



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:35 AM UTC

PDB ID : 8FKQ / pdb_00008fkq
EMDB ID : EMD-29253
Title : Human nucleolar pre-60S ribosomal subunit (State A2)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.76 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:

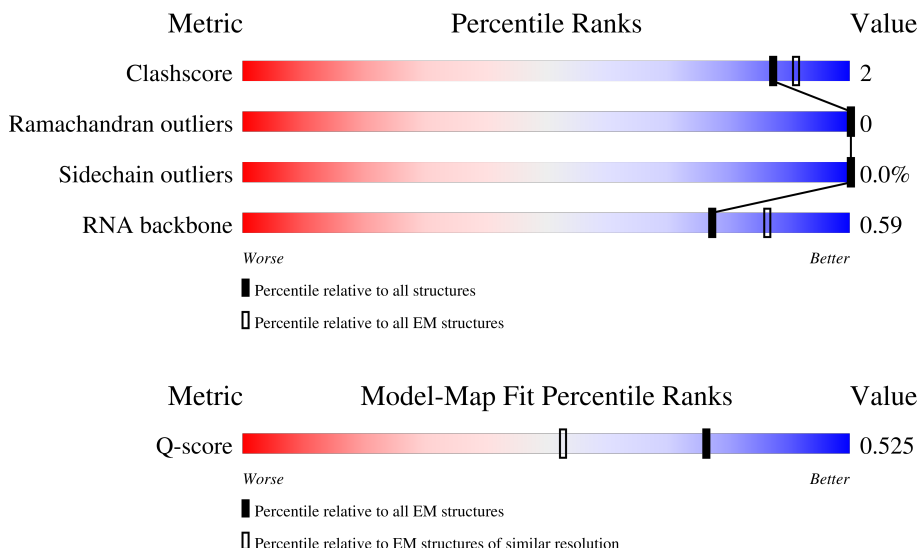
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.76 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	10642 (2.26 - 3.26)

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	L1	157	13% 83% 11% • •
2	L2	1167	5% 94%
3	L3	5070	25% 5% 69%

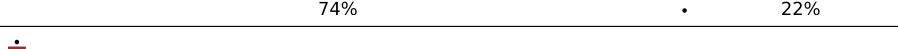
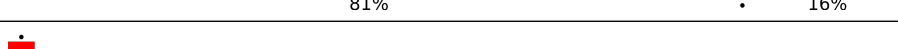
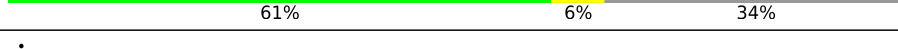
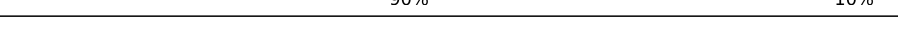
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Mol	Chain	Length	Quality of chain
4	L6	211	
5	L7	203	
6	L8	215	
7	L9	204	
8	LA	184	
9	LB	188	
10	LC	176	
11	LE	160	
12	LG	140	
13	LH	156	
14	LI	145	
15	LK	148	
16	LL	137	
17	LN	403	
18	LQ	135	
19	LS	123	
20	LT	110	
21	LU	105	
22	LW	97	
23	NE	361	
24	NG	282	
25	NN	473	
26	SA	427	
27	SC	288	
28	SD	248	

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Mol	Chain	Length	Quality of chain
29	SE	266	
30	SH	293	
31	SI	255	
32	SJ	847	
33	SK	245	
34	SL	490	
35	SM	588	
36	SN	306	
37	SO	353	
38	SR	634	
39	SS	746	
40	ST	365	
41	SV	163	
42	SW	670	
43	SZ	178	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 93805 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 RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	150	Total	C	N	O	P	0	0
			3189	1423	561	1055	150		

- Molecule 2 is a RNA chain called ITS2 rRNA.

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

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	1565	Total	C	N	O	P	0	0
			33557	14935	6157	10900	1565		

- Molecule 4 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L6	114	Total	C	N	O	S	0	0
			936	583	206	146	1		

- Molecule 5 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L7	184	Total	C	N	O	S	0	0
			1507	976	290	237	4		

- Molecule 6 is a protein called 60S ribosomal protein L14.

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

- Molecule 7 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L9	183	Total	C	N	O	S	1	0
			1553	979	327	243	4		

- Molecule 8 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LA	121	Total	C	N	O	S	0	0
			981	616	182	176	7		

- Molecule 9 is a protein called 60S ribosomal protein L18.

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

- Molecule 10 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LC	173	Total	C	N	O	S	0	0
			1431	908	281	231	11		

- Molecule 11 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	LE	108	Total	C	N	O	0	0
			702	430	138	134		

- Molecule 12 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LG	114	Total	C	N	O	S	0	0
			844	532	155	152	5		

- Molecule 13 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	LH	20	Total	C	N	O	0	0
			146	95	29	22		

- Molecule 14 is a protein called 60S ribosomal protein L26.

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

- Molecule 15 is a protein called 60S ribosomal protein L27a.

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

- Molecule 16 is a protein called 60S ribosomal protein L28.

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

- Molecule 17 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LN	377	Total	C	N	O	S	0	0
			3044	1937	566	527	14		

- Molecule 18 is a protein called 60S ribosomal protein L32.

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

- Molecule 19 is a protein called 60S ribosomal protein L35.

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

- Molecule 20 is a protein called 60S ribosomal protein L35a.

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

- Molecule 21 is a protein called 60S ribosomal protein L36.

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

- Molecule 22 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LW	69	Total	C	N	O	S	0	0
			563	346	126	86	5		

- Molecule 23 is a protein called Surfeit locus protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	NE	156	Total	C	N	O	S	0	0
			1331	810	293	226	2		

- Molecule 24 is a protein called RRP15-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	NG	89	Total	C	N	O	S	0	0
			738	456	145	133	4		

- Molecule 25 is a protein called Suppressor of SWI4 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	NN	244	Total	C	N	O	S	0	0
			1950	1230	371	338	11		

- Molecule 26 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SA	329	Total	C	N	O	S	0	0
			2645	1675	522	435	13		

- Molecule 27 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SC	211	Total	C	N	O	S	0	0
			1692	1090	320	278	4		

- Molecule 28 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SD	212	Total	C	N	O	S	0	0
			1755	1127	334	285	9		

- Molecule 29 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SE	186	Total	C	N	O	S	0	0
			1498	951	290	253	4		

- Molecule 30 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

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

- Molecule 31 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SI	199	Total	C	N	O	S	1	0
			1661	1076	311	270	4		

- Molecule 32 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SJ	72	Total	C	N	O		0	0
			609	385	114	110			

- Molecule 33 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SK	226	Total	C	N	O	S	0	0
			1721	1070	296	343	12		

- Molecule 34 is a protein called Ribosomal L1 domain-containing protein 1.

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

- Molecule 35 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SM	437	Total	C	N	O	S	0	0
			3452	2229	603	609	11		

- Molecule 36 is a protein called Probable rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SN	168	Total	C	N	O	S	0	0
			1308	821	247	235	5		

- Molecule 37 is a protein called Ribosome biogenesis protein BRX1 homolog.

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

- Molecule 38 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SR	77	Total	C	N	O	S	0	0
			642	411	107	122	2		

- Molecule 39 is a protein called Ribosome biogenesis protein BOP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	SS	235	Total	C	N	O	P	S	0	0
			1955	1238	348	360	2	7		

- Molecule 40 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	ST	36	Total	C	N	O	S	0	0
			263	160	51	51	1		

- Molecule 41 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 42 is a protein called ATP-dependent RNA helicase DDX18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SW	445	Total	C	N	O	S	0	0
			3560	2288	609	646	17		

- Molecule 43 is a protein called Nucleolar protein 16.

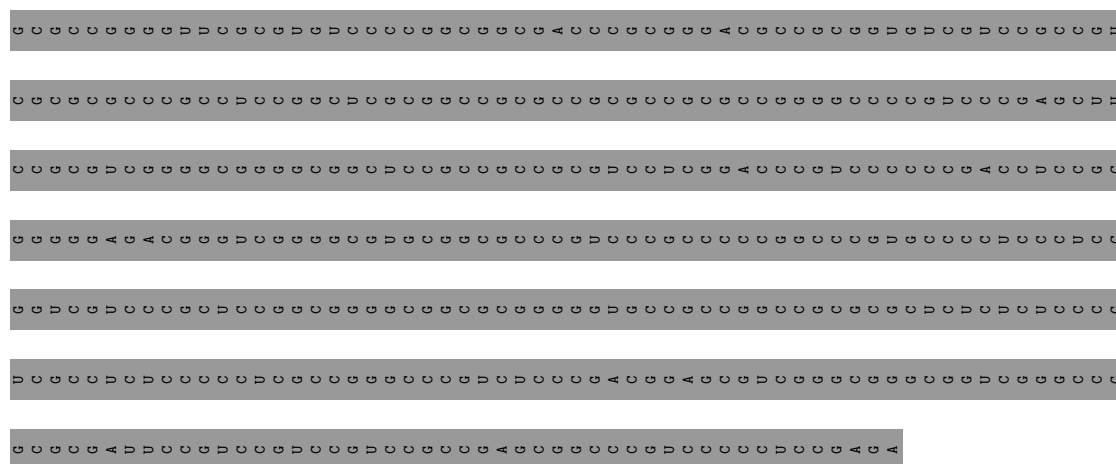
Mol	Chain	Residues	Atoms					AltConf	Trace
43	SZ	160	Total	C	N	O	S	0	0
			1338	835	260	238	5		

- Molecule 44 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

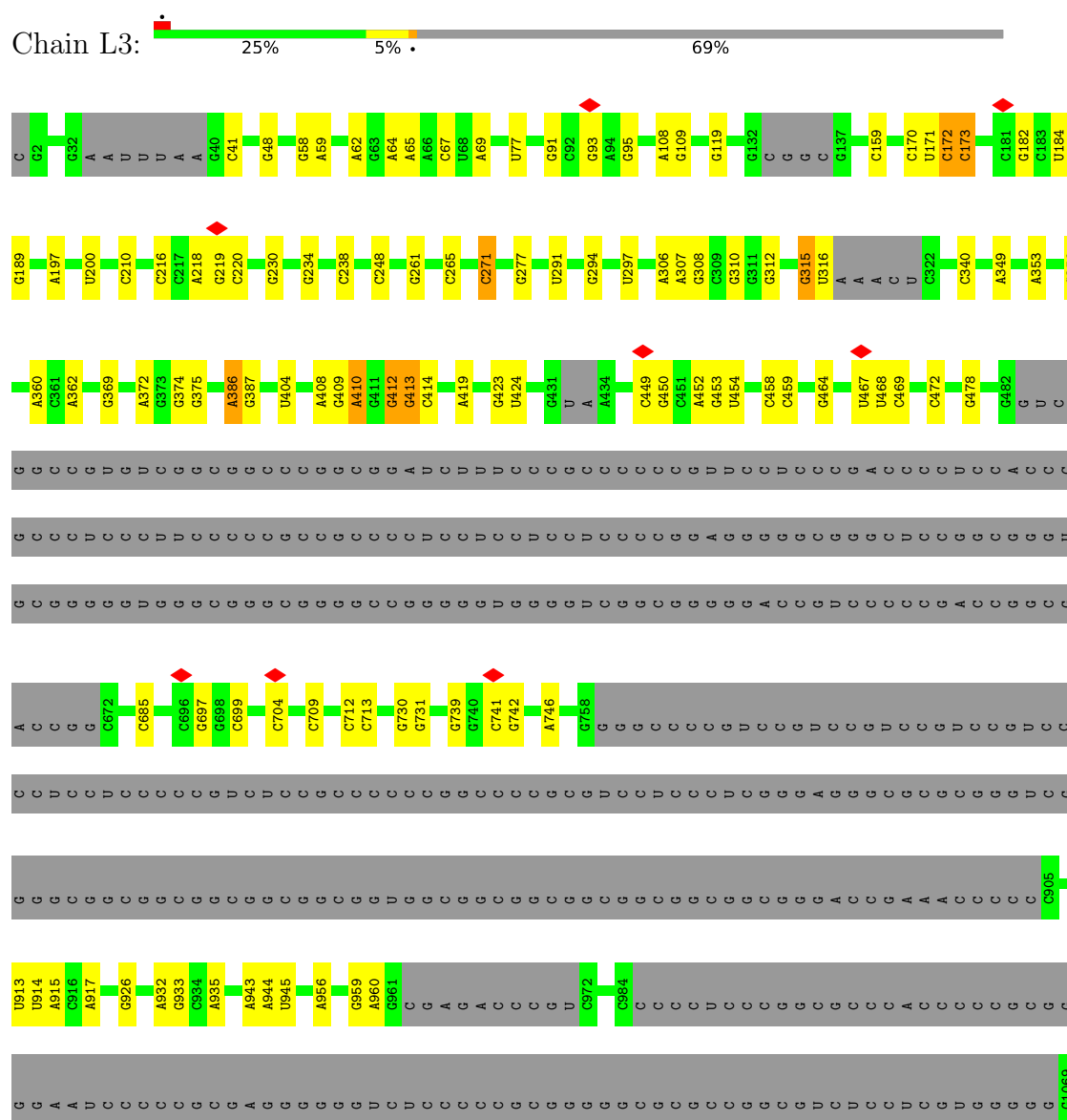
Mol	Chain	Residues	Atoms		AltConf
44	L1	4	Total	Mg	0
			4	4	
44	L2	1	Total	Mg	0
			1	1	
44	L3	42	Total	Mg	0
			42	42	
44	L9	1	Total	Mg	0
			1	1	
44	LQ	1	Total	Mg	0
			1	1	
44	LT	1	Total	Mg	0
			1	1	
44	SA	1	Total	Mg	0
			1	1	

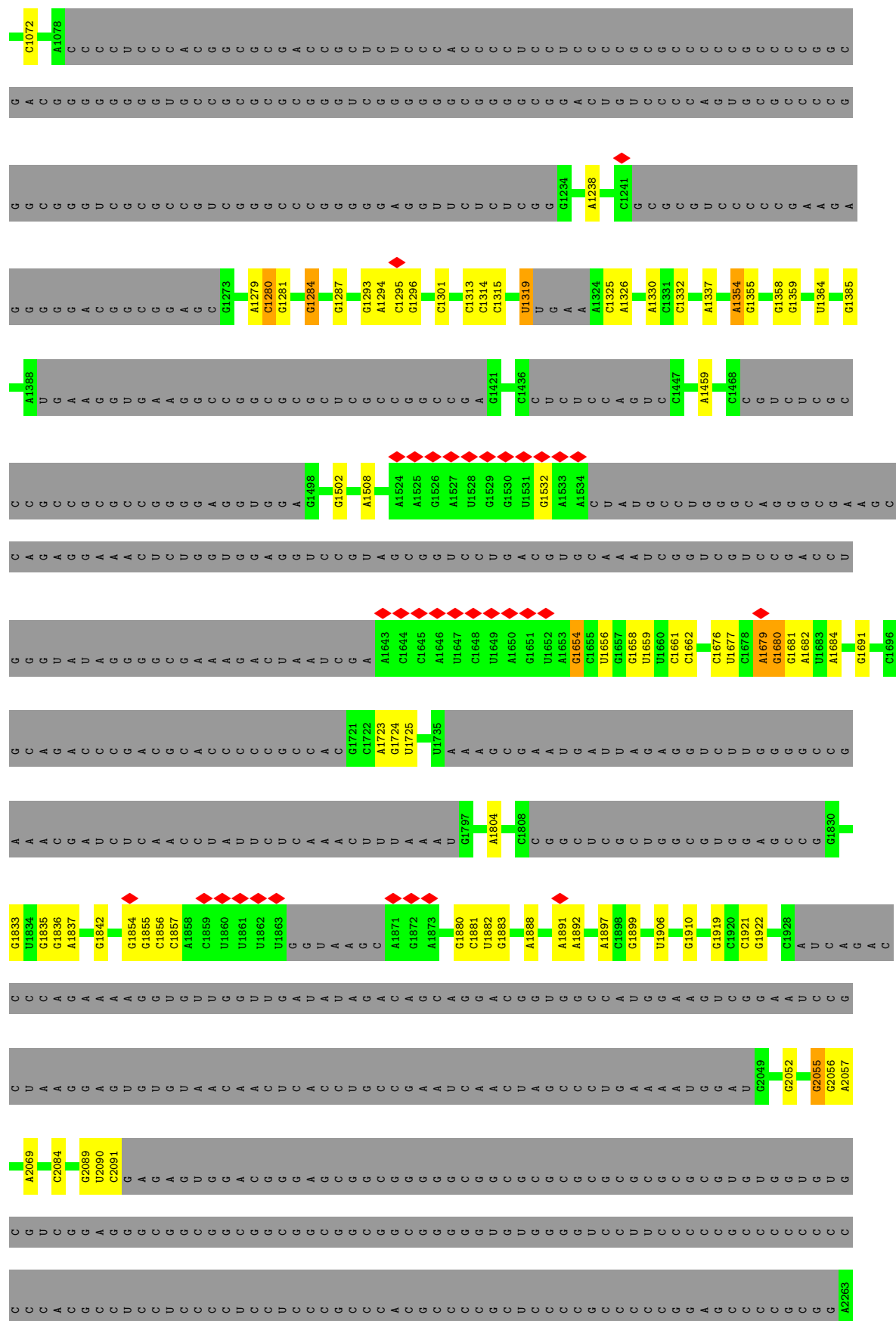
- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

