD23	42:SM:244:LEU:HD11	2.00	0.41
43:SN:111:GLN:OE1	44:SO:209:THR:HG22	2.20	0.41
43:SN:113:GLN:HG2	44:SO:227:ALA:HB1	2.02	0.41
1:BA:32:ILE:HD13	1:BA:39:PRO:HA	2.02	0.41
5:L3:4597:U:O2'	46:SR:399:ARG:NH2	2.52	0.41
19:LN:56:ILE:HD12	19:LN:365:LEU:HD22	2.01	0.41
26:NA:580:ASN:C	26:NA:580:ASN:HD22	2.27	0.41
31:NK:82:ASN:O	31:NK:86:LEU:N	2.46	0.41
5:L3:4763:U:O2'	12:LC:174:THR:OG1	2.24	0.41
29:NH:81:LEU:HD21	29:NH:89:LEU:HD21	2.02	0.41
40:SK:85:ARG:NH2	40:SK:89:PRO:O	2.53	0.41
52:SY:429:LEU:HD12	52:SY:439:ILE:HD11	2.02	0.41
5:L3:4715:C:H5''	19:LN:278:THR:HG21	2.01	0.41
23:LT:37:ASP:OD1	23:LT:38:GLU:N	2.54	0.41
39:SJ:176:ARG:HH12	39:SJ:201:LEU:HG	1.85	0.41
45:SQ:209:ASP:OD2	45:SQ:211:GLN:N	2.53	0.41
52:SY:227:MET:HE1	52:SY:269:ARG:HD3	2.02	0.41
5:L3:374:G:OP2	25:LW:56:ARG:NH1	2.45	0.41
5:L3:730:G:OP2	34:SD:76:ARG:NE	2.52	0.41
5:L3:308:G:OP2	5:L3:308:G:N2	2.39	0.41
5:L3:976:G:H4'	32:SA:326:LEU:HD13	2.02	0.41
30:NI:205:ARG:HH11	30:NI:205:ARG:HA	1.86	0.41
40:SK:49:VAL:HG12	40:SK:50:HIS:O	2.20	0.41
52:SY:326:GLN:O	52:SY:330:ASN:ND2	2.53	0.41
5:L3:4478:G:N2	5:L3:4608:G:O2'	2.54	0.41
19:LN:86:VAL:HG13	19:LN:162:VAL:CG1	2.50	0.41
4:L2:91:C:OP2	41:SL:176:ARG:NH2	2.54	0.41
5:L3:1279:A:O2'	5:L3:1281:G:N7	2.37	0.41
5:L3:1449:C:OP1	11:LB:132:LYS:NZ	2.54	0.41
5:L3:2072:C:OP1	11:LB:2:GLY:N	2.54	0.41
5:L3:4468:U:O2'	31:NK:2:ALA:N	2.53	0.41
5:L3:4493:U:C5	5:L3:4512:U:H2'	2.56	0.41
11:LB:86:ILE:HD13	11:LB:100:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LQ:124:ASN:OD1	21:LQ:124:ASN:N	2.54	0.41
35:SE:109:GLU:OE2	42:SM:102:ASN:ND2	2.54	0.41
38:SI:155:LYS:NZ	42:SM:270:GLU:OE1	2.35	0.41
46:SR:101:ILE:HG22	46:SR:105:LEU:HD13	2.02	0.41
51:SW:229:LYS:NZ	51:SW:333:ASP:OD2	2.53	0.41
52:SY:314:THR:HG22	52:SY:324:LEU:HD23	2.02	0.41
40:SK:19:LEU:HB3	40:SK:198:VAL:HG22	2.03	0.41
40:SK:79:GLN:OE1	50:SV:1:MET:N	2.54	0.41
5:L3:3837:C:H5''	30:NI:205:ARG:HD2	2.02	0.40
12:LC:92:ASN:ND2	27:NB:49:GLY:O	2.54	0.40
32:SA:340:ILE:CG2	33:SC:50:LEU:HD13	2.41	0.40
45:SQ:86:LYS:H	45:SQ:89:LEU:HD12	1.85	0.40
1:BA:92:ARG:NH2	5:L3:1980:U:OP2	2.54	0.40
1:BA:131:GLU:OE2	5:L3:1973:G:N3	2.55	0.40
40:SK:61:ARG:O	40:SK:105:GLY:N	2.52	0.40
49:SU:556:LEU:HD21	49:SU:603:VAL:HG22	2.03	0.40
1:BA:15:LEU:HD23	1:BA:16:ARG:N	2.35	0.40
19:LN:25:HIS:HD1	19:LN:274:TYR:HH	1.63	0.40
19:LN:312:LYS:NZ	19:LN:368:ILE:O	2.55	0.40
40:SK:101:LEU:HB3	40:SK:107:VAL:HG21	2.04	0.40
1:BA:45:ASP:OD2	1:BA:71:ILE:HD12	2.22	0.40
5:L3:958:G:N2	5:L3:1285:U:OP1	2.44	0.40
5:L3:4433:G:H21	28:NF:191:THR:HG21	1.86	0.40
36:SG:63:ASN:ND2	36:SG:66:GLU:OE1	2.55	0.40
40:SK:121:LEU:O	40:SK:139:ARG:NH2	2.53	0.40
46:SR:292:ASP:OD1	46:SR:293:VAL:N	2.54	0.40
49:SU:416:VAL:HG22	49:SU:417:ARG:N	2.37	0.40
5:L3:1669:A:H2'	5:L3:1670:G:O4'	2.21	0.40
5:L3:4688:C:O2'	36:SG:155:SER:OG	2.38	0.40
11:LB:88:ASP:OD2	11:LB:108:ARG:NH1	2.55	0.40
13:LE:84:ILE:O	13:LE:84:ILE:HG23	2.21	0.40
26:NA:295:LEU:HD21	26:NA:320:VAL:HG11	2.02	0.40
33:SC:211:HIS:NE2	33:SC:249:ASP:OD1	2.51	0.40
41:SL:255:THR:HG22	41:SL:256:GLU:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	158/165 (96%)	158 (100%)	0	0	100	100
2	BB	211/217 (97%)	206 (98%)	5 (2%)	0	100	100
6	L6	118/211 (56%)	115 (98%)	3 (2%)	0	100	100
7	L7	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
8	L8	133/215 (62%)	129 (97%)	4 (3%)	0	100	100
9	L9	179/204 (88%)	179 (100%)	0	0	100	100
10	LA	134/184 (73%)	132 (98%)	2 (2%)	0	100	100
11	LB	149/188 (79%)	149 (100%)	0	0	100	100
12	LC	174/176 (99%)	174 (100%)	0	0	100	100
13	LE	107/160 (67%)	106 (99%)	1 (1%)	0	100	100
14	LG	132/140 (94%)	130 (98%)	2 (2%)	0	100	100
15	LH	129/156 (83%)	129 (100%)	0	0	100	100
16	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
17	LK	104/148 (70%)	101 (97%)	3 (3%)	0	100	100
18	LL	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
19	LN	352/403 (87%)	351 (100%)	1 (0%)	0	100	100
20	LP	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
21	LQ	126/135 (93%)	126 (100%)	0	0	100	100
22	LS	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
23	LT	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
24	LU	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
25	LW	72/97 (74%)	72 (100%)	0	0	100	100
26	NA	480/749 (64%)	480 (100%)	0	0	100	100
27	NB	63/549 (12%)	61 (97%)	2 (3%)	0	100	100
28	NF	210/260 (81%)	207 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	NH	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
30	NI	633/881 (72%)	628 (99%)	5 (1%)	0	100	100
31	NK	65/129 (50%)	65 (100%)	0	0	100	100
32	SA	356/427 (83%)	353 (99%)	3 (1%)	0	100	100
33	SC	197/288 (68%)	194 (98%)	3 (2%)	0	100	100
34	SD	223/248 (90%)	220 (99%)	3 (1%)	0	100	100
35	SE	183/266 (69%)	182 (100%)	1 (0%)	0	100	100
36	SG	189/192 (98%)	185 (98%)	4 (2%)	0	100	100
37	SH	148/293 (50%)	146 (99%)	2 (1%)	0	100	100
38	SI	220/255 (86%)	216 (98%)	4 (2%)	0	100	100
39	SJ	305/847 (36%)	299 (98%)	6 (2%)	0	100	100
40	SK	242/245 (99%)	237 (98%)	5 (2%)	0	100	100
41	SL	241/490 (49%)	236 (98%)	5 (2%)	0	100	100
42	SM	445/588 (76%)	445 (100%)	0	0	100	100
43	SN	169/306 (55%)	169 (100%)	0	0	100	100
44	SO	292/353 (83%)	288 (99%)	4 (1%)	0	100	100
45	SQ	216/239 (90%)	213 (99%)	3 (1%)	0	100	100
46	SR	460/634 (73%)	452 (98%)	8 (2%)	0	100	100
47	SS	237/746 (32%)	236 (100%)	1 (0%)	0	100	100
48	ST	120/365 (33%)	118 (98%)	2 (2%)	0	100	100
49	SU	558/800 (70%)	548 (98%)	10 (2%)	0	100	100
50	SV	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
51	SW	440/670 (66%)	431 (98%)	9 (2%)	0	100	100
52	SY	376/812 (46%)	374 (100%)	2 (0%)	0	100	100
53	SZ	156/178 (88%)	156 (100%)	0	0	100	100
All	All	10696/15900 (67%)	10576 (99%)	120 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	BA	132/137 (96%)	132 (100%)	0	100	100
6	L6	104/177 (59%)	104 (100%)	0	100	100
7	L7	171/174 (98%)	171 (100%)	0	100	100
8	L8	115/161 (71%)	115 (100%)	0	100	100
9	L9	155/172 (90%)	155 (100%)	0	100	100
10	LA	121/163 (74%)	121 (100%)	0	100	100
11	LB	136/165 (82%)	136 (100%)	0	100	100
12	LC	157/157 (100%)	157 (100%)	0	100	100
13	LE	101/140 (72%)	101 (100%)	0	100	100
14	LG	102/107 (95%)	102 (100%)	0	100	100
15	LH	39/133 (29%)	39 (100%)	0	100	100
16	LI	124/135 (92%)	124 (100%)	0	100	100
17	LK	29/121 (24%)	29 (100%)	0	100	100
18	LL	106/121 (88%)	106 (100%)	0	100	100
19	LN	313/348 (90%)	313 (100%)	0	100	100
21	LQ	114/121 (94%)	114 (100%)	0	100	100
22	LS	109/110 (99%)	109 (100%)	0	100	100
23	LT	88/89 (99%)	88 (100%)	0	100	100
24	LU	87/89 (98%)	87 (100%)	0	100	100
25	LW	63/80 (79%)	63 (100%)	0	100	100
26	NA	362/656 (55%)	362 (100%)	0	100	100
27	NB	61/485 (13%)	61 (100%)	0	100	100
28	NF	193/228 (85%)	193 (100%)	0	100	100
29	NH	155/155 (100%)	155 (100%)	0	100	100
30	NI	553/730 (76%)	553 (100%)	0	100	100
31	NK	62/115 (54%)	62 (100%)	0	100	100
32	SA	298/348 (86%)	297 (100%)	1 (0%)	86	94
33	SC	180/252 (71%)	180 (100%)	0	100	100
34	SD	194/215 (90%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	SE	158/223 (71%)	158 (100%)	0	100	100
36	SG	170/171 (99%)	170 (100%)	0	100	100
37	SH	140/274 (51%)	140 (100%)	0	100	100
38	SI	200/228 (88%)	200 (100%)	0	100	100
39	SJ	268/733 (37%)	268 (100%)	0	100	100
40	SK	212/213 (100%)	212 (100%)	0	100	100
41	SL	226/437 (52%)	226 (100%)	0	100	100
42	SM	401/509 (79%)	401 (100%)	0	100	100
43	SN	133/260 (51%)	133 (100%)	0	100	100
44	SO	274/319 (86%)	274 (100%)	0	100	100
45	SQ	195/214 (91%)	195 (100%)	0	100	100
46	SR	422/574 (74%)	422 (100%)	0	100	100
47	SS	214/648 (33%)	214 (100%)	0	100	100
48	ST	78/300 (26%)	78 (100%)	0	100	100
49	SU	486/733 (66%)	486 (100%)	0	100	100
50	SV	127/149 (85%)	127 (100%)	0	100	100
51	SW	393/591 (66%)	393 (100%)	0	100	100
52	SY	325/685 (47%)	325 (100%)	0	100	100
53	SZ	141/158 (89%)	141 (100%)	0	100	100
All	All	8987/13503 (67%)	8986 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
32	SA	278	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	68	GLN
1	BA	97	ASN
6	L6	15	HIS
8	L8	34	ASN
8	L8	69	HIS