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



• Molecule 3: 28S rRNA

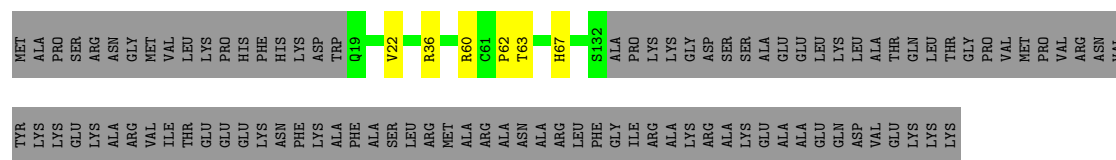




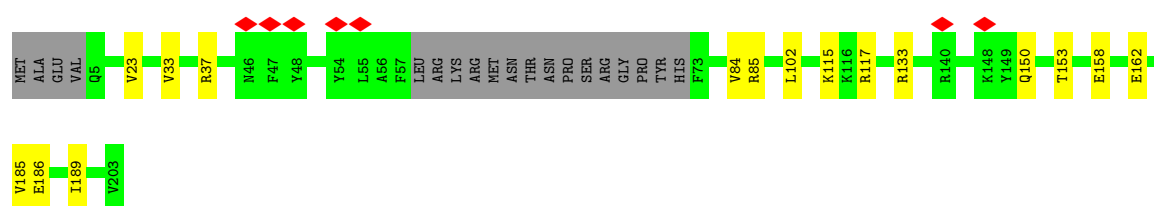
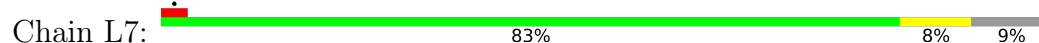




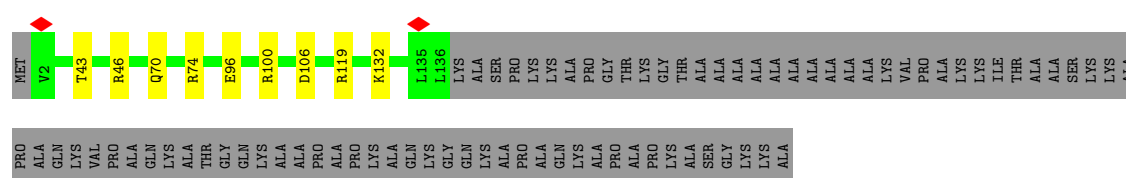
- Molecule 4: 60S ribosomal protein L13



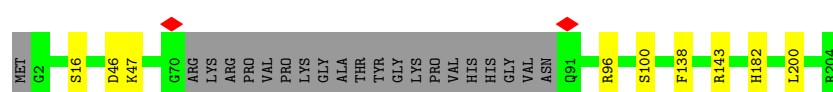
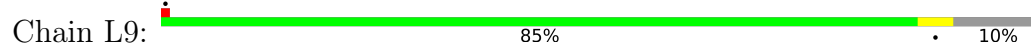
- Molecule 5: 60S ribosomal protein L13a



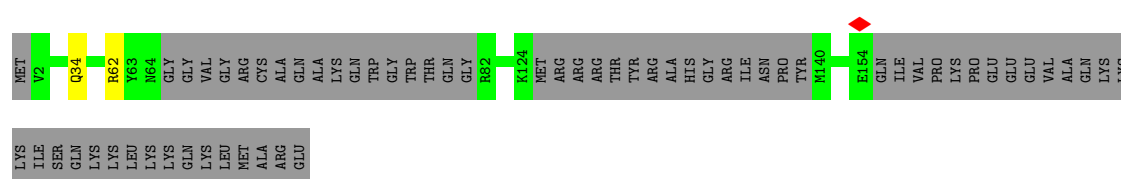
- Molecule 6: 60S ribosomal protein L14



- Molecule 7: 60S ribosomal protein L15

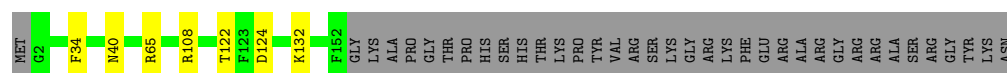


- Molecule 8: 60S ribosomal protein L17

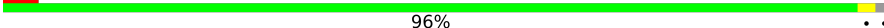


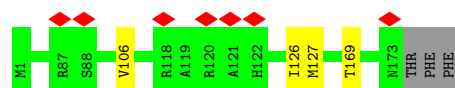
- Molecule 9: 60S ribosomal protein L18

Chain LB:  77% 20%



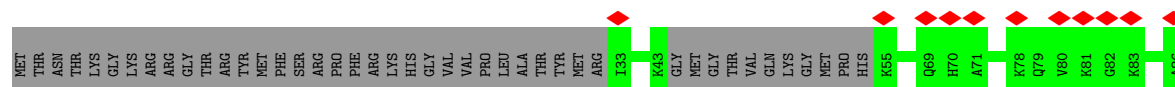
- Molecule 10: 60S ribosomal protein L18a

Chain LC:  96%



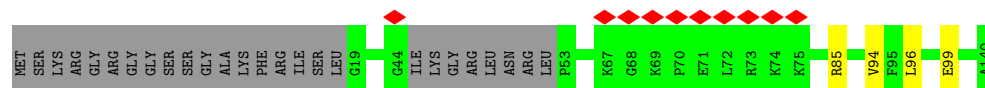
- Molecule 11: 60S ribosomal protein L21

Chain LE:  11% 66% 32%



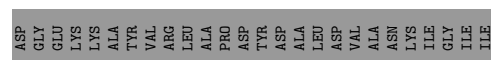
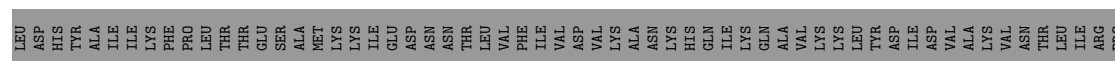
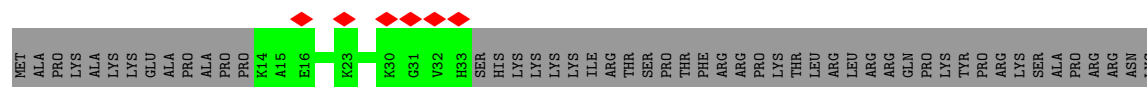
- Molecule 12: 60S ribosomal protein L23

Chain LG:  7% 79% 19%



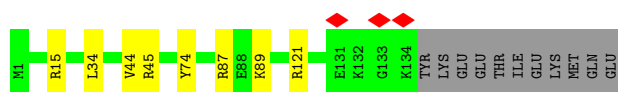
- Molecule 13: 60S ribosomal protein L23a

Chain LH:  13% 87%

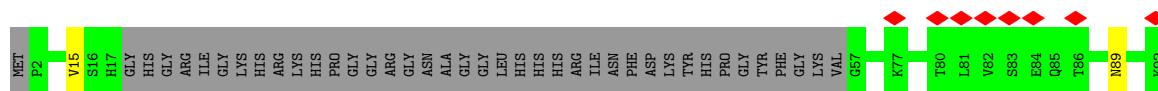
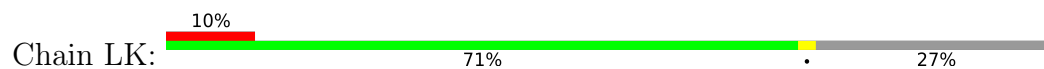


- Molecule 14: 60S ribosomal protein L26

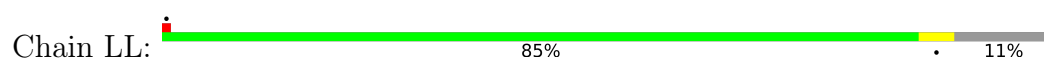
Chain LI:  87% 6% 8%



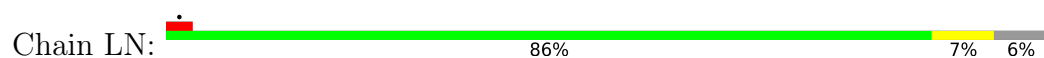
- Molecule 15: 60S ribosomal protein L27a



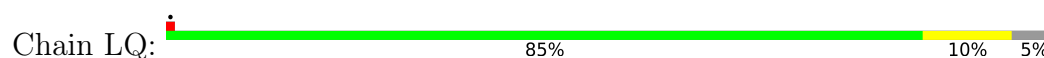
- Molecule 16: 60S ribosomal protein L28



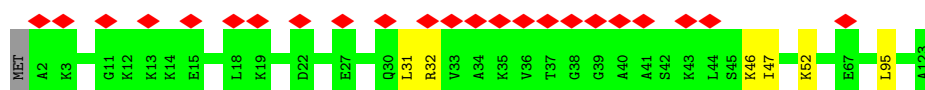
- Molecule 17: 60S ribosomal protein L3



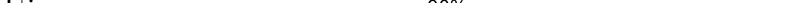
- Molecule 18: 60S ribosomal protein L32



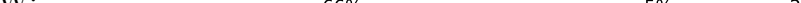
- Molecule 19: 60S ribosomal protein L35



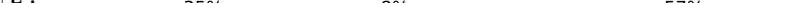
- Molecule 20: 60S ribosomal protein L35a

- Chain LU: 

Amino Acid	Count	Color	Red Diamond
A2	10	Green	Yes
L3	8	Green	Yes
R4	7	Green	Yes
M7	5	Green	Yes
G10	10	Green	Yes
L11	8	Green	Yes
N12	7	Green	Yes
K13	6	Green	Yes
E46	4	Yellow	No
V47	3	Green	No
C48	2	Yellow	No
G49	3	Yellow	No
F50	2	Yellow	No
Y53	1	Yellow	No
V77	2	Green	No
R82	3	Yellow	No
V93	4	Green	No
M97	3	Green	No
K103	10	Green	Yes
LYS	0	Grey	No
ASP	0	Grey	No

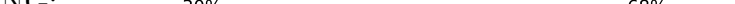
- Chain LW: 

[illegible]

- Chain NE: 

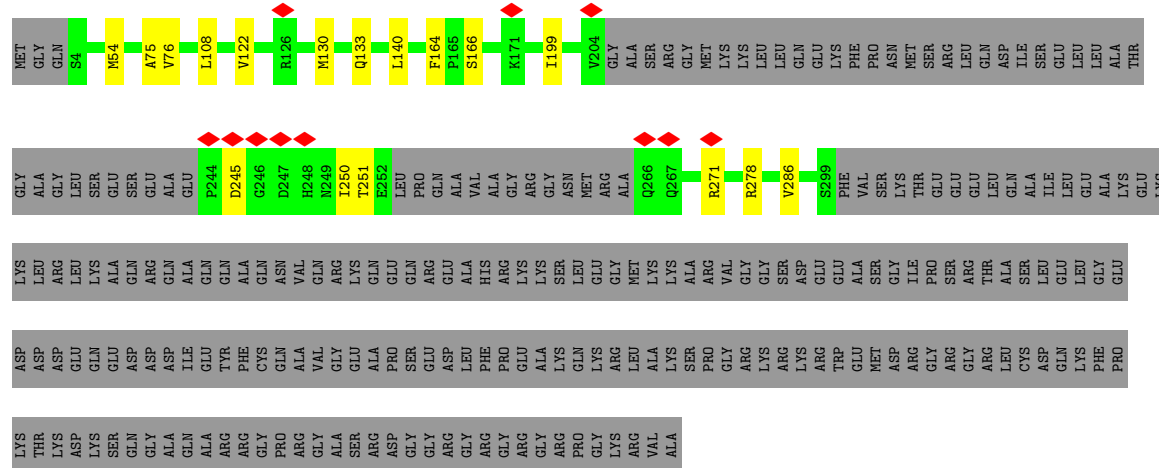
LEU	HIS	ALA	LYS	MET
GLU	GLU	ALA	ALA	ALA
LYS	LYS	GLU	GLU	SER
ILE	ILE	HIS	HIS	LEU
GLN	GLN	LYS	LYS	ALA
GLU	GLU	ALA	LYS	ASP
GLU	ARG	ARG	SER	ALA
GLY	GLY	LEU	LEU	TYR
GLN	GLN	GLY	GLY	LEU
GLY	GLY	GLU	GLN	GLN
SER	SER	LYS	SER	SER
ALA	ALA	SER	LEU	LEU
LYS	LYS	PRO	ALA	ALA
GLU	GLU	ALA	LYS	LYS
LEU	LEU	ALA	ALA	LYS
SER	SER	SER	SER	ILE
PRO	PRO	GLY	CYS	CYS
ALA	ALA	ALA	SER	SER
ALA	ALA	ARG	HIS	HIS
LEU	LEU	ARG	SER	SER
GLU	GLU	PRO	ALA	ALA
LYS	LYS	GLU	PRO	PRO
ARG	ARG	GLU	GLU	GLU
ARG	ARG	ALA	GLN	GLN
ARG	ARG	LYS	GLN	ALA
LYS	LYS	GLU	ARG	ALA
GLN	GLN	ALA	THR	THR
GLU	GLU	ALA	ARG	ALA
ASP	ASP	ALA	GLY	LYS
ARG	ARG	SER	LYS	THR
LYS	LYS	SER	THR	GLN
LYS	LYS	ALA	GLY	GLY
ARG	ARG	ALA	SER	GLY
LYS	LYS	GLU	GLU	PRO
LYS	LYS	ASN	GLU	PRO
GLU	GLU	PRO	THR	THR
ALA	ALA	ALA	ALA	GLY
ASP	ASP	LYS	GLY	PRO
LEU	LEU	GLY	PRO	PRO
ALA	ALA	LEU	LYS	LYS
LYS	LYS	THR	LYS	LYS
GLU	GLU	THR	LYS	LYS
LYS	LYS	GLU	ARG	ARG
ALA	ALA	PRO	LYS	LYS
ARG	ARG	GLU	LYS	LYS
THR	THR	ASP	PHE	PHE
GLU	GLU	VAL	THR	THR
ALA	ALA	GLN	GLN	GLN
GLU	GLU	ALA	LYS	LYS
ALA	ALA	LEU	LYS	LYS
THR	THR	ASP	PHE	PHE
GLU	GLU	VAL	ARG	ARG
GLN	GLN	LEU	LYS	LYS
ALA	ALA	GLN	ARG	ARG
GLU	GLU	GLN	GLY	GLY
ALA	ALA	ARG	ALA	ALA

Gene	Category	Value
V280	Low	0.00
K281	Low	0.00
I282	Low	0.00
R283	Low	0.00
R310	Low	0.00
R321	Low	0.00
K332	Low	0.00
R336	Low	0.00
A337	Low	0.00
E338	Low	0.00
R339	Low	0.00
R340	Low	0.00
R343	Low	0.00
A344	Low	0.00
R345	Low	0.00
K346	Low	0.00
K347	Low	0.00
G348	Low	0.00
R349	Low	0.00
I350	Low	0.00
L351	Low	0.00
P352	Low	0.00
Q353	Low	0.00
D354	Low	0.00
L355	Low	0.00
E356	Low	0.00
R357	Low	0.00
ALA	Low	0.00
GLY	Low	0.00
LEU	Low	0.00
VAL	Low	0.00
VAL	High	0.00
GLU	High	0.00
ALA	High	0.00
THR	High	0.00
PRO	High	0.00
GLU	High	0.00
GLY	High	0.00
CYS	High	0.00
THR	High	0.00
GLU	High	0.00
PRO	High	0.00
ARG	High	0.00
GLU	High	0.00
PRO	High	0.00
P196	High	0.00
K202	High	0.00
V205	High	0.00
SER	High	0.00
GLU	High	0.00
ASP	High	0.00
GLU	High	0.00
PRO	High	0.00
ALA	High	0.00
S212	High	0.00
R216	High	0.00
R221	High	0.00
V224	High	0.00
N227	High	0.00
L228	High	0.00
T232	High	0.00
G233	High	0.00
L250	High	0.00
L253	High	0.00
D257	High	0.00
L264	High	0.00
E265	High	0.00
A266	High	0.00
K267	High	0.00
K268	High	0.00
K269	High	0.00
K270	High	0.00
T271	High	0.00
N272	High	0.00
L273	High	0.00
L274	High	0.00
Y275	High	0.00
K276	High	0.00

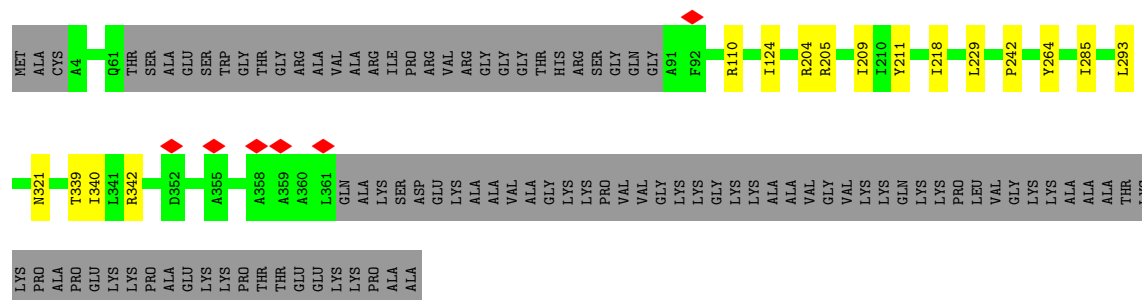
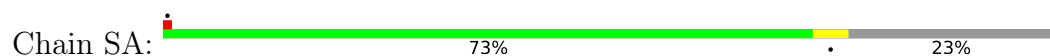
- Chain NG: 

[illegible]

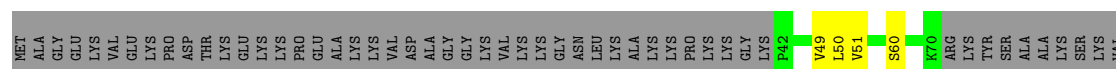
- Molecule 25: Suppressor of SWI4 1 homolog



- Molecule 26: 60S ribosomal protein L4



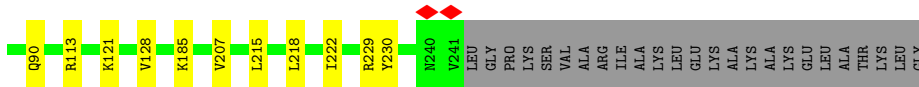
- Molecule 27: 60S ribosomal protein L6



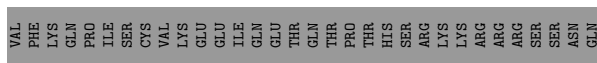
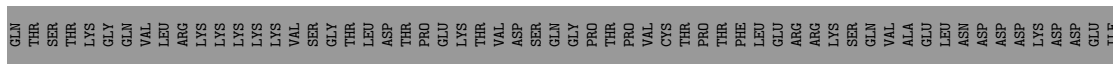


- | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|
| MET | GLU | GLY | VAL | GLU | GLU | GLY | LYS | LYS | LYS | GLU | VAL | PRO | ALA | ALA | VAL | PRO | THR | LEU | LYS | LYS | LYS | LYS | ARG | ARG | ASN | PHE | ALA | GLU | LEU | LYS | LYS | ILE | GLU | ARG | ARG | ARG | LYS | LYS | LYS | F37 | K107 | V108 | D171 | M172 | A176 | G180 | D232 | R236 | V238 |
|------|------|------|------|------|------|------|------|------|

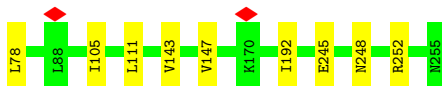
- [illegible]



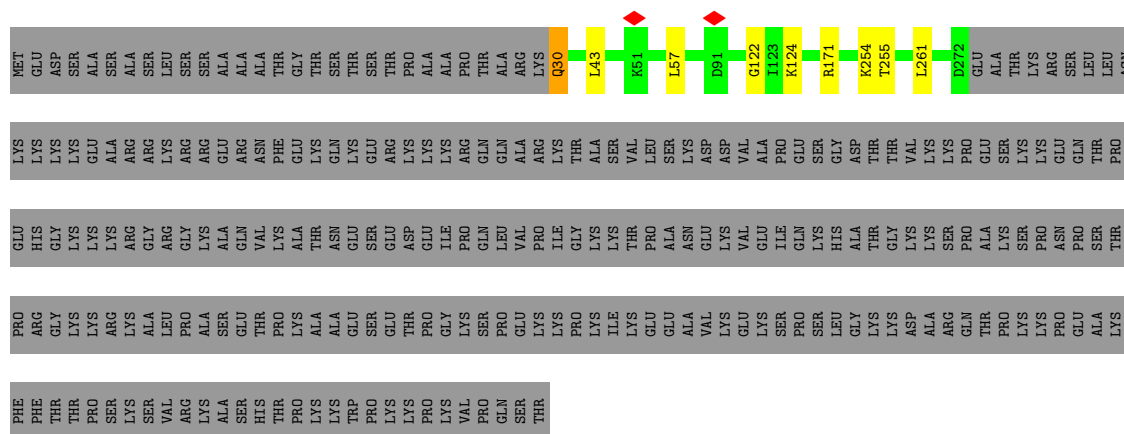
- | | | | | | | | | | | | |
|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|
| Met | Ala | Thr | Phe | Ser | Gly | Pro | Ala | Gly | Pro | Leu | Ser | Leu | Asn | Pro | Gly | Gln | Asp | Val | Gly | Phe | Gln | Lys | Gly | Val | Ala | Gln | Val | Arg | Lys | Arg | Lys | Gln | Lys | Gln | Gly | Gln | 142 | D133 | 1136 | K168 | Q191 | Gly | Thr | Ser | Ser | Lys | Thr | Asn | Arg |
|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|



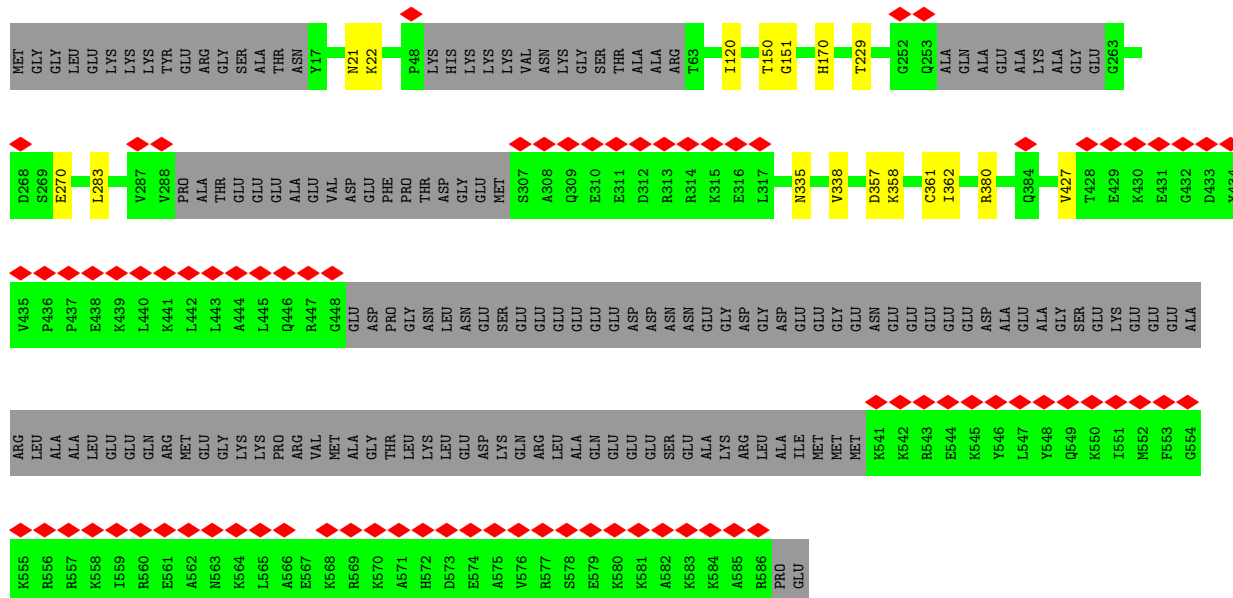
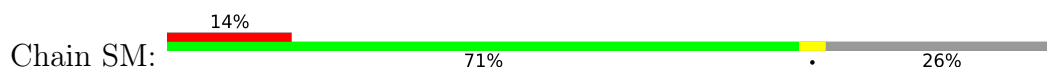
- [illegible]



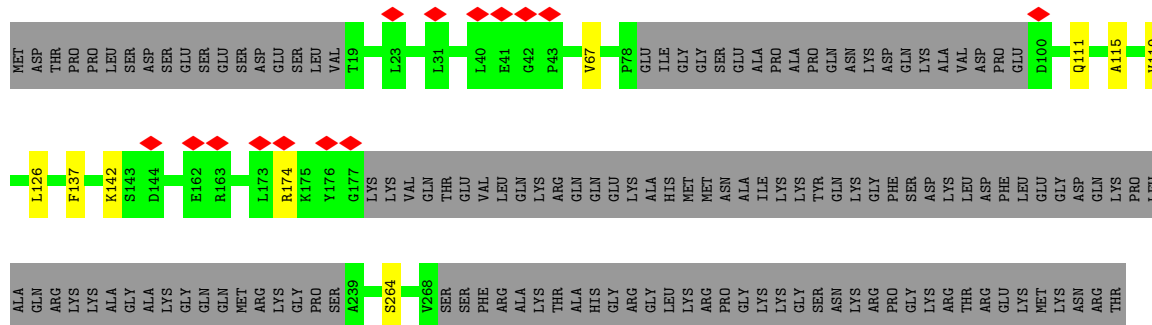




• Molecule 35: Pescadillo homolog

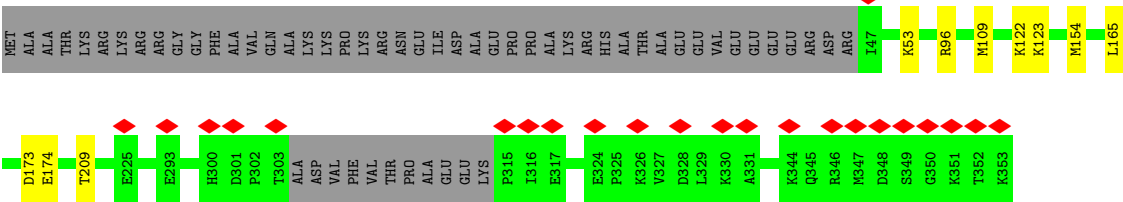
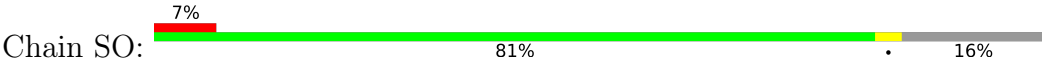