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Mol	Chain	Res	Type
9	L9	32	GLN
10	LA	54	GLN
10	LA	97	ASN
11	LB	7	HIS
12	LC	37	HIS
13	LE	70	HIS
13	LE	127	GLN
13	LE	131	GLN
16	LI	127	GLN
17	LK	66	ASN
18	LL	70	GLN
18	LL	95	HIS
18	LL	121	GLN
19	LN	109	HIS
19	LN	121	ASN
19	LN	184	GLN
19	LN	203	GLN
19	LN	275	HIS
22	LS	20	GLN
23	LT	21	GLN
23	LT	24	HIS
23	LT	78	HIS
23	LT	99	HIS
24	LU	15	HIS
24	LU	20	ASN
24	LU	26	HIS
24	LU	36	HIS
25	LW	48	ASN
26	NA	376	HIS
26	NA	572	GLN
26	NA	580	ASN
28	NF	33	HIS
28	NF	127	GLN
28	NF	223	ASN
29	NH	111	ASN
30	NI	329	HIS
30	NI	333	ASN
30	NI	588	GLN
30	NI	707	GLN
30	NI	775	GLN
30	NI	832	GLN
31	NK	90	HIS

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Mol	Chain	Res	Type
32	SA	278	ASN
32	SA	329	ASN
34	SD	56	HIS
35	SE	64	GLN
35	SE	208	ASN
37	SH	119	HIS
38	SI	94	HIS
38	SI	219	HIS
38	SI	225	HIS
39	SJ	712	HIS
39	SJ	726	HIS
40	SK	162	HIS
41	SL	225	HIS
42	SM	154	HIS
42	SM	211	HIS
42	SM	572	HIS
44	SO	204	HIS
44	SO	219	ASN
45	SQ	47	ASN
46	SR	37	HIS
46	SR	157	HIS
46	SR	209	HIS
46	SR	228	HIS
46	SR	246	HIS
46	SR	342	HIS
47	SS	269	GLN
47	SS	310	HIS
48	ST	200	GLN
48	ST	208	HIS
49	SU	217	HIS
49	SU	246	GLN
49	SU	355	HIS
49	SU	491	HIS
49	SU	583	HIS
49	SU	592	HIS
49	SU	597	ASN
49	SU	636	HIS
50	SV	17	HIS
50	SV	76	ASN
50	SV	115	ASN
50	SV	129	GLN
50	SV	132	HIS

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Mol	Chain	Res	Type
51	SW	499	GLN
52	SY	315	ASN
52	SY	430	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L1	150/157 (95%)	18 (12%)	0
4	L2	65/1167 (5%)	10 (15%)	0
5	L3	2234/5070 (44%)	303 (13%)	6 (0%)
All	All	2449/6394 (38%)	331 (13%)	6 (0%)

All (331) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L1	34	U
3	L1	52	A
3	L1	54	C
3	L1	55	U
3	L1	59	A
3	L1	62	A
3	L1	63	U
3	L1	82	A
3	L1	83	C
3	L1	84	A
3	L1	86	U
3	L1	94	G
3	L1	103	A
3	L1	105	C
3	L1	110	U
3	L1	111	U
3	L1	114	G
3	L1	156	U
4	L2	2	C
4	L2	11	C
4	L2	48	G
4	L2	49	G
4	L2	62	U
4	L2	87	G
4	L2	94	U
4	L2	95	A

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Mol	Chain	Res	Type
4	L2	96	A
4	L2	101	A
5	L3	41	C
5	L3	48	G
5	L3	56	A
5	L3	58	G
5	L3	59	A
5	L3	64	A
5	L3	65	A
5	L3	69	A
5	L3	89	C
5	L3	91	G
5	L3	92	C
5	L3	93	G
5	L3	95	G
5	L3	116	G
5	L3	119	G
5	L3	159	C
5	L3	170	C
5	L3	171	U
5	L3	172	C
5	L3	173	C
5	L3	181	C
5	L3	186	G
5	L3	197	A
5	L3	200	U
5	L3	210	C
5	L3	218	A
5	L3	233	U
5	L3	234	G
5	L3	257	C
5	L3	261	G
5	L3	264	C
5	L3	265	C
5	L3	281	U
5	L3	315	G
5	L3	340	C
5	L3	349	A
5	L3	362	A
5	L3	386	A
5	L3	387	G
5	L3	399	G

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Mol	Chain	Res	Type
5	L3	410	A
5	L3	413	G
5	L3	414	C
5	L3	431	G
5	L3	449	C
5	L3	450	G
5	L3	452	A
5	L3	453	G
5	L3	454	U
5	L3	464	G
5	L3	467	U
5	L3	468	U
5	L3	472	C
5	L3	685	C
5	L3	697	G
5	L3	699	C
5	L3	704	C
5	L3	730	G
5	L3	731	G
5	L3	739	G
5	L3	742	G
5	L3	746	A
5	L3	913	U
5	L3	914	U
5	L3	915	A
5	L3	917	A
5	L3	926	G
5	L3	932	A
5	L3	933	G
5	L3	943	A
5	L3	944	A
5	L3	945	U
5	L3	956	A
5	L3	959	G
5	L3	960	A
5	L3	1072	C
5	L3	1280	C
5	L3	1284	G
5	L3	1287	G
5	L3	1293	G
5	L3	1294	A
5	L3	1295	C

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Mol	Chain	Res	Type
5	L3	1296	G
5	L3	1301	C
5	L3	1313	C
5	L3	1314	C
5	L3	1337	A
5	L3	1354	A
5	L3	1358	G
5	L3	1359	G
5	L3	1378	C
5	L3	1379	C
5	L3	1435	G
5	L3	1447	C
5	L3	1448	G
5	L3	1497	A
5	L3	1498	G
5	L3	1500	A
5	L3	1525	A
5	L3	1654	G
5	L3	1661	C
5	L3	1670	G
5	L3	1682	A
5	L3	1691	G
5	L3	1726	U
5	L3	1804	A
5	L3	1810	G
5	L3	1836	G
5	L3	1837	A
5	L3	1842	G
5	L3	1853	G
5	L3	1856	C
5	L3	1870	C
5	L3	1881	C
5	L3	1891	A
5	L3	1897	A
5	L3	1910	G
5	L3	1918	U
5	L3	1921	C
5	L3	1922	G
5	L3	1925	G
5	L3	1931	C
5	L3	1935	C
5	L3	1938	C