• Molecule 36: Probable rRNA-processing protein EBP2

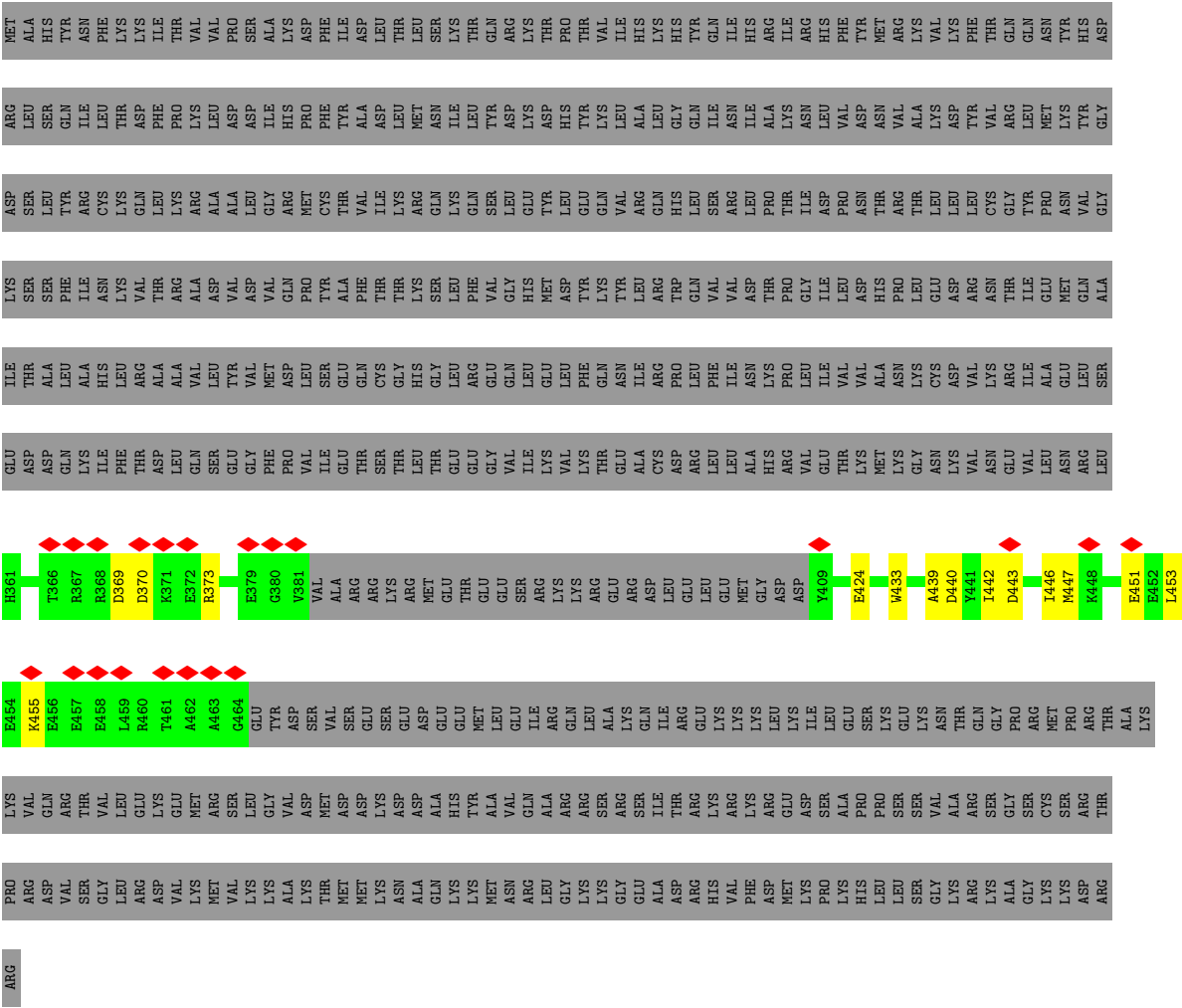


HIS

- Molecule 37: Ribosome biogenesis protein BRX1 homolog

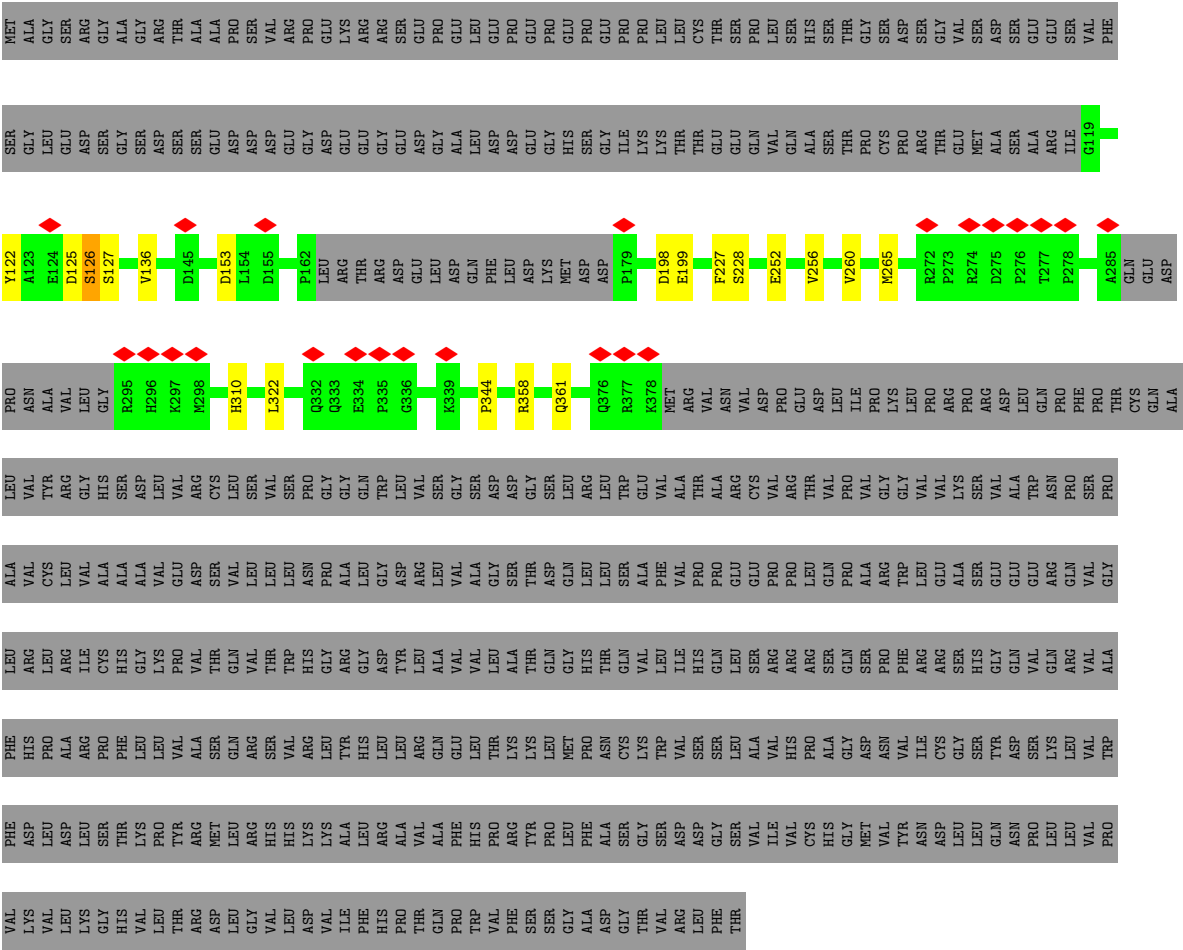


- Molecule 38: GTP-binding protein 4

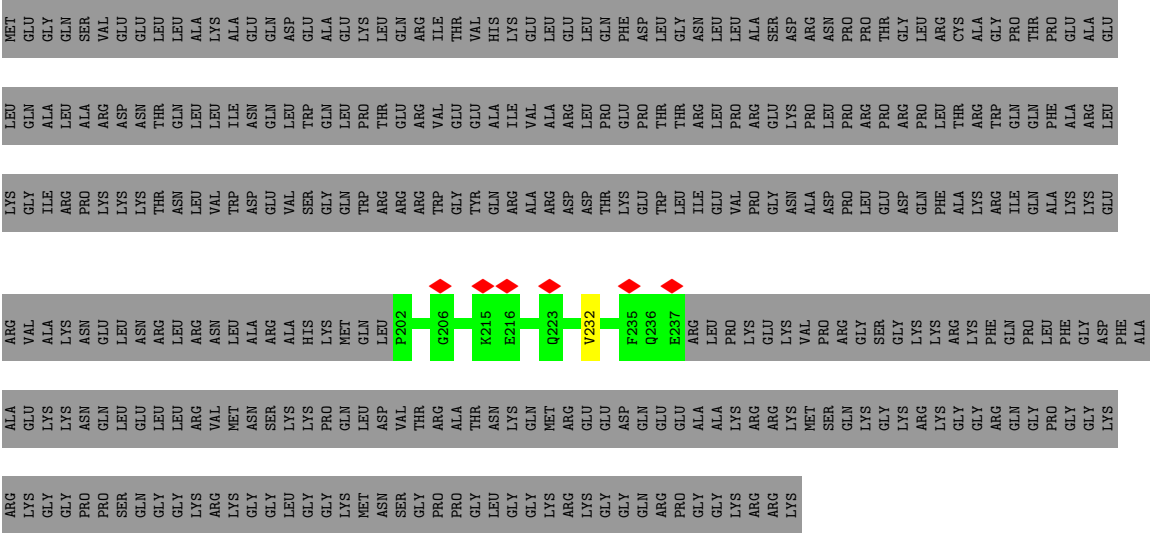


- Molecule 39: Ribosome biogenesis protein BOP1

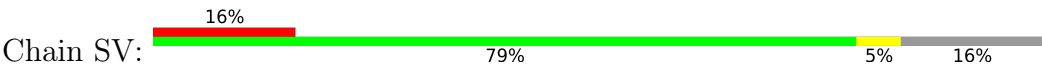




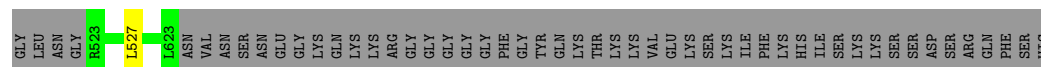
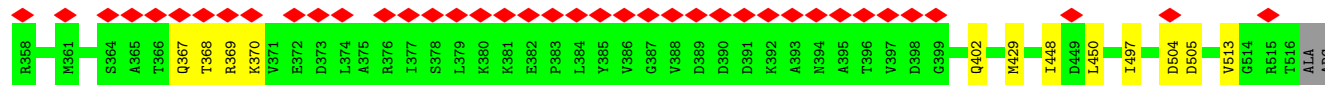
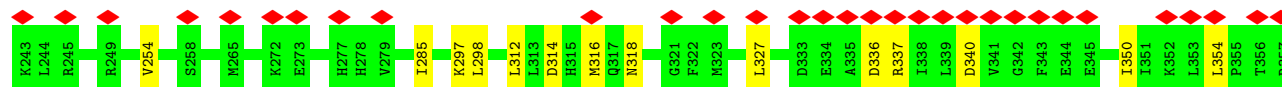
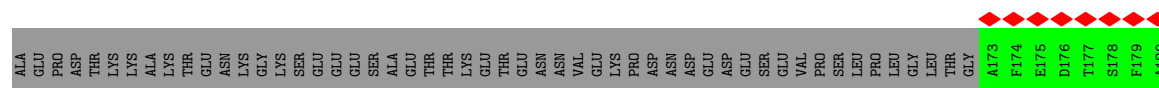
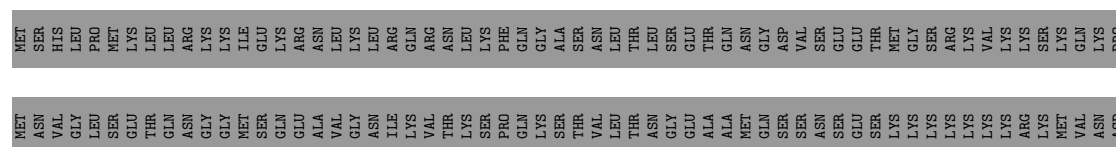
● Molecule 40: Ribosome biogenesis regulatory protein homolog



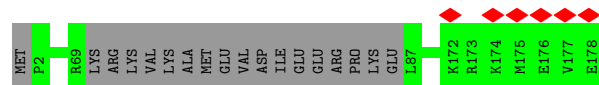
● Molecule 41: Probable ribosome biogenesis protein RLP24



- Molecule 42: ATP-dependent RNA helicase DDX18



- Molecule 43: Nucleolar protein 16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68600	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	6.040	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	0.75	Depositor
Map size ($\text{\AA}$)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ZN, SEP, HIC, MG

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	L1	0.12	0/3559	0.24	0/5539
2	L2	0.15	0/1634	0.27	0/2538
3	L3	0.13	0/37504	0.26	0/58442
4	L6	0.15	0/953	0.33	0/1276
5	L7	0.16	0/1534	0.37	0/2049
6	L8	0.12	0/1133	0.28	0/1516
7	L9	0.15	0/1595	0.33	0/2132
8	LA	0.13	0/997	0.30	0/1334
9	LB	0.15	0/1239	0.31	0/1658
10	LC	0.16	0/1469	0.31	0/1971
11	LE	0.16	0/708	0.41	0/958
12	LG	0.14	0/856	0.35	0/1149
13	LH	0.14	0/146	0.26	0/190
14	LI	0.15	0/1132	0.33	0/1504
15	LK	0.18	0/648	0.40	0/880
16	LL	0.16	0/995	0.35	0/1334
17	LN	0.15	0/3092	0.33	0/4133
18	LQ	0.13	0/1071	0.30	0/1429
19	LS	0.12	0/1023	0.30	0/1351
20	LT	0.14	0/895	0.30	0/1198
21	LU	0.15	0/854	0.34	0/1129
22	LW	0.11	0/573	0.33	0/755
23	NE	0.12	0/1339	0.27	0/1767
24	NG	0.12	0/743	0.27	0/986
25	NN	0.16	0/1988	0.36	0/2678
26	SA	0.14	0/2694	0.29	0/3617
27	SC	0.13	0/1725	0.32	0/2316
28	SD	0.13	0/1789	0.29	0/2388
29	SE	0.15	0/1524	0.33	0/2056
30	SH	0.15	0/1298	0.30	0/1742
31	SI	0.14	0/1702	0.31	0/2289
32	SJ	0.13	0/623	0.37	0/836

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SK	0.15	0/1745	0.36	0/2374
34	SL	0.14	0/1994	0.31	0/2684
35	SM	0.11	0/3530	0.25	0/4779
36	SN	0.12	0/1327	0.30	0/1774
37	SO	0.13	0/2521	0.31	0/3384
38	SR	0.20	0/657	0.45	0/887
39	SS	0.14	0/1994	0.32	0/2703
40	ST	0.10	0/267	0.25	0/357
41	SV	0.16	0/1194	0.33	0/1582
42	SW	0.12	0/3631	0.28	0/4900
43	SZ	0.12	0/1364	0.27	0/1826
All	All	0.14	0/99259	0.29	0/142390