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Mol	Chain	Res	Type
5	L3	1941	A
5	L3	1944	A
5	L3	1945	G
5	L3	1969	G
5	L3	1984	A
5	L3	1997	U
5	L3	2002	A
5	L3	2024	G
5	L3	2025	A
5	L3	2026	A
5	L3	2044	U
5	L3	2046	G
5	L3	2055	G
5	L3	2056	G
5	L3	2069	A
5	L3	2084	C
5	L3	2085	G
5	L3	2089	G
5	L3	2090	U
5	L3	2091	C
5	L3	2268	A
5	L3	2289	C
5	L3	2300	A
5	L3	2301	G
5	L3	2313	A
5	L3	2314	G
5	L3	2348	G
5	L3	2351	C
5	L3	2374	A
5	L3	2378	G
5	L3	2382	A
5	L3	2383	C
5	L3	2384	U
5	L3	2395	A
5	L3	2396	A
5	L3	2397	G
5	L3	2398	U
5	L3	2474	G
5	L3	2484	A
5	L3	2485	U
5	L3	2490	U
5	L3	2492	C

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Mol	Chain	Res	Type
5	L3	2493	G
5	L3	2500	U
5	L3	2574	G
5	L3	2769	U
5	L3	2796	G
5	L3	2798	A
5	L3	2799	G
5	L3	2814	C
5	L3	2818	C
5	L3	2844	A
5	L3	2845	A
5	L3	2848	G
5	L3	2852	U
5	L3	2853	C
5	L3	3630	A
5	L3	3835	C
5	L3	3836	A
5	L3	3845	A
5	L3	3853	U
5	L3	3868	G
5	L3	3877	A
5	L3	3878	C
5	L3	3879	G
5	L3	3881	G
5	L3	3887	C
5	L3	3889	G
5	L3	3894	A
5	L3	3895	G
5	L3	3906	A
5	L3	3907	G
5	L3	3908	A
5	L3	3920	U
5	L3	3926	C
5	L3	3930	U
5	L3	3938	G
5	L3	3939	G
5	L3	3940	U
5	L3	3941	G
5	L3	3942	A
5	L3	3967	G
5	L3	4049	U
5	L3	4064	C

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Mol	Chain	Res	Type
5	L3	4183	G
5	L3	4348	A
5	L3	4349	C
5	L3	4350	C
5	L3	4357	G
5	L3	4372	U
5	L3	4373	G
5	L3	4376	A
5	L3	4380	A
5	L3	4385	A
5	L3	4390	A
5	L3	4392	G
5	L3	4393	G
5	L3	4398	C
5	L3	4401	G
5	L3	4433	G
5	L3	4437	U
5	L3	4438	U
5	L3	4439	U
5	L3	4441	A
5	L3	4442	U
5	L3	4451	G
5	L3	4464	A
5	L3	4466	C
5	L3	4475	G
5	L3	4476	C
5	L3	4480	A
5	L3	4494	G
5	L3	4495	G
5	L3	4496	A
5	L3	4499	G
5	L3	4512	U
5	L3	4513	A
5	L3	4518	A
5	L3	4521	U
5	L3	4522	G
5	L3	4523	A
5	L3	4538	G
5	L3	4540	C
5	L3	4541	G
5	L3	4545	G
5	L3	4546	A

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Mol	Chain	Res	Type
5	L3	4548	A
5	L3	4549	G
5	L3	4550	G
5	L3	4551	U
5	L3	4552	U
5	L3	4568	A
5	L3	4584	A
5	L3	4590	A
5	L3	4608	G
5	L3	4652	G
5	L3	4653	C
5	L3	4656	A
5	L3	4657	U
5	L3	4670	C
5	L3	4671	C
5	L3	4672	A
5	L3	4678	G
5	L3	4684	A
5	L3	4708	A
5	L3	4709	U
5	L3	4719	G
5	L3	4720	C
5	L3	4721	G
5	L3	4741	C
5	L3	4742	G
5	L3	4745	G
5	L3	4751	G
5	L3	4754	G
5	L3	4757	C
5	L3	4759	C
5	L3	4765	G
5	L3	4772	C
5	L3	4773	C
5	L3	4870	G
5	L3	4871	C
5	L3	4880	C
5	L3	4882	U
5	L3	4883	C
5	L3	4900	C
5	L3	4901	G
5	L3	4910	G
5	L3	4914	C

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Mol	Chain	Res	Type
5	L3	4943	A
5	L3	4976	U
5	L3	5006	U
5	L3	5013	C
5	L3	5014	A
5	L3	5020	G
5	L3	5026	U
5	L3	5030	U
5	L3	5041	G
5	L3	5050	C
5	L3	5062	G

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L3	2267	U
5	L3	2798	A
5	L3	3835	C
5	L3	4347	G
5	L3	4520	G
5	L3	5013	C

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

2 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	$\# Z > 2$
47	SEP	SS	127	47	8,9,10	1.60	1 (12%)	7,12,14	1.26	1 (14%)
47	SEP	SS	126	47	8,9,10	1.59	1 (12%)	7,12,14	1.25	1 (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
47	SEP	SS	127	47	-	1/6/8/10	-
47	SEP	SS	126	47	-	0/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	SS	127	SEP	P-O1P	3.48	1.61	1.50
47	SS	126	SEP	P-O1P	3.47	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	SS	126	SEP	OG-CB-CA	2.61	110.68	108.14
47	SS	127	SEP	OG-CB-CA	2.60	110.67	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	SS	127	SEP	N-CA-CB-OG

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 64 ligands modelled in this entry, 62 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	GDP	SR	1001	58,54	29,30,30	3.03	12 (41%)	45,47,47	2.66	17 (37%)
56	ADP	NI	1001	54	28,29,29	1.37	4 (14%)	43,45,45	1.90	10 (23%)

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
57	GDP	SR	1001	58,54	-	0/16/32/32	0/3/3/3
56	ADP	NI	1001	54	-	6/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	SR	1001	GDP	O6-C6	8.77	1.40	1.23
57	SR	1001	GDP	C5-N7	6.53	1.52	1.39
57	SR	1001	GDP	PA-O3A	5.01	1.64	1.59
57	SR	1001	GDP	C2-N2	4.78	1.45	1.34
56	NI	1001	ADP	C5-C4	4.38	1.46	1.39
57	SR	1001	GDP	C8-N9	-4.05	1.28	1.37
57	SR	1001	GDP	C4-N9	-3.88	1.28	1.38
57	SR	1001	GDP	C5-C4	3.75	1.49	1.38
57	SR	1001	GDP	C4-N3	2.81	1.40	1.34
56	NI	1001	ADP	C5-C6	2.57	1.48	1.41
57	SR	1001	GDP	PB-O2B	-2.33	1.46	1.54
57	SR	1001	GDP	PB-O3B	-2.32	1.46	1.54
56	NI	1001	ADP	C5-N7	-2.31	1.34	1.39
56	NI	1001	ADP	C8-N7	2.27	1.36	1.31
57	SR	1001	GDP	O4'-C1'	2.25	1.47	1.42
57	SR	1001	GDP	C2'-C3'	-2.09	1.47	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	SR	1001	GDP	C8-N9-C4	7.84	120.73	106.03
57	SR	1001	GDP	C5-C4-N3	-6.72	117.69	128.39
57	SR	1001	GDP	N9-C4-N3	6.72	139.38	125.95
56	NI	1001	ADP	C5-C4-N3	-5.79	118.75	126.72
57	SR	1001	GDP	C2-N3-C4	5.30	121.44	112.30
57	SR	1001	GDP	C6-C5-N7	4.71	138.87	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	NI	1001	ADP	N3-C4-N9	4.66	135.09	127.17
57	SR	1001	GDP	C4-C5-N7	-4.59	103.40	110.67
56	NI	1001	ADP	C2-N3-C4	3.88	121.31	111.83
56	NI	1001	ADP	N3-C2-N1	-3.73	122.93	128.58
56	NI	1001	ADP	C4-C5-N7	-3.48	106.60	110.58
56	NI	1001	ADP	C4-N9-C8	3.08	108.97	105.74
57	SR	1001	GDP	N9-C8-N7	-3.04	107.77	113.40
57	SR	1001	GDP	C2-N1-C6	-2.96	119.74	125.11
57	SR	1001	GDP	O2B-PB-O3A	2.88	114.28	104.64
57	SR	1001	GDP	O3B-PB-O3A	2.78	113.96	104.64
56	NI	1001	ADP	C5-N7-C8	2.75	107.77	103.45
57	SR	1001	GDP	C1'-N9-C4	-2.57	118.90	126.49
57	SR	1001	GDP	C5-C6-N1	2.56	119.77	113.25
57	SR	1001	GDP	C3'-C2'-C1'	2.47	106.13	101.46
57	SR	1001	GDP	C2'-C3'-C4'	2.46	107.37	102.61
56	NI	1001	ADP	N9-C8-N7	-2.43	110.49	113.94
57	SR	1001	GDP	O6-C6-C5	-2.41	120.16	126.53
57	SR	1001	GDP	O2A-PA-O1A	-2.32	101.64	112.44
57	SR	1001	GDP	C1'-N9-C8	-2.25	120.35	126.73
56	NI	1001	ADP	C3'-C2'-C1'	2.21	105.64	101.46
56	NI	1001	ADP	C6-C5-N7	2.18	136.30	132.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

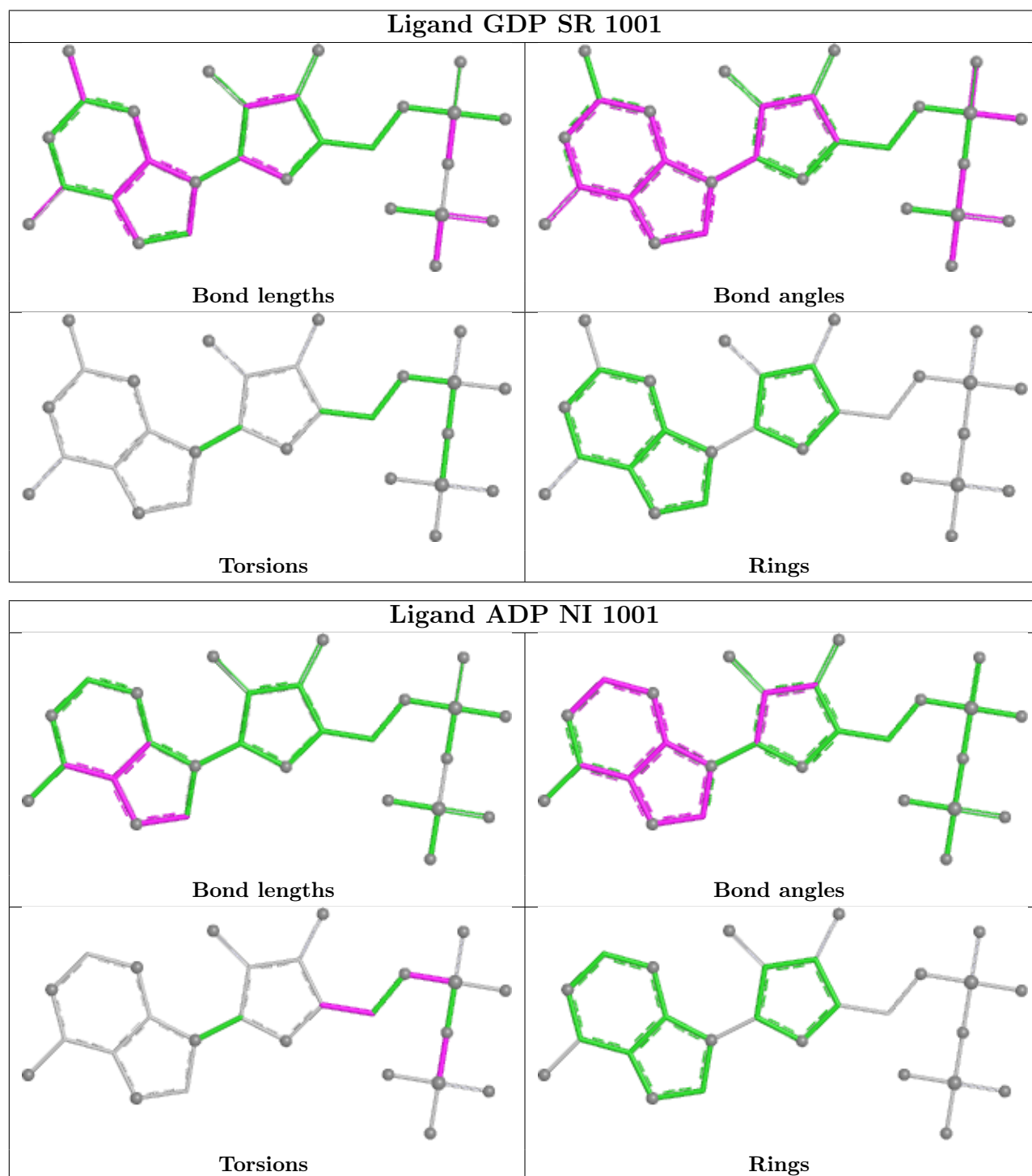
Mol	Chain	Res	Type	Atoms
56	NI	1001	ADP	C5'-O5'-PA-O2A
56	NI	1001	ADP	O4'-C4'-C5'-O5'
56	NI	1001	ADP	C3'-C4'-C5'-O5'
56	NI	1001	ADP	PA-O3A-PB-O1B
56	NI	1001	ADP	PA-O3A-PB-O2B
56	NI	1001	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	L3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L3	2403:A	O3'	2473:A	P	61.05

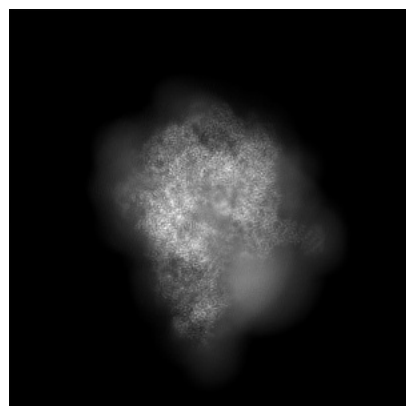
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29259. These allow visual inspection of the internal detail of the map and identification of artifacts.

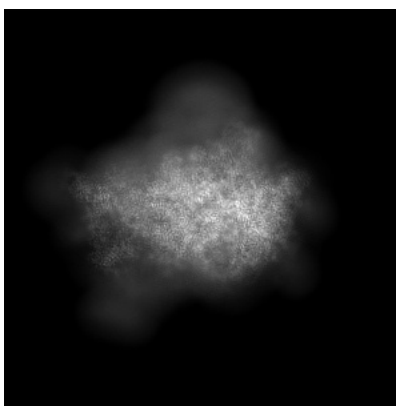
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

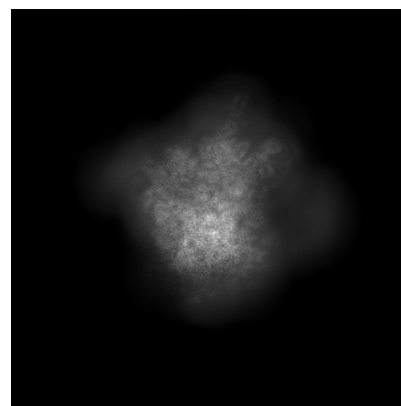
6.1.1 Primary map



X

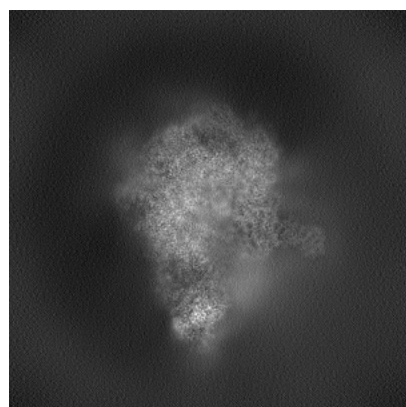


Y

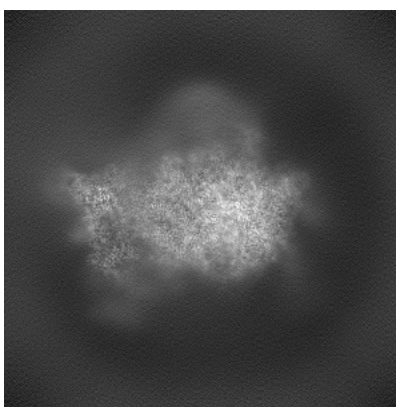


Z

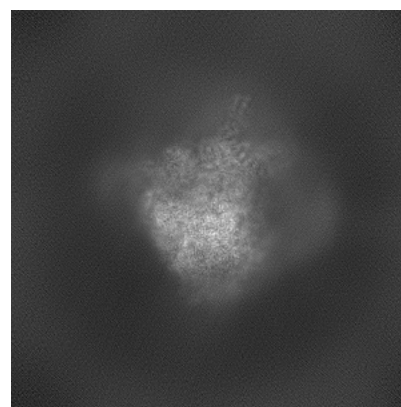
6.1.2 Raw map



X



Y

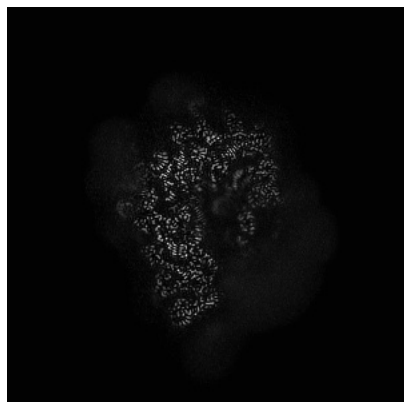


Z

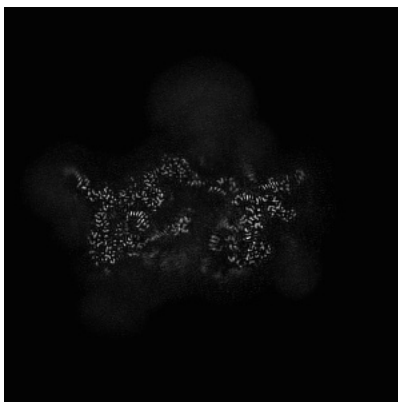
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