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	L1	3189	0	1618	7	0
2	L2	1468	0	755	3	0
3	L3	33557	0	17010	107	0
4	L6	936	0	1017	4	0
5	L7	1507	0	1649	13	0
6	L8	1111	0	1174	8	0
7	L9	1553	0	1592	8	0
8	LA	981	0	1013	2	0
9	LB	1223	0	1330	6	0
10	LC	1431	0	1477	5	0
11	LE	702	0	561	3	0
12	LG	844	0	883	3	0
13	LH	146	0	176	0	0
14	LI	1115	0	1205	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	LK	642	0	455	2	0
16	LL	980	0	1041	5	0
17	LN	3044	0	3178	24	0
18	LQ	1053	0	1147	10	0
19	LS	1015	0	1148	5	0
20	LT	876	0	912	5	0
21	LU	840	0	930	8	0
22	LW	563	0	596	5	0
23	NE	1331	0	1430	25	0
24	NG	738	0	786	8	0
25	NN	1950	0	2005	16	0
26	SA	2645	0	2823	11	0
27	SC	1692	0	1839	18	0
28	SD	1755	0	1859	5	0
29	SE	1498	0	1601	9	0
30	SH	1267	0	1291	2	0
31	SI	1661	0	1752	7	0
32	SJ	609	0	600	1	0
33	SK	1721	0	1695	15	0
34	SL	1960	0	2052	7	0
35	SM	3452	0	3376	11	0
36	SN	1308	0	1286	8	0
37	SO	2460	0	2551	9	0
38	SR	642	0	630	11	0
39	SS	1955	0	1871	14	0
40	ST	263	0	260	1	0
41	SV	1171	0	1232	10	0
42	SW	3560	0	3641	24	0
43	SZ	1338	0	1352	0	0
44	L1	4	0	0	0	0
44	L2	1	0	0	0	0
44	L3	42	0	0	0	0
44	L9	1	0	0	0	0
44	LQ	1	0	0	0	0
44	LT	1	0	0	0	0
44	SA	1	0	0	0	0
45	LW	1	0	0	0	0
45	SV	1	0	0	0	0
All	All	93805	0	76799	328	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 (328) 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)
34:SL:30:GLN:HE21	34:SL:30:GLN:N	1.69	0.90
3:L3:404:U:O2'	14:LI:87:ARG:NH2	2.13	0.81
23:NE:228:LEU:HD21	23:NE:271:THR:HG21	1.64	0.80
3:L3:2055:G:OP2	5:L7:133:ARG:NH1	2.17	0.78
12:LG:85:ARG:NH1	12:LG:99:GLU:O	2.17	0.77
3:L3:271:C:OP1	42:SW:297:LYS:NZ	2.17	0.77
33:SK:178:GLN:OE1	38:SR:373:ARG:NH1	2.17	0.77
3:L3:375:G:OP2	22:LW:52:LYS:NZ	2.17	0.77
3:L3:172:C:O2'	3:L3:173:C:O5'	2.02	0.77
3:L3:4598:C:O2	3:L3:4612:C:N4	2.18	0.76
31:SI:252:ARG:NH1	35:SM:270:GLU:OE1	2.19	0.76
3:L3:1355:G:OP1	9:LB:108:ARG:NH2	2.19	0.76
4:L6:60:ARG:NH2	4:L6:67:HIS:O	2.19	0.76
1:L1:153:C:OP1	29:SE:185:LYS:NZ	2.18	0.75
3:L3:4940:C:OP1	27:SC:156:ARG:NH1	2.21	0.74
3:L3:1680:G:N7	23:NE:349:ARG:NH1	2.35	0.74
3:L3:478:G:OP1	16:LL:66:ARG:NH1	2.24	0.71
1:L1:75:G:OP2	14:LI:74:TYR:OH	2.09	0.71
3:L3:458:C:O2'	27:SC:110:ARG:NH1	2.23	0.71
3:L3:412:G:O2'	3:L3:413:G:OP2	2.07	0.71
17:LN:95:THR:OG1	17:LN:98:GLY:O	2.06	0.70
23:NE:202:LYS:O	25:NN:166:SER:OG	2.06	0.70
3:L3:62:A:N3	3:L3:77:U:O2'	2.22	0.70
36:SN:67:VAL:HG22	36:SN:126:LEU:HD13	1.74	0.69
3:L3:1280:C:O2'	26:SA:321:ASN:OD1	2.09	0.69
3:L3:713:C:O2	27:SC:130:LYS:NZ	2.26	0.69
26:SA:340:ILE:HG21	27:SC:50:LEU:HD13	1.73	0.69
2:L2:52:G:N7	34:SL:171:ARG:NH1	2.41	0.69
3:L3:172:C:HO2'	3:L3:173:C:P	2.15	0.69
3:L3:386:A:OP2	14:LI:89:LYS:NZ	2.26	0.69
3:L3:469:C:N3	27:SC:105:ARG:NH2	2.41	0.68
34:SL:30:GLN:N	34:SL:30:GLN:NE2	2.42	0.68
38:SR:451:GLU:OE2	38:SR:455:LYS:NZ	2.26	0.68
3:L3:291:U:O2'	7:L9:182[A]:HIS:NE2	2.24	0.68
35:SM:120:ILE:HD11	35:SM:229:THR:HG23	1.76	0.67
3:L3:2267:U:OP1	16:LL:37:SER:OG	2.07	0.67
3:L3:2361:G:O2'	3:L3:3859:G:O6	2.08	0.67
3:L3:4669:A:O2'	3:L3:4671:C:OP2	2.10	0.67
23:NE:275:TYR:HB2	23:NE:282:ILE:HD11	1.77	0.67
42:SW:402:GLN:NE2	42:SW:513:VAL:HG21	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SI:143:VAL:O	31:SI:147:VAL:HG12	1.95	0.66
25:NN:122:VAL:HG21	25:NN:130:MET:HE2	1.78	0.66
3:L3:306:A:OP1	21:LU:53:TYR:OH	2.14	0.65
3:L3:386:A:O2'	14:LI:87:ARG:NH1	2.28	0.65
3:L3:248:C:O2	14:LI:121:ARG:NH2	2.27	0.65
3:L3:4751:G:N7	20:LT:52:LYS:NZ	2.45	0.65
3:L3:3863:C:OP1	23:NE:321:ARG:NH1	2.30	0.65
3:L3:1238:A:OP2	27:SC:60:SER:OG	2.12	0.64
29:SE:90:GLN:OE1	31:SI:60:ARG:NH2	2.30	0.64
39:SS:358:ARG:NH1	39:SS:361:GLN:OE1	2.30	0.64
3:L3:4946:U:HO2'	20:LT:2:SER:N	1.96	0.64
2:L2:66:A:OP2	30:SH:168:LYS:NZ	2.25	0.63
42:SW:241:ILE:HD11	42:SW:254:VAL:HG23	1.80	0.63
3:L3:4972:U:OP1	17:LN:249:ARG:NH1	2.31	0.63
3:L3:1833:G:N2	3:L3:1835:G:O4'	2.33	0.62
6:L8:106:ASP:OD2	27:SC:161:ARG:NH2	2.31	0.62
36:SN:119:VAL:HG21	37:SO:165:LEU:HD13	1.80	0.62
7:L9:46:ASP:OD1	7:L9:47:LYS:N	2.33	0.62
3:L3:2834:C:O2	17:LN:234:ARG:NH2	2.33	0.62
16:LL:20:ARG:NH1	18:LQ:78:LEU:O	2.32	0.62
3:L3:5001:U:OP1	17:LN:385:LYS:NZ	2.29	0.61
17:LN:219:VAL:HG11	17:LN:337:VAL:CG2	2.31	0.61
28:SD:232:ASP:OD1	28:SD:236:ARG:NH2	2.32	0.61
42:SW:312:LEU:HD23	42:SW:316:MET:HE2	1.83	0.61
3:L3:4589:A:N1	3:L3:4621:C:O2'	2.33	0.60
21:LU:50:PHE:HZ	21:LU:93:VAL:HG11	1.66	0.60
9:LB:40:ASN:OD1	9:LB:132:LYS:NZ	2.33	0.60
3:L3:315:G:N7	37:SO:96:ARG:NH2	2.49	0.60
3:L3:4761:G:OP1	5:L7:37:ARG:NH2	2.33	0.60
3:L3:4724:A:O2'	17:LN:104:THR:HG22	2.00	0.60
3:L3:4567:G:OP1	17:LN:21:ARG:N	2.33	0.59
27:SC:201:ILE:HG22	27:SC:264:ILE:HD12	1.84	0.59
42:SW:327:LEU:HD22	42:SW:354:LEU:HD12	1.84	0.59
7:L9:96:ARG:NH1	7:L9:100:SER:OG	2.36	0.58
42:SW:219:LEU:HD21	42:SW:221:ALA:HB2	1.85	0.58
3:L3:458:C:OP1	16:LL:87:ARG:NH2	2.36	0.58
29:SE:207:VAL:HG21	29:SE:215:LEU:HD22	1.85	0.58
33:SK:177:LEU:HD23	33:SK:181:LEU:HD21	1.84	0.58
39:SS:125:ASP:OD1	39:SS:126:SEP:N	2.35	0.58
10:LC:106:VAL:HG13	10:LC:126:ILE:CD1	2.34	0.58
24:NG:170:VAL:HG21	25:NN:199:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:SR:440:ASP:O	41:SV:75:ARG:NE	2.29	0.57
29:SE:113:ARG:NH2	39:SS:252:GLU:OE2	2.38	0.57
10:LC:127:MET:CE	11:LE:154:ILE:HG22	2.35	0.57
21:LU:93:VAL:HG12	21:LU:97:MET:HE3	1.87	0.57
27:SC:50:LEU:HD12	27:SC:51:VAL:N	2.19	0.57
3:L3:2363:A:O2'	23:NE:310:ARG:NH2	2.38	0.57
10:LC:127:MET:HE2	11:LE:154:ILE:HG22	1.87	0.57
3:L3:1508:A:OP1	26:SA:110:ARG:NH2	2.37	0.56
23:NE:275:TYR:CB	23:NE:282:ILE:HD11	2.34	0.56
36:SN:111:GLN:OE1	37:SO:209:THR:HG22	2.04	0.56
23:NE:250:LEU:HD11	23:NE:268:MET:HE1	1.87	0.56
1:L1:102:G:OP2	1:L1:104:A:O2'	2.22	0.56
3:L3:4679:G:O2'	3:L3:4680:G:OP1	2.22	0.56
9:LB:122:THR:OG1	9:LB:124:ASP:OD1	2.19	0.56
33:SK:28:ILE:HG23	33:SK:28:ILE:O	2.06	0.56
23:NE:276:LYS:HG3	23:NE:282:ILE:HD12	1.88	0.56
20:LT:43:LEU:O	20:LT:109:ARG:NH1	2.38	0.56
17:LN:234:ARG:HD2	25:NN:75:ALA:HB1	1.88	0.56
27:SC:202:ASP:O	27:SC:260:LYS:NZ	2.40	0.55
3:L3:374:G:OP2	22:LW:56:ARG:NH1	2.38	0.55
3:L3:4662:C:OP2	3:L3:4663:G:N2	2.39	0.55
5:L7:189:ILE:HD11	6:L8:119:ARG:HG2	1.89	0.55
35:SM:170:HIS:HB3	35:SM:283:LEU:HD11	1.89	0.55
42:SW:182:LEU:HD21	42:SW:211:ARG:HE	1.70	0.55
3:L3:712:C:O2	3:L3:1284:G:N2	2.19	0.55
3:L3:1883:G:OP1	18:LQ:47:ARG:NH1	2.39	0.55
10:LC:106:VAL:HG13	10:LC:126:ILE:HD13	1.89	0.55
3:L3:423:G:OP1	8:LA:62:ARG:NH1	2.40	0.55
3:L3:458:C:O3'	27:SC:110:ARG:NH1	2.40	0.54
3:L3:4598:C:OP2	3:L3:4599:A:O2'	2.13	0.54
32:SJ:709:GLU:OE2	32:SJ:713:ARG:NE	2.41	0.54
3:L3:1319:U:O3'	23:NE:339:ARG:NH1	2.41	0.54
5:L7:85:ARG:NH1	36:SN:264:SER:O	2.40	0.54
35:SM:427:VAL:HG21	39:SS:310:HIS:CE1	2.43	0.54
7:L9:143:ARG:NH1	19:LS:95:LEU:HD12	2.23	0.54
3:L3:4895:C:O3'	6:L8:132:LYS:NZ	2.41	0.54
3:L3:709:C:OP1	20:LT:89:ARG:NH2	2.41	0.53
37:SO:53:LYS:NZ	39:SS:153:ASP:OD2	2.35	0.53
42:SW:285:ILE:HD11	42:SW:298:LEU:HD21	1.90	0.53
33:SK:155:SER:OG	33:SK:156:ASN:N	2.40	0.53
39:SS:198:ASP:OD2	39:SS:199:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LS:31:LEU:HD21	19:LS:46:LYS:HB3	1.91	0.53
3:L3:1659:U:H2'	15:LK:15:VAL:HG23	1.91	0.53
3:L3:5005:G:N2	3:L3:5041:G:O2'	2.42	0.53
23:NE:253:LEU:HD12	23:NE:264:LEU:HD12	1.89	0.53
21:LU:50:PHE:CZ	21:LU:93:VAL:HG11	2.45	0.52
3:L3:4741:C:O2'	3:L3:4742:G:OP1	2.25	0.52
42:SW:340:ASP:OD1	42:SW:370:LYS:NZ	2.30	0.52
17:LN:47:LEU:HD11	17:LN:181:MET:SD	2.49	0.52
1:L1:62:A:OP1	19:LS:52:LYS:NZ	2.42	0.52
3:L3:1855:G:OP1	23:NE:343:ARG:NH1	2.39	0.52
3:L3:1656:U:OP1	23:NE:336:ARG:NH1	2.42	0.52
3:L3:4760:G:OP1	5:L7:117:ARG:NH2	2.43	0.52
36:SN:115:ALA:O	36:SN:119:VAL:HG22	2.09	0.52
3:L3:307:A:N3	3:L3:310:G:O2'	2.42	0.52
3:L3:1662:C:OP2	18:LQ:39:ARG:NH2	2.44	0.51
5:L7:189:ILE:HD11	6:L8:119:ARG:CG	2.41	0.51
29:SE:58:PRO:HG2	29:SE:61:ILE:HD12	1.92	0.51
2:L2:1:G:O2'	2:L2:2:C:OP1	2.24	0.51
3:L3:4728:U:OP2	17:LN:132:LYS:NZ	2.44	0.51
26:SA:339:THR:HG22	26:SA:342:ARG:HH22	1.76	0.51
29:SE:218:LEU:O	29:SE:222:ILE:HD12	2.10	0.51
38:SR:424:GLU:OE2	41:SV:83:ARG:NH2	2.36	0.50
33:SK:177:LEU:CD2	33:SK:181:LEU:HD21	2.41	0.50
42:SW:182:LEU:O	42:SW:186:VAL:HG12	2.11	0.50
3:L3:238:C:OP2	14:LI:45:ARG:NH2	2.44	0.50
42:SW:314:ASP:OD1	42:SW:318:ASN:ND2	2.44	0.50
1:L1:94:G:N3	22:LW:82:THR:HG23	2.25	0.50
35:SM:120:ILE:HD11	35:SM:229:THR:CG2	2.42	0.50
3:L3:935:A:O2'	6:L8:46:ARG:NH1	2.45	0.50
3:L3:316:U:OP2	37:SO:122:LYS:NZ	2.25	0.50
3:L3:1337:A:N1	3:L3:1658:G:O2'	2.39	0.50
27:SC:203:ILE:O	27:SC:203:ILE:HG22	2.12	0.49
31:SI:192:ILE:HD11	35:SM:380:ARG:HE	1.76	0.49
42:SW:336:ASP:OD1	42:SW:337:ARG:N	2.46	0.49
3:L3:4875:G:H2'	10:LC:169:THR:HG22	1.93	0.49
24:NG:159:GLU:OE2	25:NN:278:ARG:NH1	2.44	0.49
42:SW:187:ASN:OD1	42:SW:188:GLU:N	2.44	0.49
21:LU:46:GLU:OE1	39:SS:228:SER:N	2.40	0.49
24:NG:167:THR:O	24:NG:171:VAL:HG23	2.11	0.49
38:SR:453:LEU:HD22	41:SV:71:PHE:CE2	2.48	0.49
25:NN:133:GLN:OE1	25:NN:133:GLN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:4745:G:H22	3:L3:4955:A:H2	1.61	0.49
38:SR:447:MET:SD	38:SR:447:MET:N	2.86	0.49
26:SA:204:ARG:NH1	26:SA:205:ARG:O	2.45	0.49
3:L3:1723:A:O2'	28:SD:107:LYS:NZ	2.46	0.48
3:L3:230:G:OP1	14:LI:15:ARG:NH1	2.43	0.48
3:L3:2296:G:O2'	26:SA:242:PRO:O	2.31	0.48
3:L3:1364:U:OP2	4:L6:36:ARG:NH1	2.41	0.48
3:L3:1459:A:OP1	9:LB:65:ARG:NH1	2.46	0.48
17:LN:219:VAL:HG11	17:LN:337:VAL:HG21	1.94	0.48
38:SR:443:ASP:HB3	38:SR:446:ILE:HG23	1.96	0.48
17:LN:223:THR:HG22	17:LN:338:VAL:HG23	1.96	0.48
18:LQ:103:VAL:O	18:LQ:108:ARG:NH2	2.45	0.48
17:LN:29:VAL:HG23	17:LN:346:THR:HG21	1.96	0.48
42:SW:197:MET:HE1	42:SW:231:LEU:HD21	1.95	0.48
42:SW:504:ASP:OD1	42:SW:505:ASP:N	2.47	0.48
23:NE:228:LEU:HD21	23:NE:271:THR:CG2	2.41	0.48
3:L3:1532:G:OP2	22:LW:31:LYS:NZ	2.45	0.47
27:SC:278:THR:OG1	27:SC:281:ILE:HD12	2.14	0.47
28:SD:171:ASP:OD2	28:SD:172:ASN:N	2.47	0.47
42:SW:312:LEU:CD2	42:SW:316:MET:HE2	2.44	0.47
27:SC:281:ILE:HG23	27:SC:286:LEU:HD21	1.95	0.47
12:LG:96:LEU:HD12	41:SV:20:MET:SD	2.54	0.47
38:SR:369:ASP:OD2	38:SR:370:ASP:N	2.47	0.47
42:SW:327:LEU:HD22	42:SW:354:LEU:CD1	2.45	0.47
24:NG:170:VAL:HG22	25:NN:140:LEU:HD23	1.96	0.47
25:NN:108:LEU:HD22	25:NN:286:VAL:HG22	1.97	0.47
4:L6:62:PRO:O	4:L6:63:THR:OG1	2.28	0.47
23:NE:232:THR:HG21	23:NE:280:VAL:CG1	2.45	0.47
3:L3:4993:G:H22	3:L3:5058:A:H2	1.62	0.47
21:LU:46:GLU:OE1	39:SS:227:PHE:N	2.45	0.47
33:SK:166:SER:OG	33:SK:168:GLU:OE2	2.33	0.47
35:SM:21:ASN:OD1	35:SM:22:LYS:N	2.48	0.47
42:SW:429:MET:HB3	42:SW:497:ILE:HD13	1.97	0.47
3:L3:4971:A:OP1	17:LN:246:ARG:NH1	2.47	0.46
30:SH:133:ASP:OD1	30:SH:136:ILE:HD12	2.15	0.46
33:SK:112:ASP:OD2	33:SK:156:ASN:ND2	2.47	0.46
11:LE:115:LYS:O	11:LE:119:ALA:N	2.47	0.46
3:L3:184:U:O2'	3:L3:189:G:OP2	2.28	0.46
3:L3:67:C:OP2	3:L3:312:G:N2	2.45	0.46
1:L1:93:C:OP1	22:LW:76:HIS:NE2	2.36	0.46
3:L3:1354:A:N1	3:L3:1385:G:O2'	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LI:34:LEU:HD22	14:LI:44:VAL:HG13	1.98	0.46
15:LK:89:ASN:O	15:LK:93:ASN:N	2.42	0.46
37:SO:109:MET:O	39:SS:122:TYR:OH	2.24	0.46
3:L3:291:U:N3	3:L3:294:G:OP1	2.44	0.46
3:L3:4679:G:HO2'	3:L3:4680:G:P	2.38	0.46
25:NN:250:ILE:HG13	25:NN:250:ILE:O	2.16	0.46
3:L3:419:A:N3	3:L3:1332:C:O2'	2.46	0.46
23:NE:350:ILE:HG23	23:NE:350:ILE:O	2.16	0.45
1:L1:25:G:N3	3:L3:356:G:O2'	2.49	0.45
19:LS:32:ARG:HH12	19:LS:47:ILE:HG23	1.81	0.45
33:SK:107:VAL:HG12	33:SK:108:THR:HG23	1.97	0.45
17:LN:254:ILE:HG23	25:NN:76:VAL:HG21	1.97	0.45
29:SE:128:VAL:O	29:SE:128:VAL:HG13	2.16	0.45
35:SM:335:ASN:O	35:SM:338:VAL:HG22	2.16	0.45
3:L3:1279:A:O2'	3:L3:1281:G:N7	2.44	0.45
26:SA:124:ILE:HG21	26:SA:264:TYR:OH	2.17	0.45
5:L7:150:GLN:O	5:L7:153:THR:OG1	2.30	0.45
38:SR:433:TRP:CE3	41:SV:93:MET:HE3	2.51	0.45
3:L3:1654:G:N7	3:L3:1679:A:N6	2.64	0.45
3:L3:4632:U:H3'	3:L3:4633:G:H5''	1.99	0.45
17:LN:71:GLU:OE2	17:LN:366:LYS:NZ	2.34	0.45
3:L3:712:C:N3	3:L3:1284:G:N1	2.40	0.44
3:L3:4660:G:O2'	3:L3:4661:G:OP2	2.33	0.44
9:LB:122:THR:HG21	26:SA:285:ILE:HG12	1.99	0.44
18:LQ:26:ASP:OD1	18:LQ:27:ARG:N	2.50	0.44
25:NN:245:ASP:OD1	25:NN:271:ARG:NH1	2.50	0.44
36:SN:137:PHE:O	39:SS:136:VAL:HG23	2.17	0.44
20:LT:33:VAL:HG23	20:LT:38:GLU:HB2	1.99	0.44
24:NG:171:VAL:HG13	25:NN:251:THR:OG1	2.17	0.44
33:SK:2:ALA:HB3	33:SK:215:LEU:HD11	1.99	0.44
35:SM:361:CYS:SG	35:SM:362:ILE:N	2.90	0.44
42:SW:350:ILE:O	42:SW:354:LEU:HD23	2.17	0.44
5:L7:158:GLU:O	5:L7:162:GLU:OE1	2.34	0.44
6:L8:43:THR:HG22	6:L8:43:THR:O	2.17	0.44
4:L6:22:VAL:HG11	7:L9:200:LEU:HD12	2.00	0.44
9:LB:34:PHE:CD2	26:SA:293:LEU:HD22	2.52	0.44
24:NG:171:VAL:HG11	25:NN:251:THR:HG21	2.00	0.44
17:LN:29:VAL:HG13	17:LN:348:ARG:HD3	2.00	0.44
17:LN:370:THR:O	17:LN:370:THR:HG22	2.18	0.44
34:SL:122:GLY:O	34:SL:124:LYS:NZ	2.49	0.44
36:SN:142:LYS:NZ	37:SO:154:MET:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:261:G:H21	39:SS:265:MET:CE	2.31	0.44
3:L3:2052:G:O2'	3:L3:2057:A:N1	2.47	0.44
7:L9:16:SER:OG	21:LU:48:CYS:SG	2.48	0.44
39:SS:256:VAL:O	39:SS:260:VAL:HG23	2.17	0.44
3:L3:308:G:OP2	3:L3:308:G:N2	2.39	0.44
23:NE:269:LYS:O	23:NE:273:LEU:HD23	2.17	0.44
3:L3:4583:C:O4'	17:LN:97:ARG:NH1	2.50	0.43
35:SM:150:THR:HG22	35:SM:151:GLY:N	2.33	0.43
3:L3:1899:G:O2'	18:LQ:57:ASN:OD1	2.34	0.43
21:LU:77:VAL:HG11	21:LU:82:ARG:HB3	1.98	0.43
33:SK:96:ARG:HB3	41:SV:76:ASN:ND2	2.33	0.43
33:SK:161:VAL:HG22	33:SK:162:HIS:H	1.83	0.43
42:SW:186:VAL:HG11	42:SW:191:LEU:HD21	1.99	0.43
3:L3:297:U:OP2	37:SO:123:LYS:NZ	2.51	0.43
3:L3:5041:G:N1	17:LN:389:MET:O	2.46	0.43
23:NE:345:ARG:O	36:SN:174:ARG:NH2	2.51	0.43
38:SR:439:ALA:O	38:SR:442:ILE:HG22	2.19	0.43
34:SL:254:LYS:NZ	34:SL:255:THR:O	2.45	0.43
42:SW:448:ILE:O	42:SW:450:LEU:N	2.49	0.43
23:NE:233:GLY:O	23:NE:283:ARG:NH2	2.51	0.43
26:SA:211:TYR:OH	26:SA:218:ILE:HD11	2.18	0.43
6:L8:70:GLN:OE1	6:L8:74:ARG:NH2	2.51	0.43
7:L9:143:ARG:HH12	19:LS:95:LEU:HD12	1.83	0.43
42:SW:222:ALA:HB2	42:SW:367:GLN:HE22	1.83	0.43
5:L7:84:VAL:HG11	5:L7:102:LEU:HD22	2.01	0.43
6:L8:96:GLU:OE2	6:L8:100:ARG:NE	2.52	0.43
29:SE:121:LYS:HD3	39:SS:260:VAL:HG21	2.01	0.43
33:SK:54:ALA:N	33:SK:80:GLU:OE1	2.49	0.43
3:L3:1676:C:O2	23:NE:349:ARG:NH2	2.52	0.42
5:L7:115:LYS:O	5:L7:117:ARG:NH1	2.50	0.42
5:L7:185:VAL:O	5:L7:189:ILE:HG22	2.19	0.42
17:LN:47:LEU:HD13	17:LN:84:MET:HE1	2.00	0.42
23:NE:232:THR:HG21	23:NE:280:VAL:HG12	2.01	0.42
3:L3:2318:G:OP2	18:LQ:14:LYS:NZ	2.51	0.42
3:L3:5039:U:H4'	41:SV:115:ASN:OD1	2.18	0.42
31:SI:78:LEU:HD13	31:SI:111:LEU:HD23	2.00	0.42
40:ST:232:VAL:O	40:ST:232:VAL:HG12	2.19	0.42
27:SC:49:VAL:O	27:SC:49:VAL:HG23	2.18	0.42
3:L3:410:A:O2'	3:L3:414:C:O2'	2.24	0.42
3:L3:5052:C:H2'	3:L3:5053:U:O4'	2.19	0.42
23:NE:266:ALA:HB1	23:NE:270:TRP:HZ3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:SA:209:ILE:HB	26:SA:229:LEU:HD13	2.01	0.42
35:SM:357:ASP:OD1	35:SM:358:LYS:N	2.52	0.42
3:L3:4883:C:N4	27:SC:181:LEU:O	2.48	0.42
31:SI:105:ILE:O	31:SI:105:ILE:HG13	2.19	0.42
23:NE:228:LEU:HD23	23:NE:228:LEU:H	1.85	0.42
27:SC:96:VAL:HG12	27:SC:105:ARG:HD2	2.00	0.42
17:LN:67:VAL:O	17:LN:67:VAL:HG22	2.20	0.42
25:NN:122:VAL:HG21	25:NN:130:MET:CE	2.48	0.42
25:NN:54:MET:HE1	25:NN:164:PHE:CZ	2.55	0.41
28:SD:176:ALA:O	28:SD:180:GLY:N	2.52	0.41
3:L3:1725:U:O2'	28:SD:108:VAL:HG22	2.20	0.41
3:L3:369:G:N2	3:L3:372:A:OP2	2.41	0.41
16:LL:112:ARG:NH1	27:SC:117:PRO:O	2.47	0.41
31:SI:245:GLU:O	31:SI:248:ASN:ND2	2.52	0.41
3:L3:353:A:N1	3:L3:360:A:O2'	2.44	0.41
24:NG:170:VAL:HG21	25:NN:199:ILE:CD1	2.51	0.41
33:SK:108:THR:HG22	33:SK:117:VAL:HG12	2.01	0.41
37:SO:173:ASP:OD1	37:SO:174:GLU:N	2.53	0.41
3:L3:424:U:OP1	8:LA:34:GLN:NE2	2.53	0.41
3:L3:2303:C:OP1	18:LQ:107:ASN:ND2	2.50	0.41
17:LN:29:VAL:CG2	17:LN:346:THR:HG21	2.50	0.41
18:LQ:124:ASN:OD1	18:LQ:124:ASN:N	2.53	0.41
12:LG:94:VAL:HG11	41:SV:20:MET:CE	2.51	0.41
18:LQ:84:GLU:O	18:LQ:87:VAL:HG22	2.21	0.41
24:NG:159:GLU:OE1	24:NG:159:GLU:HA	2.20	0.41
29:SE:229:ARG:NH1	29:SE:230:TYR:OH	2.54	0.41
33:SK:201:ASP:OD1	33:SK:202:TRP:N	2.54	0.41
38:SR:453:LEU:HD22	41:SV:71:PHE:HE2	1.83	0.41
7:L9:138:PHE:HA	7:L9:143:ARG:HE	1.86	0.40
3:L3:5029:C:HO2'	3:L3:5030:U:H6	1.67	0.40
17:LN:93:VAL:HG12	17:LN:157:CYS:HA	2.03	0.40
23:NE:221:ARG:O	23:NE:224:VAL:HG22	2.21	0.40
34:SL:57:LEU:HD11	42:SW:527:LEU:HD22	2.02	0.40
39:SS:322:LEU:HD13	39:SS:344:PRO:HD2	2.03	0.40
3:L3:412:G:HO2'	3:L3:413:G:P	2.36	0.40
5:L7:23:VAL:HG13	5:L7:33:VAL:HG11	2.03	0.40
23:NE:232:THR:HG22	23:NE:281:LYS:O	2.21	0.40
41:SV:84:GLU:OE1	41:SV:84:GLU:HA	2.21	0.40
34:SL:43:LEU:HG	34:SL:261:LEU:HD12	2.03	0.40
5:L7:186:GLU:HA	5:L7:189:ILE:HG22	2.02	0.40
33:SK:109:THR:OG1	33:SK:149:GLY:HA2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:SW:368:THR:HG22	42:SW:369:ARG:N	2.36	0.40

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	
4	L6	112/211 (53%)	110 (98%)	2 (2%)	0	100	100
5	L7	180/203 (89%)	179 (99%)	1 (1%)	0	100	100
6	L8	133/215 (62%)	131 (98%)	2 (2%)	0	100	100
7	L9	180/204 (88%)	179 (99%)	1 (1%)	0	100	100
8	LA	115/184 (62%)	113 (98%)	2 (2%)	0	100	100
9	LB	149/188 (79%)	149 (100%)	0	0	100	100
10	LC	171/176 (97%)	171 (100%)	0	0	100	100
11	LE	102/160 (64%)	101 (99%)	1 (1%)	0	100	100
12	LG	110/140 (79%)	110 (100%)	0	0	100	100
13	LH	18/156 (12%)	18 (100%)	0	0	100	100
14	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
15	LK	104/148 (70%)	102 (98%)	2 (2%)	0	100	100
16	LL	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
17	LN	372/403 (92%)	367 (99%)	5 (1%)	0	100	100
18	LQ	126/135 (93%)	126 (100%)	0	0	100	100
19	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
20	LT	107/110 (97%)	107 (100%)	0	0	100	100
21	LU	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
22	LW	65/97 (67%)	65 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	NE	152/361 (42%)	150 (99%)	2 (1%)	0	100	100
24	NG	87/282 (31%)	87 (100%)	0	0	100	100
25	NN	238/473 (50%)	234 (98%)	4 (2%)	0	100	100
26	SA	325/427 (76%)	321 (99%)	4 (1%)	0	100	100
27	SC	205/288 (71%)	203 (99%)	2 (1%)	0	100	100
28	SD	210/248 (85%)	205 (98%)	5 (2%)	0	100	100
29	SE	184/266 (69%)	183 (100%)	1 (0%)	0	100	100
30	SH	148/293 (50%)	145 (98%)	3 (2%)	0	100	100
31	SI	198/255 (78%)	196 (99%)	2 (1%)	0	100	100
32	SJ	70/847 (8%)	70 (100%)	0	0	100	100
33	SK	224/245 (91%)	219 (98%)	5 (2%)	0	100	100
34	SL	241/490 (49%)	236 (98%)	5 (2%)	0	100	100
35	SM	427/588 (73%)	425 (100%)	2 (0%)	0	100	100
36	SN	162/306 (53%)	161 (99%)	1 (1%)	0	100	100
37	SO	292/353 (83%)	288 (99%)	4 (1%)	0	100	100
38	SR	73/634 (12%)	71 (97%)	2 (3%)	0	100	100
39	SS	227/746 (30%)	225 (99%)	2 (1%)	0	100	100
40	ST	34/365 (9%)	33 (97%)	1 (3%)	0	100	100
41	SV	135/163 (83%)	133 (98%)	2 (2%)	0	100	100
42	SW	441/670 (66%)	433 (98%)	8 (2%)	0	100	100
43	SZ	156/178 (88%)	155 (99%)	1 (1%)	0	100	100
All	All	6746/11718 (58%)	6669 (99%)	77 (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	
4	L6	98/177 (55%)	98 (100%)	0	100	100
5	L7	157/174 (90%)	157 (100%)	0	100	100
6	L8	115/161 (71%)	115 (100%)	0	100	100
7	L9	156/172 (91%)	156 (100%)	0	100	100
8	LA	111/163 (68%)	111 (100%)	0	100	100
9	LB	136/165 (82%)	136 (100%)	0	100	100
10	LC	154/157 (98%)	154 (100%)	0	100	100
11	LE	47/140 (34%)	47 (100%)	0	100	100
12	LG	87/107 (81%)	87 (100%)	0	100	100
13	LH	13/133 (10%)	13 (100%)	0	100	100
14	LI	124/135 (92%)	124 (100%)	0	100	100
15	LK	29/121 (24%)	29 (100%)	0	100	100
16	LL	106/121 (88%)	106 (100%)	0	100	100
17	LN	328/348 (94%)	328 (100%)	0	100	100
18	LQ	114/121 (94%)	114 (100%)	0	100	100
19	LS	109/110 (99%)	109 (100%)	0	100	100
20	LT	88/89 (99%)	88 (100%)	0	100	100
21	LU	87/89 (98%)	87 (100%)	0	100	100
22	LW	58/80 (72%)	58 (100%)	0	100	100
23	NE	136/294 (46%)	136 (100%)	0	100	100
24	NG	83/246 (34%)	83 (100%)	0	100	100
25	NN	218/398 (55%)	218 (100%)	0	100	100
26	SA	279/348 (80%)	279 (100%)	0	100	100
27	SC	187/252 (74%)	187 (100%)	0	100	100
28	SD	182/215 (85%)	182 (100%)	0	100	100
29	SE	159/223 (71%)	159 (100%)	0	100	100
30	SH	140/274 (51%)	140 (100%)	0	100	100
31	SI	182/228 (80%)	182 (100%)	0	100	100
32	SJ	64/733 (9%)	64 (100%)	0	100	100
33	SK	196/213 (92%)	196 (100%)	0	100	100
34	SL	226/437 (52%)	225 (100%)	1 (0%)	84	91
35	SM	350/509 (69%)	350 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	SN	126/260 (48%)	126 (100%)	0	100	100
37	SO	274/319 (86%)	274 (100%)	0	100	100
38	SR	69/574 (12%)	69 (100%)	0	100	100
39	SS	208/648 (32%)	208 (100%)	0	100	100
40	ST	27/300 (9%)	27 (100%)	0	100	100
41	SV	127/149 (85%)	127 (100%)	0	100	100
42	SW	394/591 (67%)	394 (100%)	0	100	100
43	SZ	141/158 (89%)	141 (100%)	0	100	100
All	All	5885/10132 (58%)	5884 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
34	SL	30	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
5	L7	90	HIS
6	L8	66	HIS
6	L8	69	HIS
9	LB	7	HIS
10	LC	122	HIS
12	LG	101	ASN
15	LK	66	ASN
17	LN	167	GLN
19	LS	108	GLN
20	LT	56	ASN
20	LT	99	HIS
21	LU	26	HIS
24	NG	172	GLN
25	NN	84	HIS
26	SA	38	ASN
26	SA	112	HIS
26	SA	215	ASN
26	SA	310	HIS
27	SC	136	HIS
27	SC	157	HIS

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Mol	Chain	Res	Type
28	SD	206	ASN
28	SD	235	ASN
29	SE	64	GLN
29	SE	208	ASN
29	SE	225	ASN
30	SH	60	GLN
30	SH	67	GLN
31	SI	255	ASN
33	SK	162	HIS
34	SL	218	HIS
35	SM	209	HIS
35	SM	240	GLN
38	SR	436	HIS
39	SS	310	HIS
40	ST	213	GLN
41	SV	17	HIS
41	SV	129	GLN
41	SV	132	HIS
42	SW	277	HIS
42	SW	402	GLN
43	SZ	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	147/157 (93%)	14 (9%)	1 (0%)
2	L2	65/1167 (5%)	9 (13%)	0
3	L3	1532/5070 (30%)	204 (13%)	5 (0%)
All	All	1744/6394 (27%)	227 (13%)	6 (0%)

All (227) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	34	U
1	L1	59	A
1	L1	62	A
1	L1	63	U
1	L1	82	A
1	L1	83	C
1	L1	84	A
1	L1	86	U

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Mol	Chain	Res	Type
1	L1	94	G
1	L1	103	A
1	L1	105	C
1	L1	111	U
1	L1	156	U
1	L1	157	U
2	L2	2	C
2	L2	11	C
2	L2	48	G
2	L2	49	G
2	L2	51	U
2	L2	62	U
2	L2	94	U
2	L2	96	A
2	L2	101	A
3	L3	41	C
3	L3	48	G
3	L3	58	G
3	L3	59	A
3	L3	64	A
3	L3	65	A
3	L3	69	A
3	L3	91	G
3	L3	93	G
3	L3	95	G
3	L3	108	A
3	L3	109	G
3	L3	119	G
3	L3	159	C
3	L3	170	C
3	L3	171	U
3	L3	172	C
3	L3	173	C
3	L3	182	G
3	L3	197	A
3	L3	200	U
3	L3	210	C
3	L3	216	C
3	L3	218	A
3	L3	219	G
3	L3	220	C
3	L3	234	G

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Mol	Chain	Res	Type
3	L3	265	C
3	L3	271	C
3	L3	277	G
3	L3	315	G
3	L3	340	C
3	L3	349	A
3	L3	362	A
3	L3	386	A
3	L3	387	G
3	L3	408	A
3	L3	409	G
3	L3	410	A
3	L3	413	G
3	L3	449	C
3	L3	450	G
3	L3	452	A
3	L3	453	G
3	L3	454	U
3	L3	459	C
3	L3	464	G
3	L3	467	U
3	L3	468	U
3	L3	472	C
3	L3	685	C
3	L3	697	G
3	L3	699	C
3	L3	704	C
3	L3	730	G
3	L3	731	G
3	L3	739	G
3	L3	741	C
3	L3	742	G
3	L3	746	A
3	L3	913	U
3	L3	914	U
3	L3	915	A
3	L3	917	A
3	L3	926	G
3	L3	932	A
3	L3	933	G
3	L3	943	A
3	L3	944	A

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Mol	Chain	Res	Type
3	L3	945	U
3	L3	956	A
3	L3	959	G
3	L3	960	A
3	L3	1072	C
3	L3	1280	C
3	L3	1284	G
3	L3	1287	G
3	L3	1293	G
3	L3	1294	A
3	L3	1295	C
3	L3	1296	G
3	L3	1301	C
3	L3	1313	C
3	L3	1314	C
3	L3	1315	C
3	L3	1319	U
3	L3	1325	C
3	L3	1326	A
3	L3	1330	A
3	L3	1354	A
3	L3	1358	G
3	L3	1359	G
3	L3	1502	G
3	L3	1654	G
3	L3	1661	C
3	L3	1677	U
3	L3	1679	A
3	L3	1680	G
3	L3	1681	G
3	L3	1682	A
3	L3	1684	A
3	L3	1691	G
3	L3	1724	G
3	L3	1804	A
3	L3	1836	G
3	L3	1837	A
3	L3	1842	G
3	L3	1854	G
3	L3	1856	C
3	L3	1857	C
3	L3	1881	C

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Mol	Chain	Res	Type
3	L3	1882	U
3	L3	1888	A
3	L3	1891	A
3	L3	1892	A
3	L3	1897	A
3	L3	1906	U
3	L3	1910	G
3	L3	1919	G
3	L3	1921	C
3	L3	1922	G
3	L3	2055	G
3	L3	2056	G
3	L3	2069	A
3	L3	2084	C
3	L3	2089	G
3	L3	2090	U
3	L3	2091	C
3	L3	2268	A
3	L3	2289	C
3	L3	2300	A
3	L3	2301	G
3	L3	2313	A
3	L3	2348	G
3	L3	2351	C
3	L3	2364	G
3	L3	2366	A
3	L3	2829	U
3	L3	2836	A
3	L3	2837	U
3	L3	2838	G
3	L3	2842	G
3	L3	3852	A
3	L3	4584	A
3	L3	4589	A
3	L3	4590	A
3	L3	4618	G
3	L3	4621	C
3	L3	4629	U
3	L3	4633	G
3	L3	4640	C
3	L3	4641	U
3	L3	4642	U

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Mol	Chain	Res	Type
3	L3	4647	G
3	L3	4648	A
3	L3	4649	G
3	L3	4651	A
3	L3	4657	U
3	L3	4658	G
3	L3	4661	G
3	L3	4672	A
3	L3	4673	U
3	L3	4680	G
3	L3	4719	G
3	L3	4741	C
3	L3	4742	G
3	L3	4747	C
3	L3	4754	G
3	L3	4757	C
3	L3	4759	C
3	L3	4761	G
3	L3	4763	U
3	L3	4765	G
3	L3	4770	U
3	L3	4773	C
3	L3	4870	G
3	L3	4871	C
3	L3	4882	U
3	L3	4883	C
3	L3	4910	G
3	L3	4912	G
3	L3	4914	C
3	L3	4934	A
3	L3	4935	C
3	L3	4943	A
3	L3	4966	A
3	L3	4976	U
3	L3	4979	A
3	L3	5013	C
3	L3	5022	U
3	L3	5025	C
3	L3	5026	U
3	L3	5027	C
3	L3	5028	G
3	L3	5030	U

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Mol	Chain	Res	Type
3	L3	5031	G
3	L3	5040	U
3	L3	5041	G
3	L3	5045	G
3	L3	5051	C
3	L3	5053	U
3	L3	5059	C
3	L3	5064	G
3	L3	5065	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	156	U
3	L3	172	C
3	L3	412	G
3	L3	1880	G
3	L3	2267	U
3	L3	4679	G

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

3 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	$\# Z > 2$
39	SEP	SS	126	39	8,9,10	1.58	1 (12%)	7,12,14	1.20	1 (14%)
39	SEP	SS	127	39	8,9,10	1.58	1 (12%)	7,12,14	1.31	1 (14%)
17	HIC	LN	245	17	10,11,12	1.51	1 (10%)	9,14,16	1.20	1 (11%)

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
39	SEP	SS	126	39	-	0/6/8/10	-
39	SEP	SS	127	39	-	3/6/8/10	-
17	HIC	LN	245	17	-	0/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	SS	126	SEP	P-O1P	3.46	1.61	1.50
39	SS	127	SEP	P-O1P	3.44	1.61	1.50
17	LN	245	HIC	CD2-CG	3.00	1.41	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	LN	245	HIC	NE2-CE1-ND1	-2.90	111.56	112.66
39	SS	127	SEP	OG-CB-CA	2.83	110.90	108.14
39	SS	126	SEP	OG-CB-CA	2.50	110.58	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	SS	127	SEP	CA-CB-OG-P
39	SS	127	SEP	N-CA-CB-OG
39	SS	127	SEP	C-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	SS	126	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 53 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

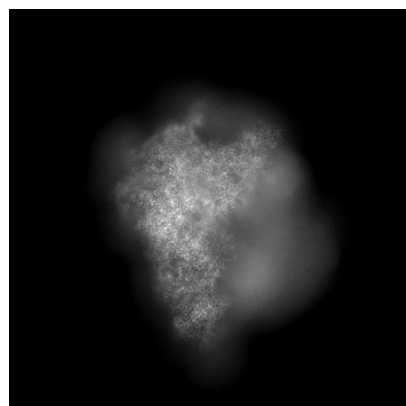
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29253. These allow visual inspection of the internal detail of the map and identification of artifacts.