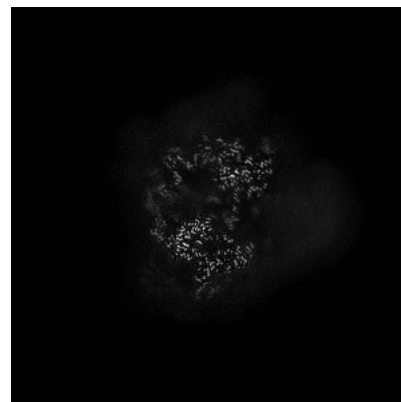
6.2.1 Primary map



X Index: 240

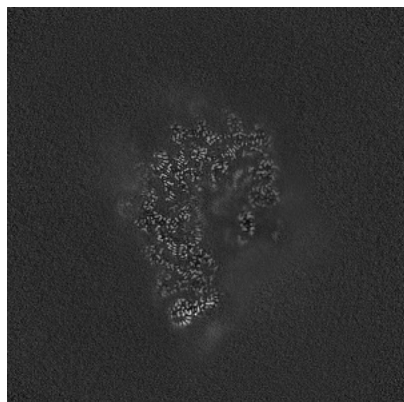


Y Index: 240

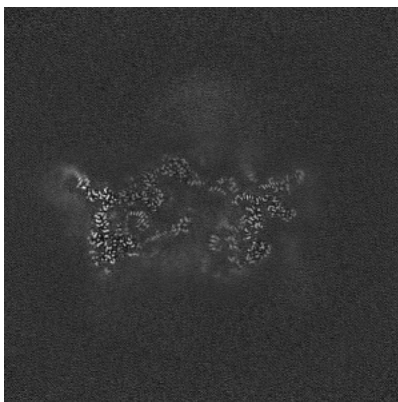


Z Index: 240

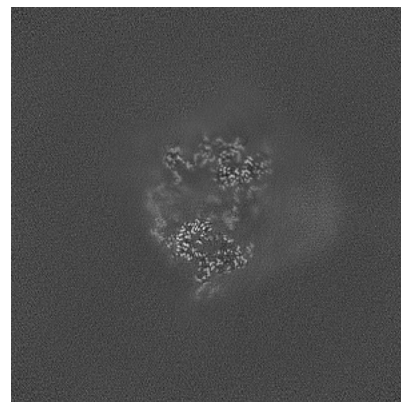
6.2.2 Raw map



X Index: 240



Y Index: 240

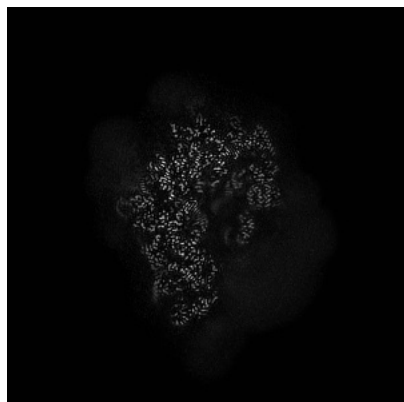


Z Index: 240

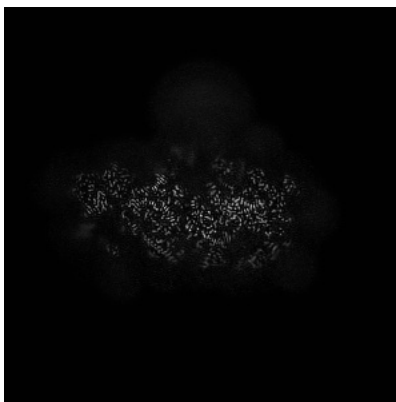
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

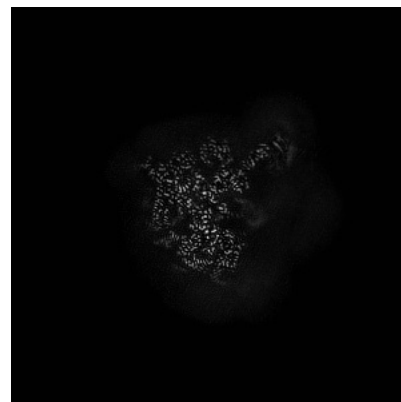
6.3.1 Primary map



X Index: 237

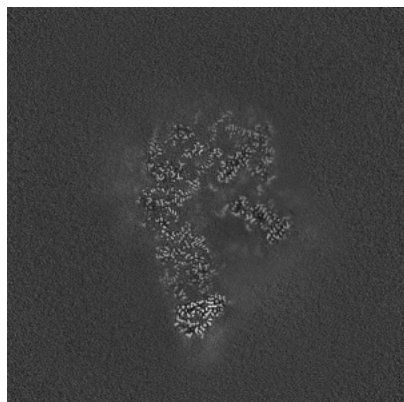


Y Index: 211

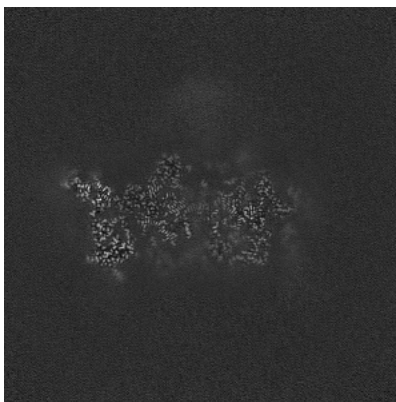


Z Index: 289

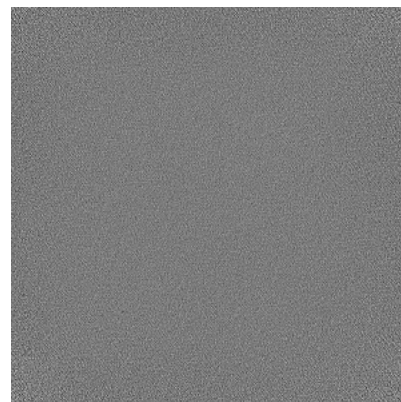
6.3.2 Raw map



X Index: 254



Y Index: 228

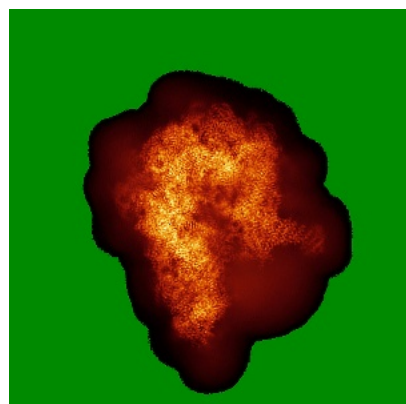


Z Index: 0

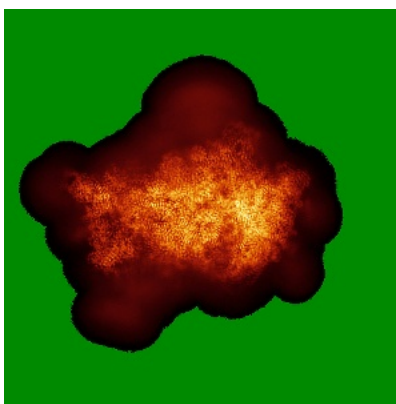
The images above show the largest variance slices of the map in three orthogonal directions.

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

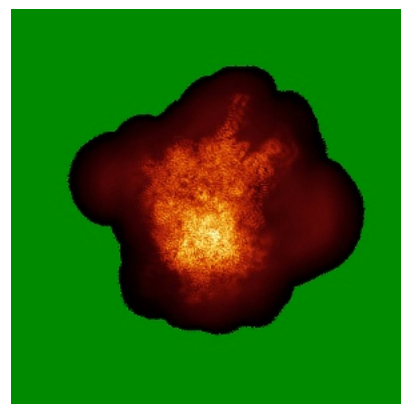
6.4.1 Primary map



X

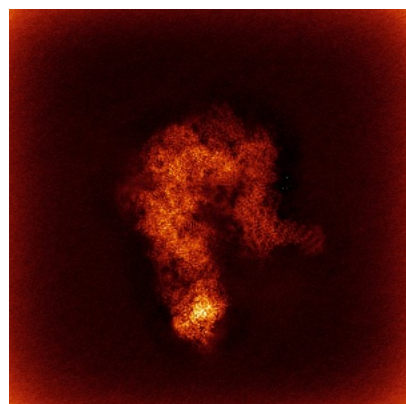


Y

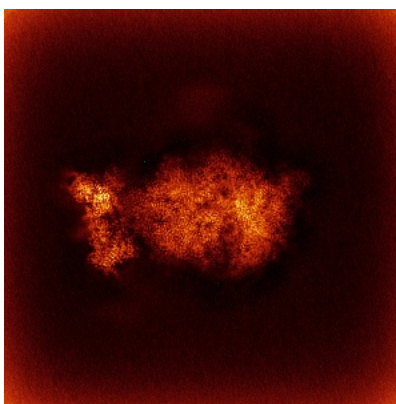


Z

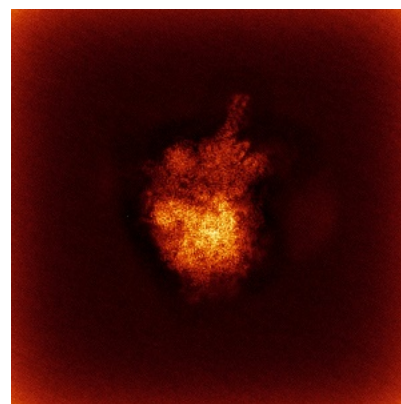
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

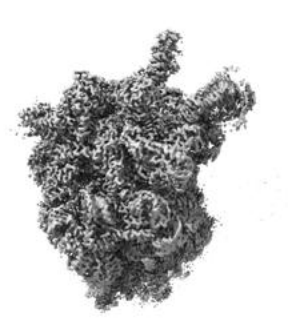
6.5.1 Primary map



X



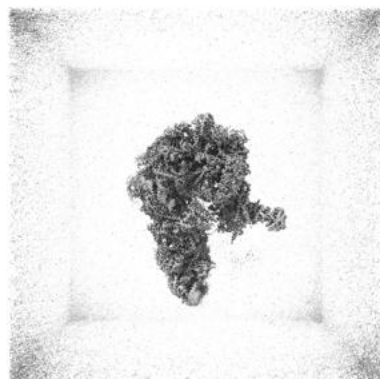
Y



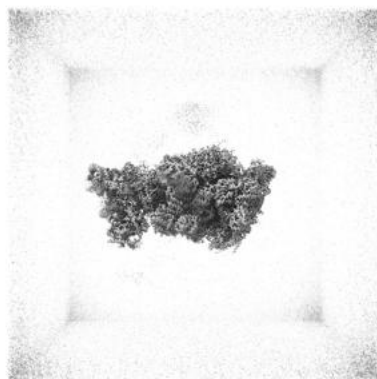
Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. 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