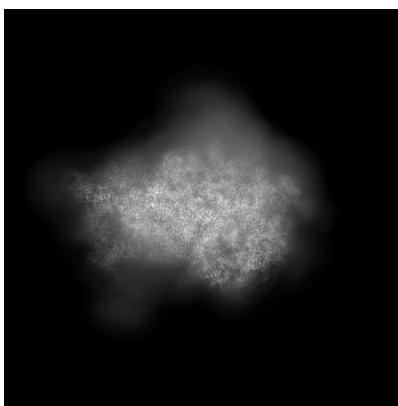
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

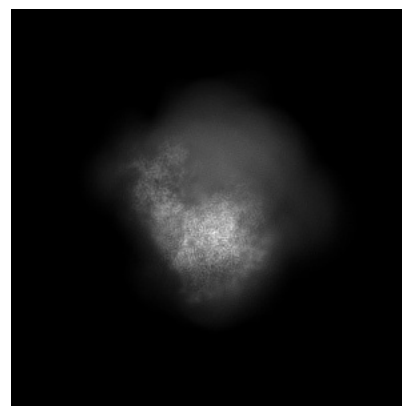
6.1.1 Primary map



X

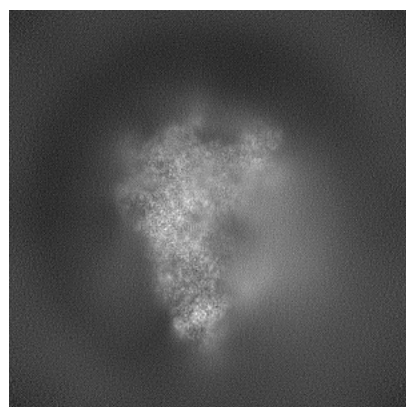


Y

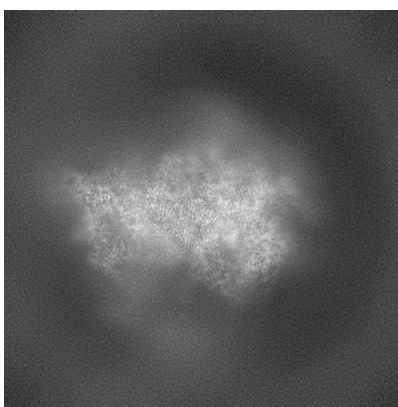


Z

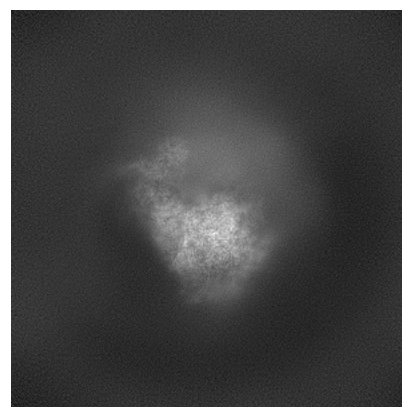
6.1.2 Raw map



X



Y

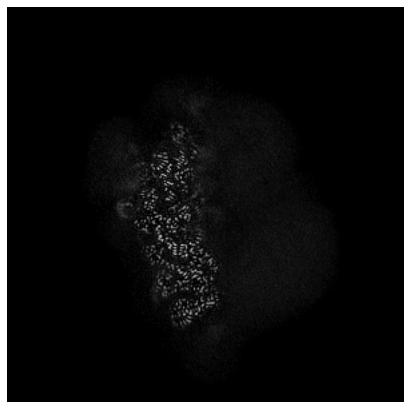


Z

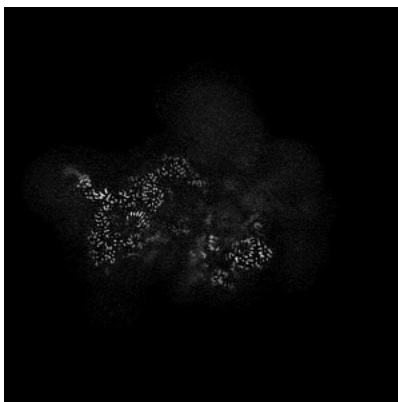
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

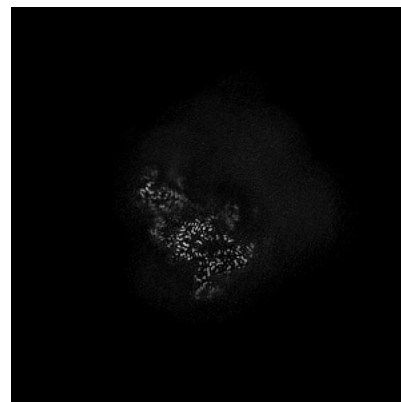
6.2.1 Primary map



X Index: 240

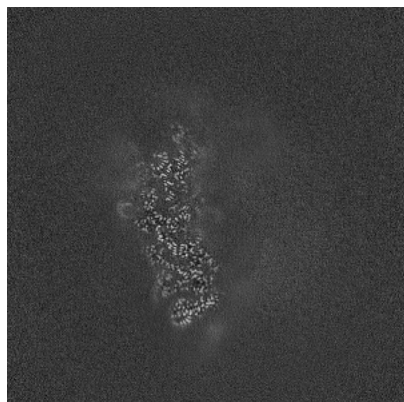


Y Index: 240

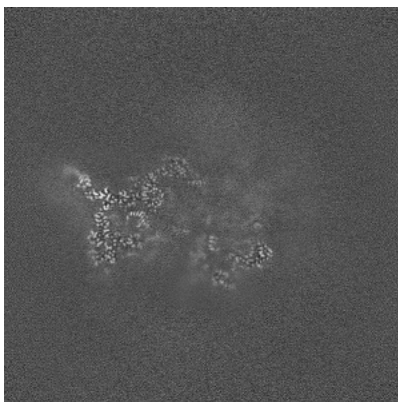


Z Index: 240

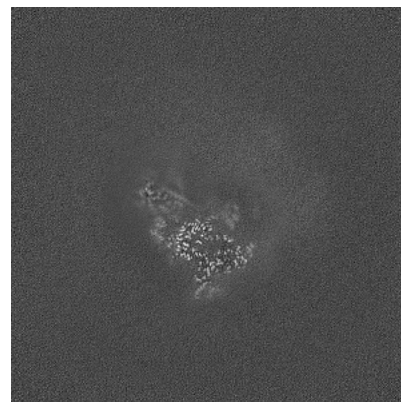
6.2.2 Raw map



X Index: 240



Y Index: 240

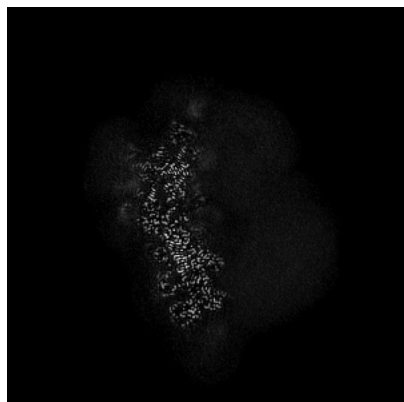


Z Index: 240

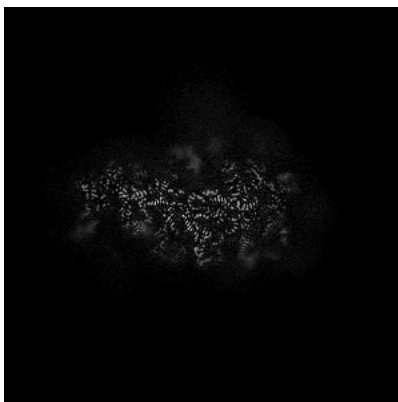
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

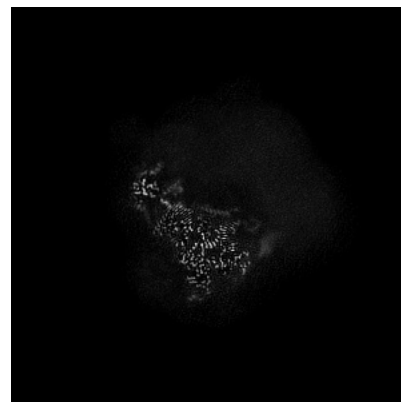
6.3.1 Primary map



X Index: 244

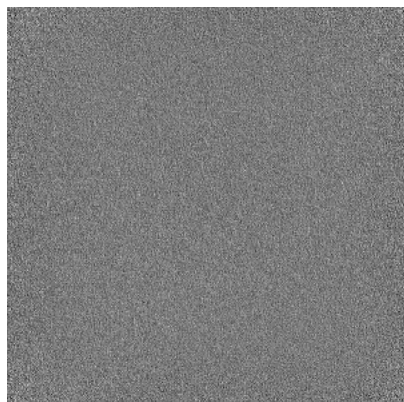


Y Index: 205

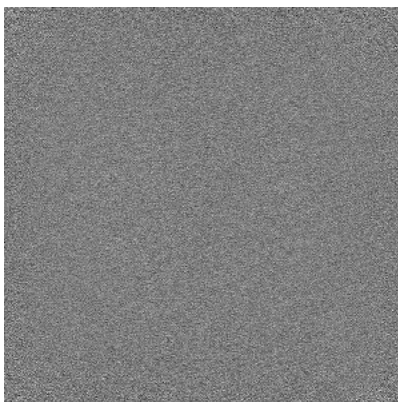


Z Index: 249

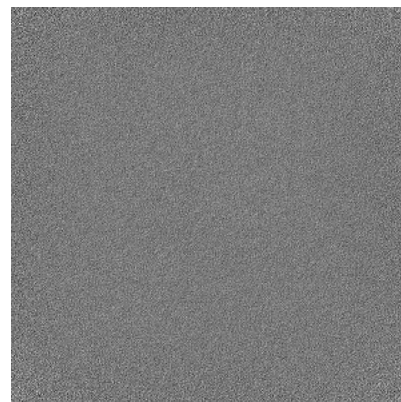
6.3.2 Raw map



X Index: 0



Y Index: 0

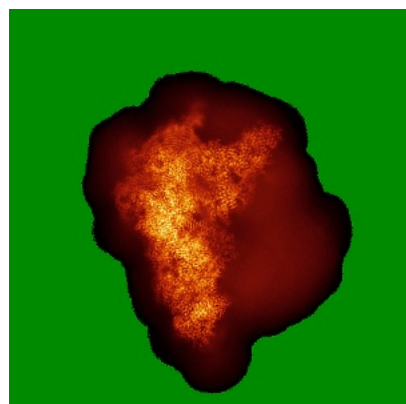


Z Index: 0

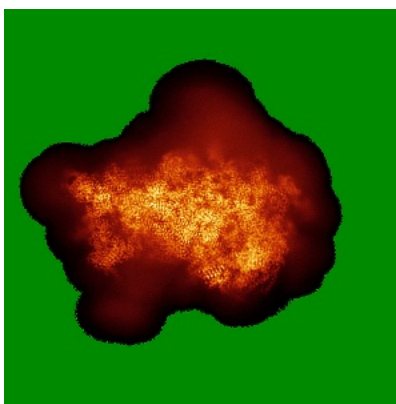
The images above show the largest variance slices of the map in three orthogonal directions.

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

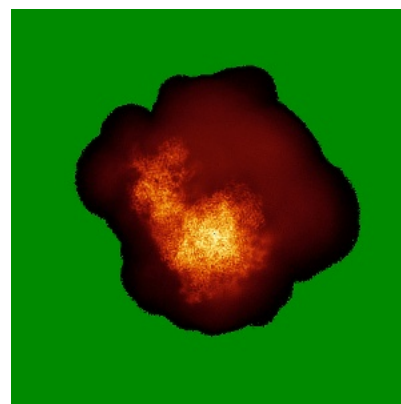
6.4.1 Primary map



X

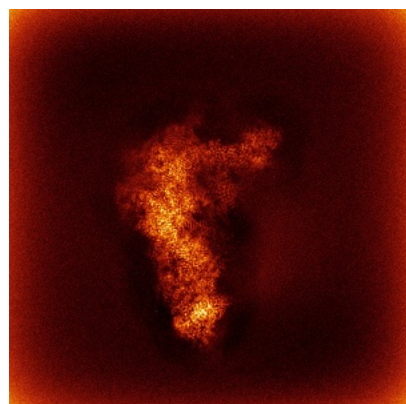


Y

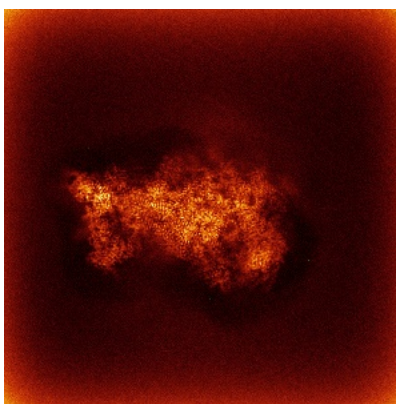


Z

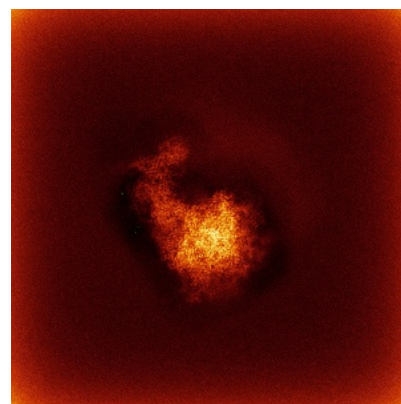
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

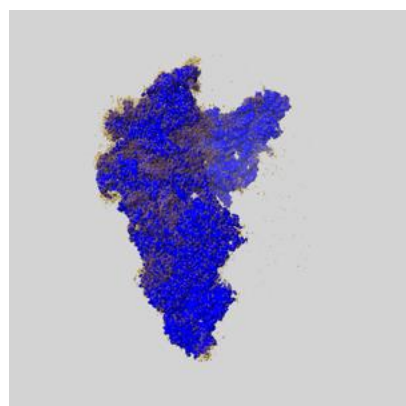
6.6 Mask visualisation [i](#)

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

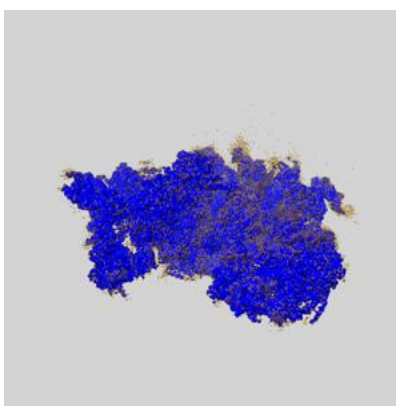
A mask typically either:

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

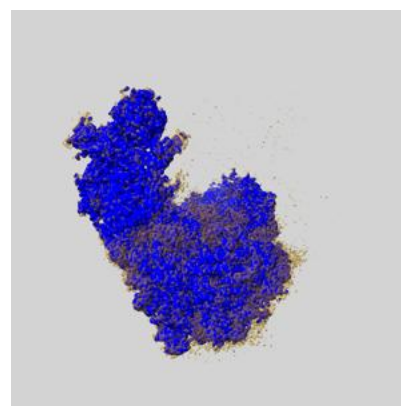
6.6.1 emd_29253_msk_1.map [i](#)