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

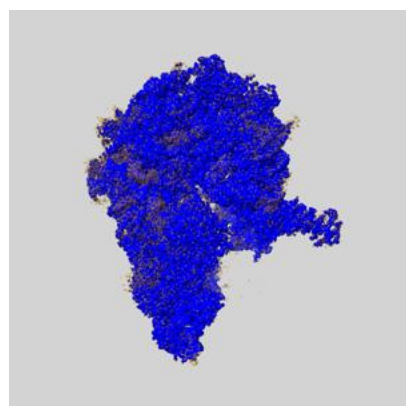
6.6 Mask visualisation [i](#)

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

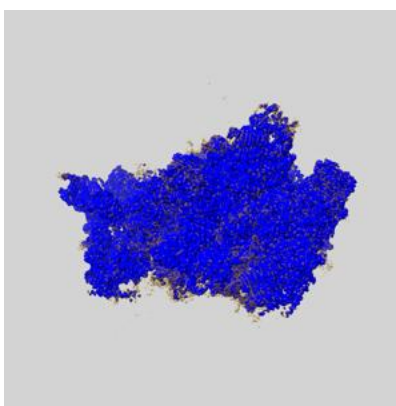
A mask typically either:

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

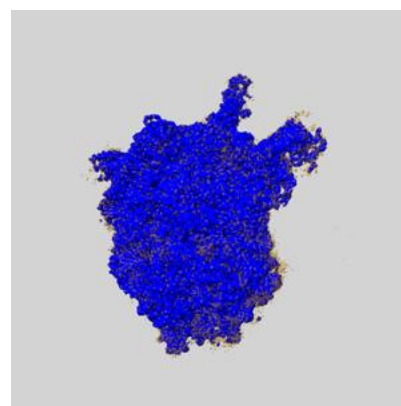
6.6.1 emd_29259_msk_1.map [i](#)



X



Y

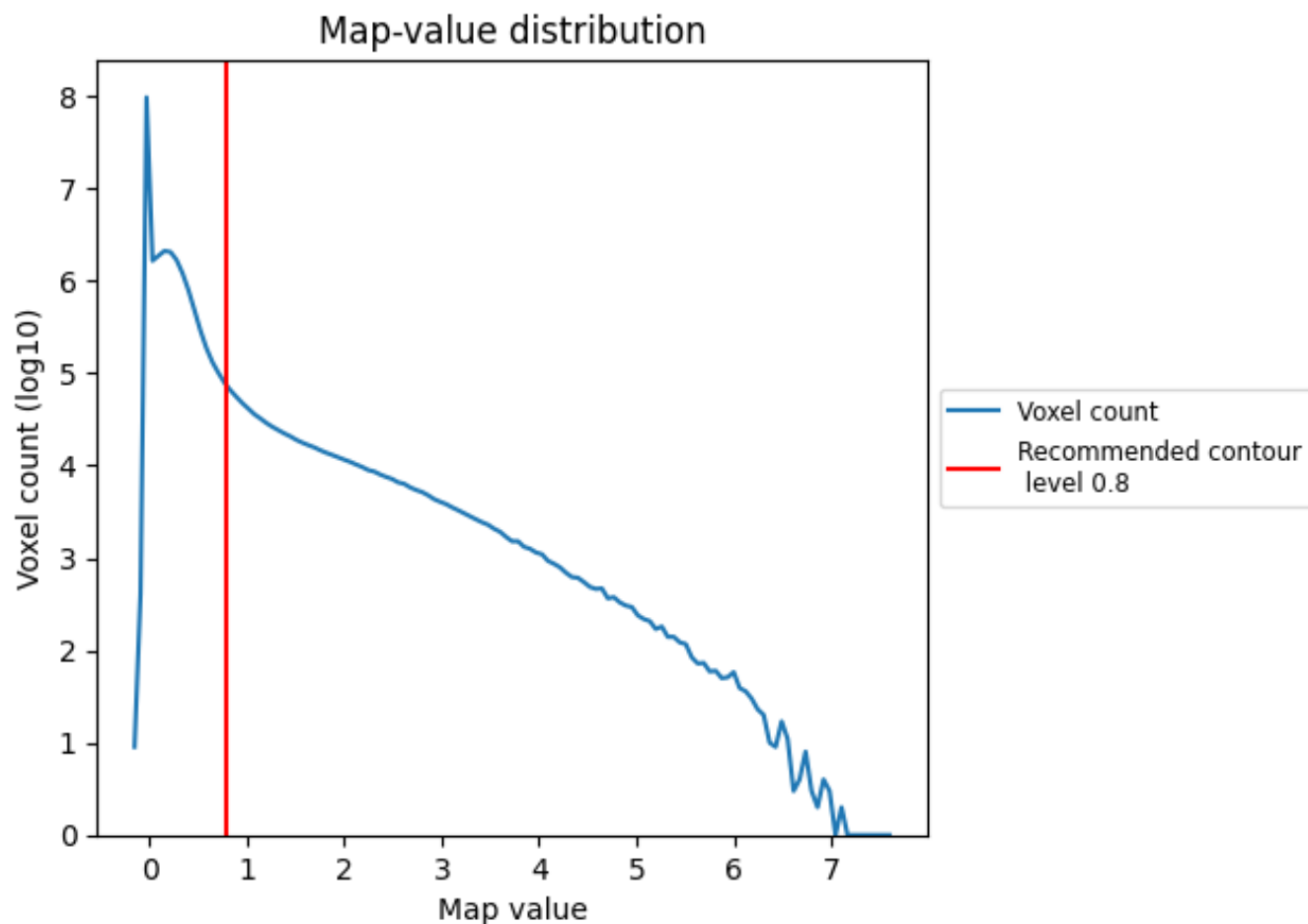


Z

7 Map analysis [i](#)

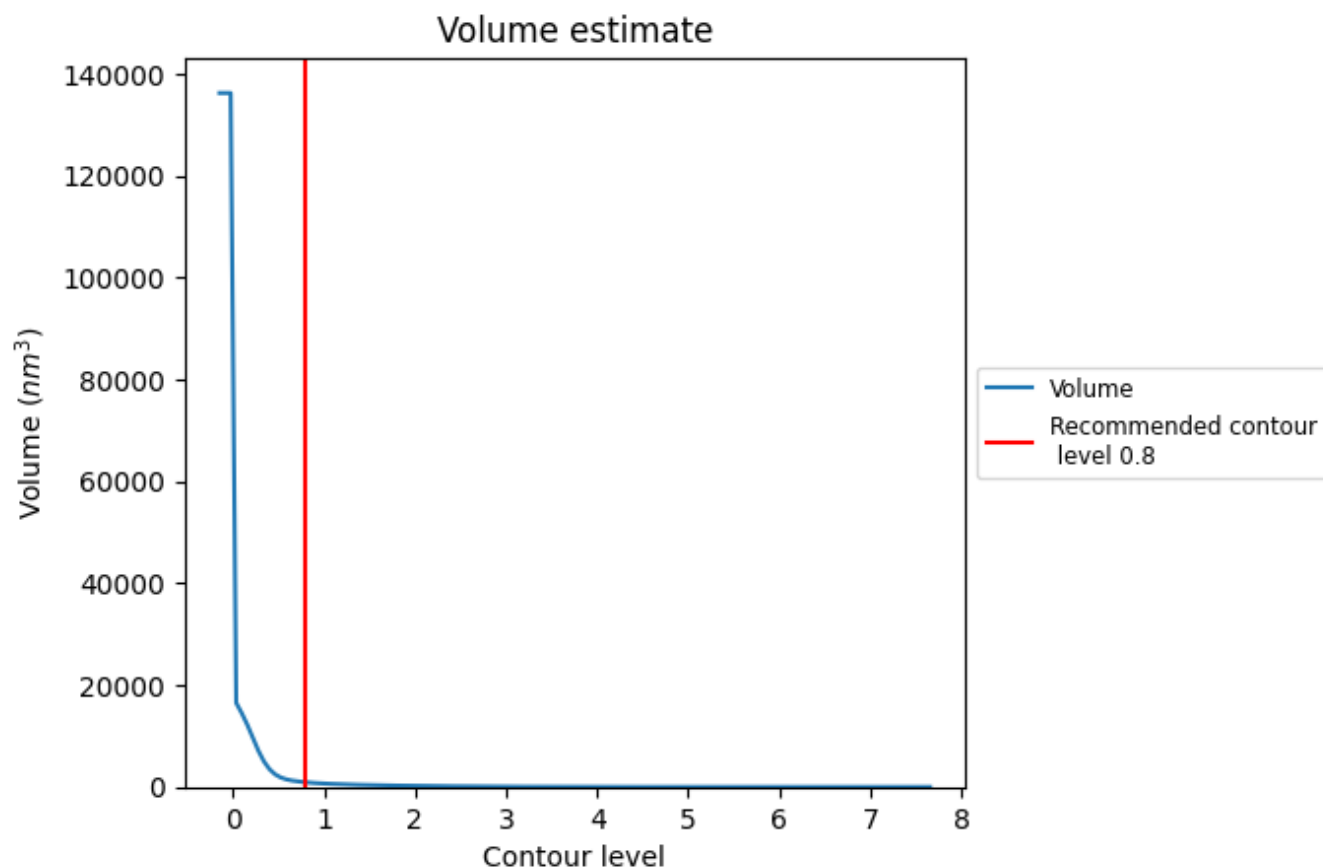
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

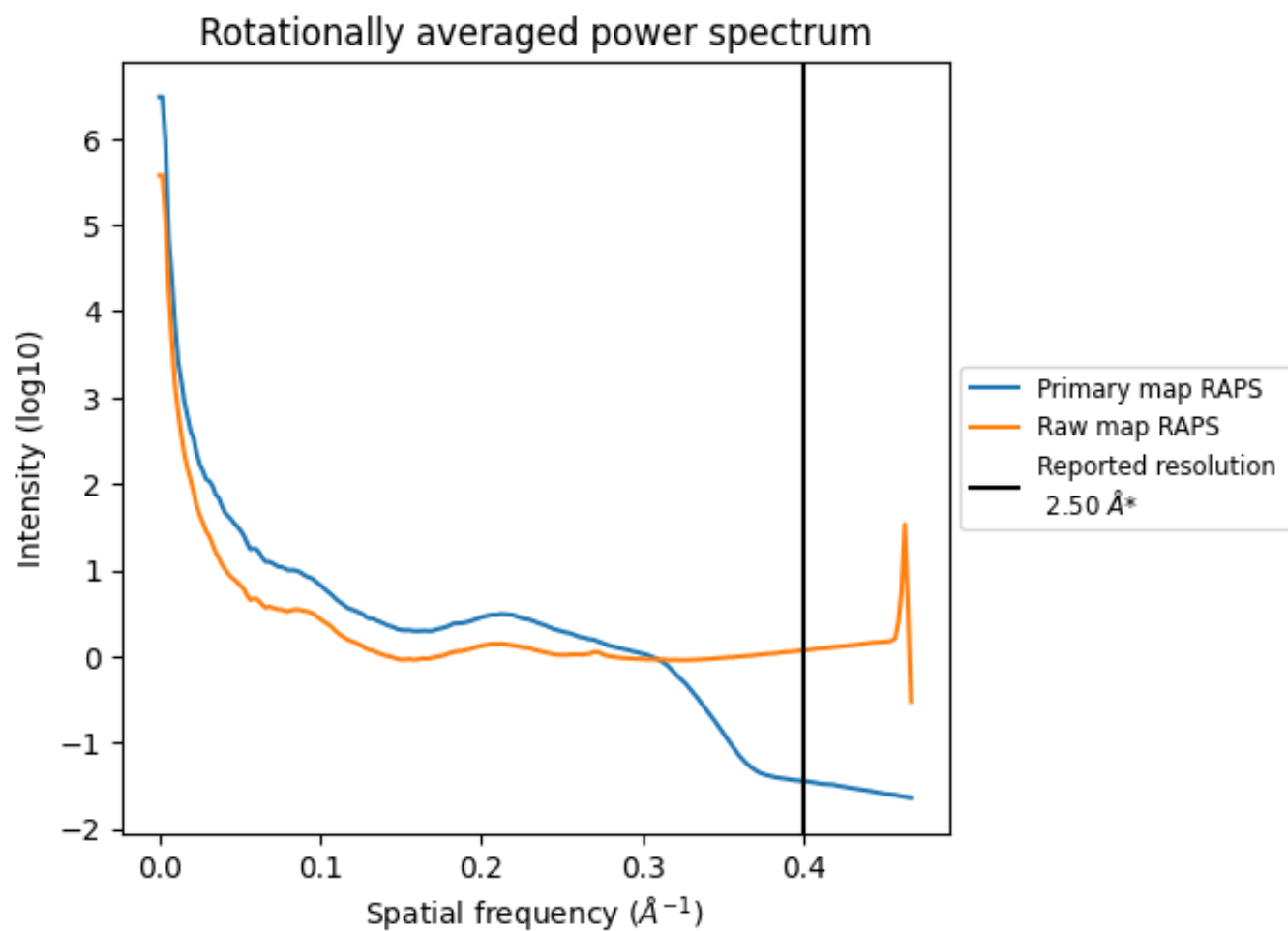
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 913 nm^3 ; this corresponds to an approximate mass of 825 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 ⓘ

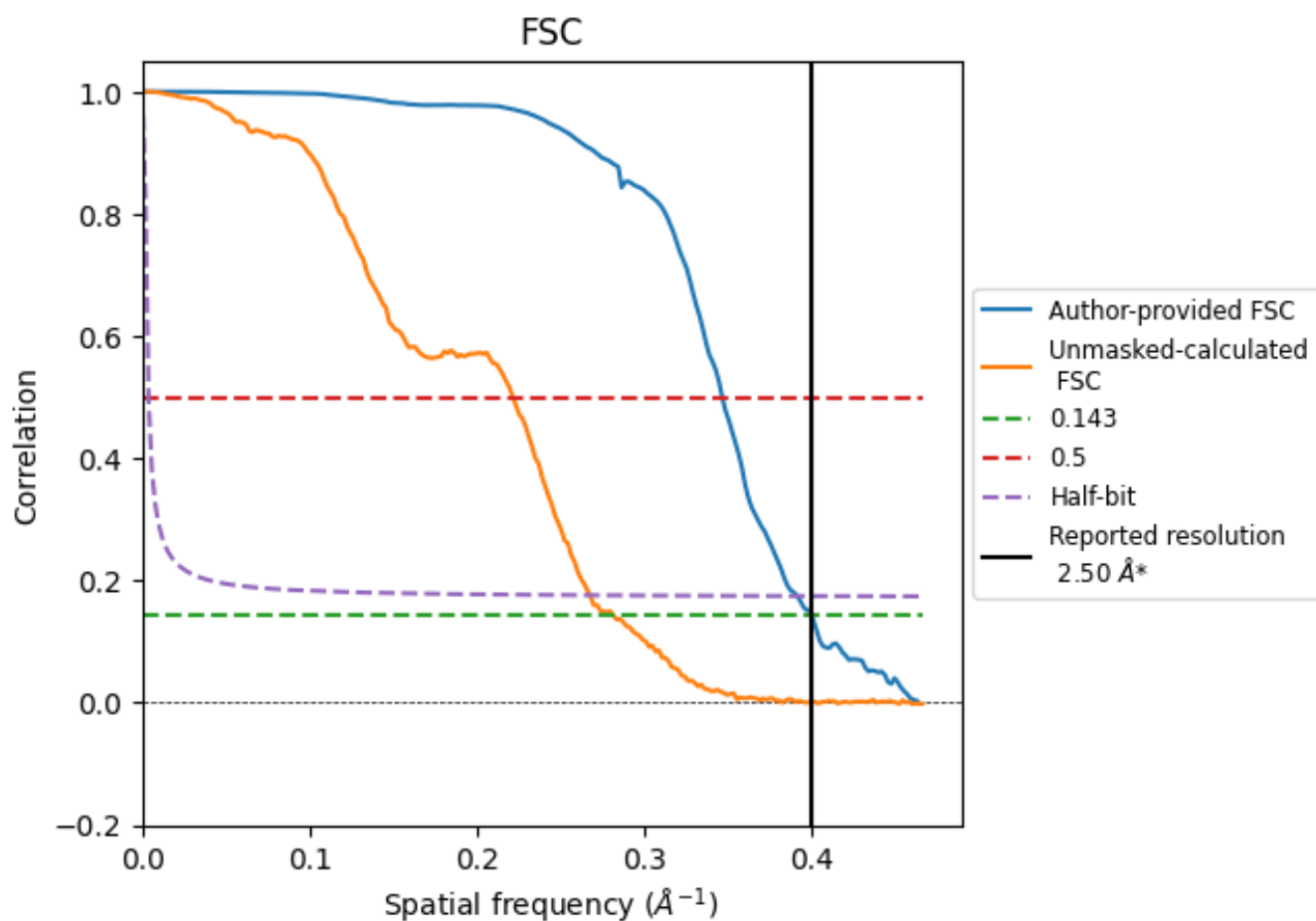


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

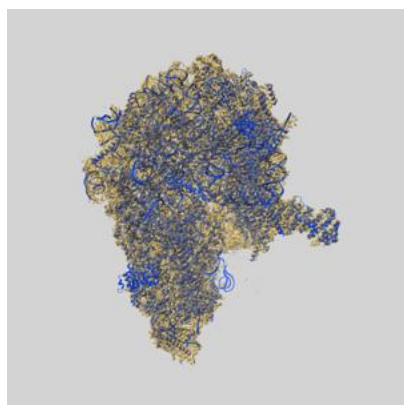
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.88	2.55
Unmasked-calculated*	3.55	4.51	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.55 differs from the reported value 2.5 by more than 10 %

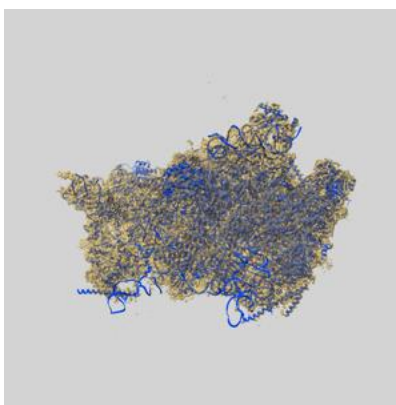
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29259 and PDB model 8FKW. Per-residue inclusion information can be found in section [3](#) on page [15](#).

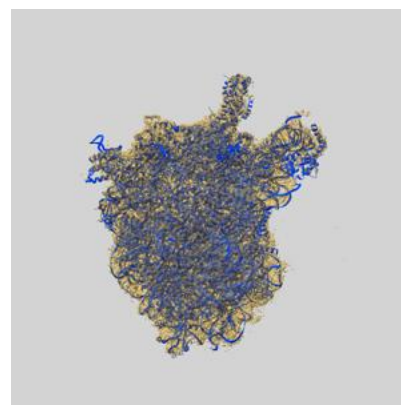
9.1 Map-model overlay [i](#)



X



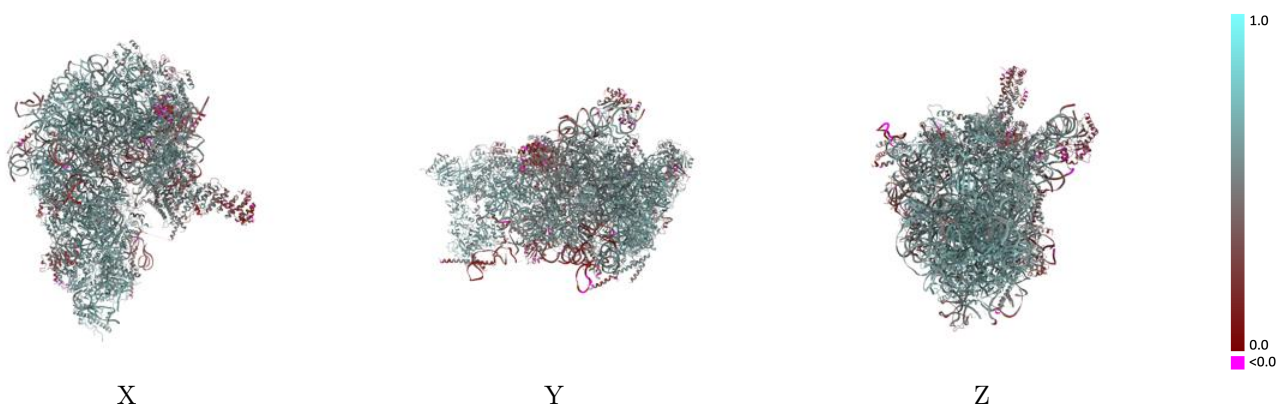
Y



Z

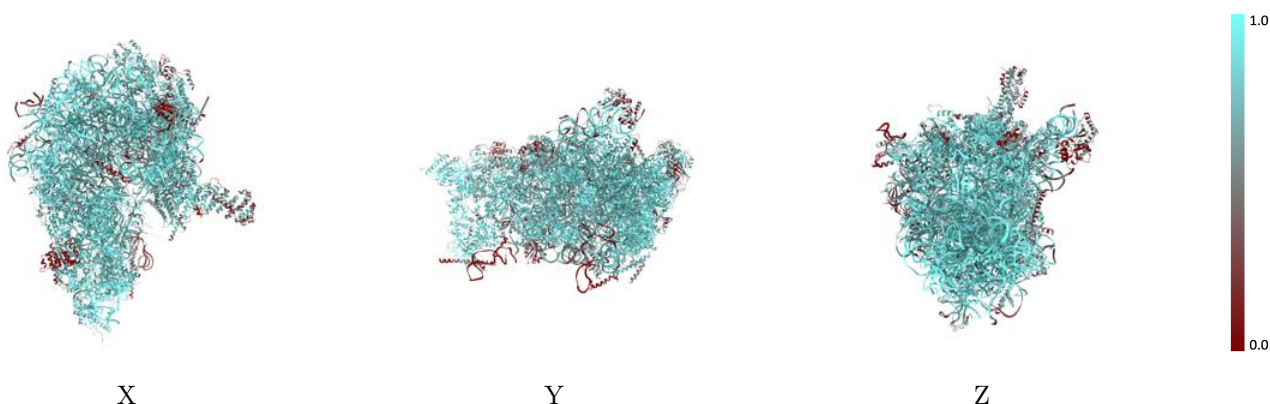
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



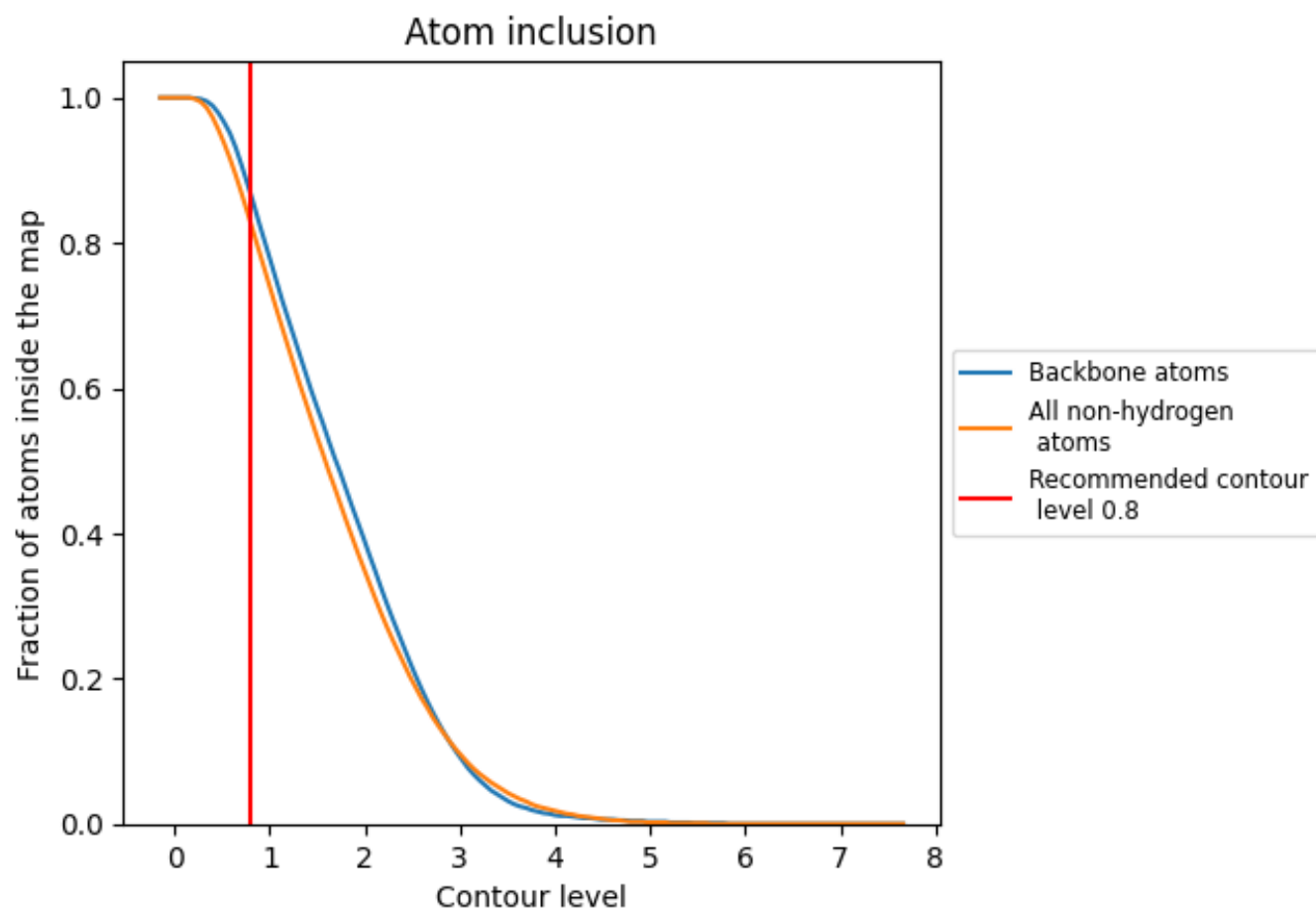
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.5460
BA	 0.4360	 0.4090
BB	 0.3090	 0.2810
L1	 0.9150	 0.5730
L2	 0.9480	 0.5970
L3	 0.8660	 0.5430
L6	 0.9360	 0.6150
L7	 0.9400	 0.6170
L8	 0.9410	 0.6270
L9	 0.9740	 0.6440
LA	 0.6690	 0.4820
LB	 0.9500	 0.6270
LC	 0.9450	 0.6280
LE	 0.6250	 0.4510
LG	 0.8590	 0.5800
LH	 0.4300	 0.3550
LI	 0.9060	 0.6060
LK	 0.7480	 0.4310
LL	 0.9490	 0.6170
LN	 0.8880	 0.6020
LP	 0.4450	 0.3580
LQ	 0.9580	 0.6320
LS	 0.8160	 0.5510
LT	 0.9700	 0.6480
LU	 0.8470	 0.5920
LW	 0.9490	 0.6130
NA	 0.7000	 0.4050
NB	 0.7510	 0.5480
NF	 0.8680	 0.5840
NH	 0.9170	 0.5700
NI	 0.8010	 0.5220
NK	 0.7500	 0.5490
SA	 0.9020	 0.6180
SC	 0.8150	 0.5660
SD	 0.9050	 0.6010



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SE	 0.9250	 0.6270
SG	 0.8970	 0.6130
SH	 0.8760	 0.6010
SI	 0.8570	 0.5870
SJ	 0.7330	 0.4850
SK	 0.8570	 0.5710
SL	 0.8420	 0.5910
SM	 0.7860	 0.5540
SN	 0.7390	 0.5040
SO	 0.8050	 0.5620
SQ	 0.7410	 0.5590
SR	 0.8230	 0.5670
SS	 0.8140	 0.5570
ST	 0.5230	 0.4510
SU	 0.7710	 0.4800
SV	 0.6940	 0.5160
SW	 0.5480	 0.4890
SY	 0.8620	 0.5560
SZ	 0.8530	 0.5630