X



Y

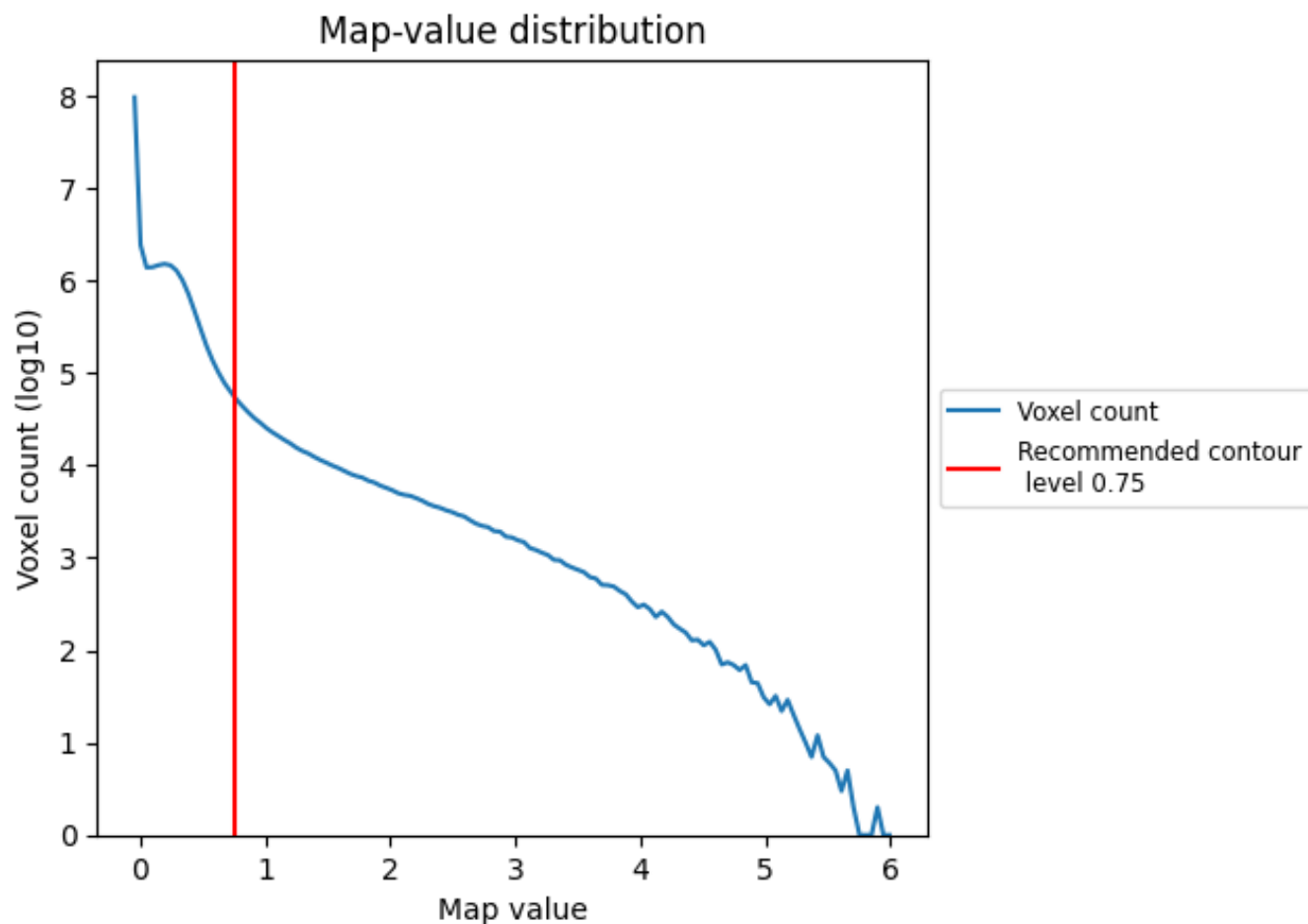


Z

7 Map analysis [i](#)

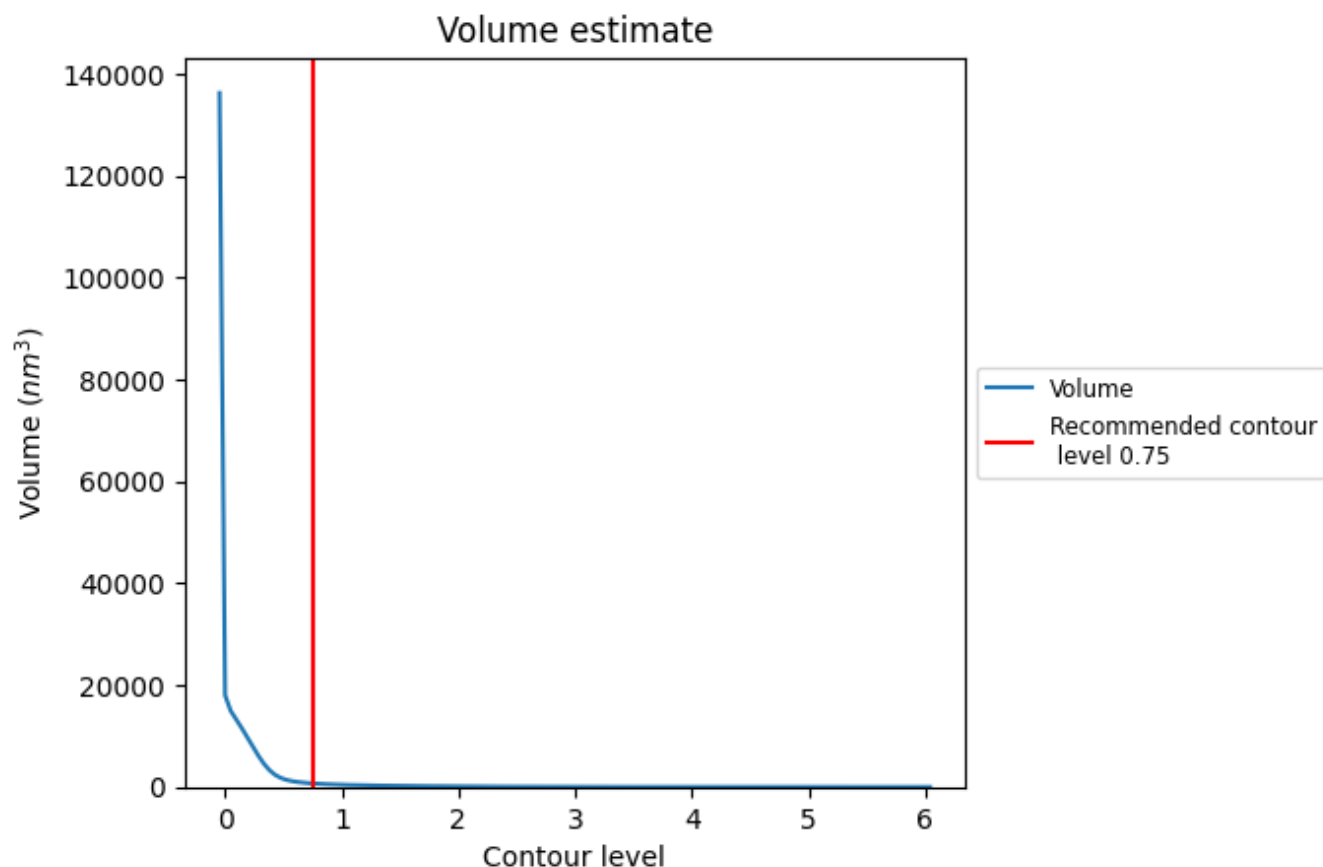
This section contains the results of statistical analysis of the map.

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.

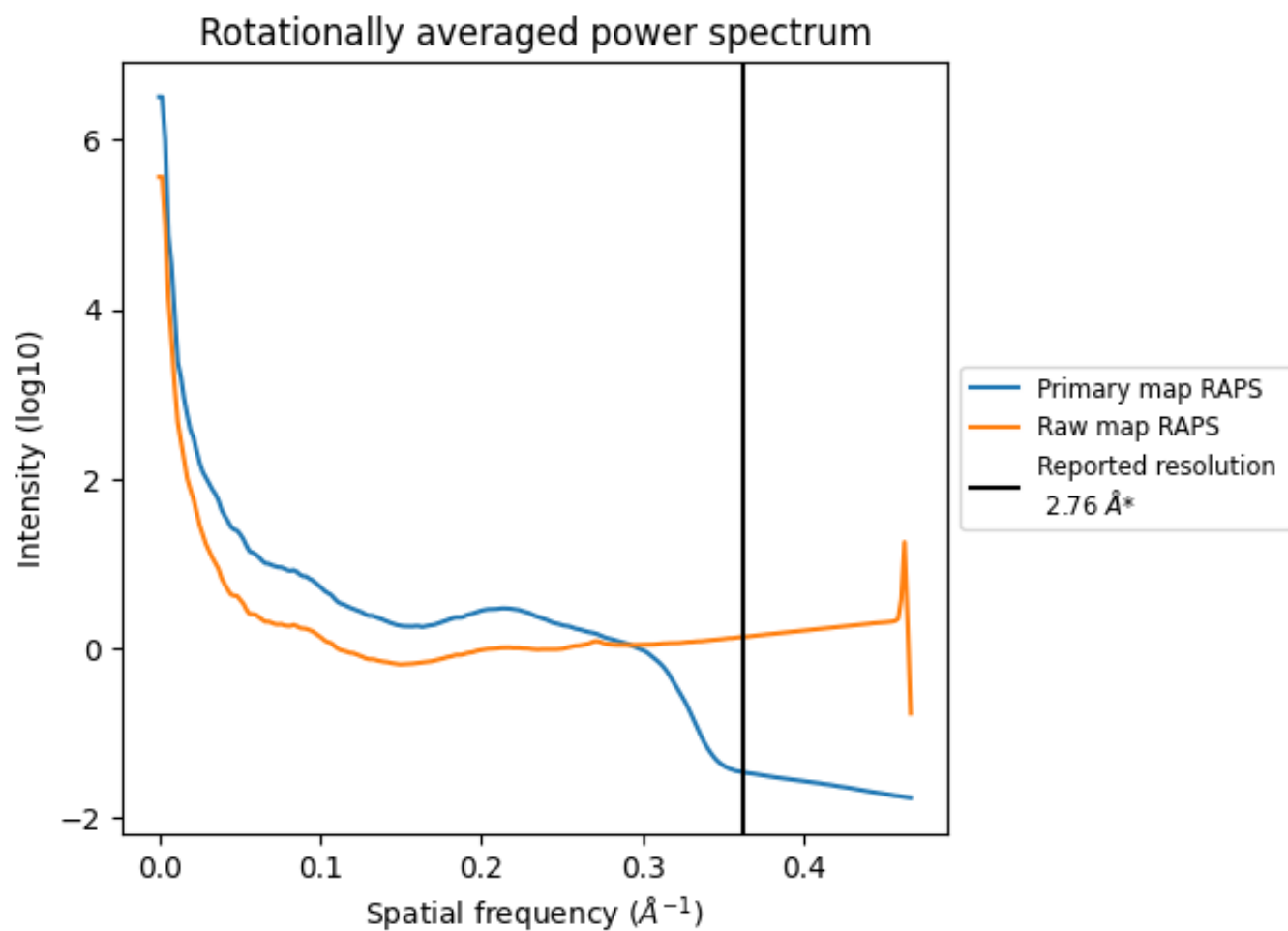
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 696 nm³; this corresponds to an approximate mass of 629 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 ⓘ

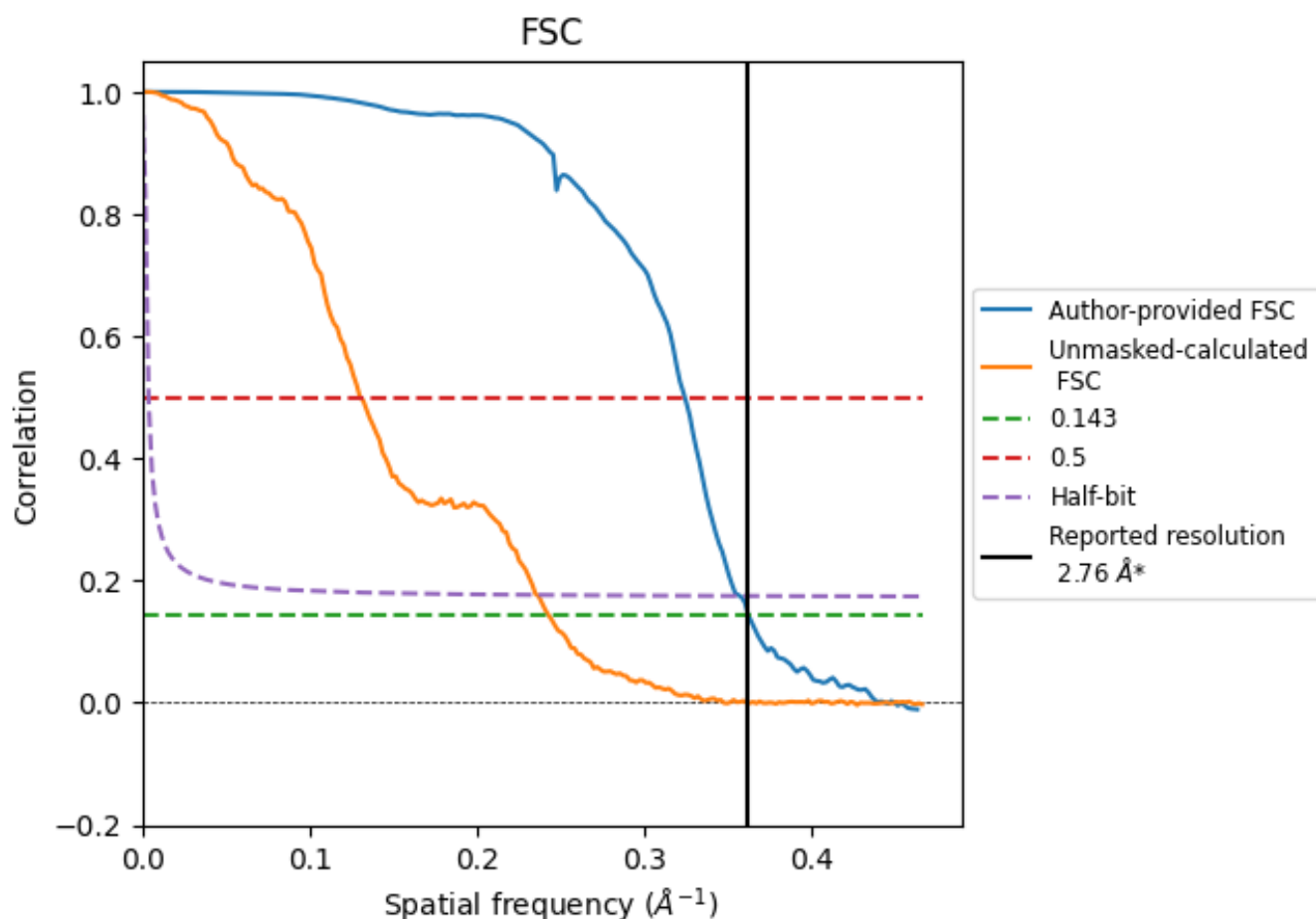


*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

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 0.362 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

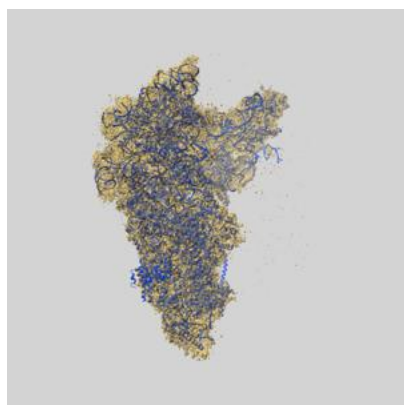
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.08	2.80
Unmasked-calculated*	4.11	7.67	4.24

*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 4.11 differs from the reported value 2.76 by more than 10 %

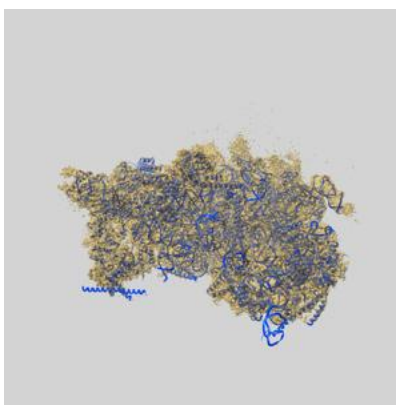
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29253 and PDB model 8FKQ. Per-residue inclusion information can be found in section 3 on page 12.

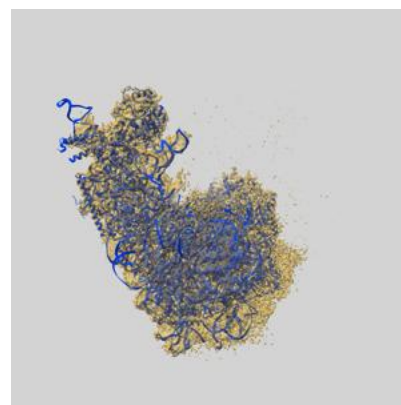
9.1 Map-model overlay [i](#)



X



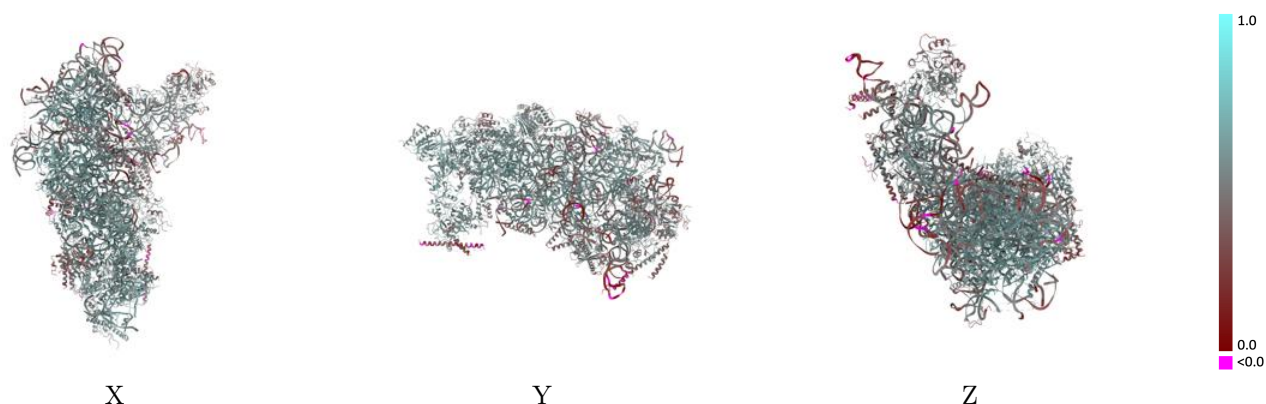
Y



Z

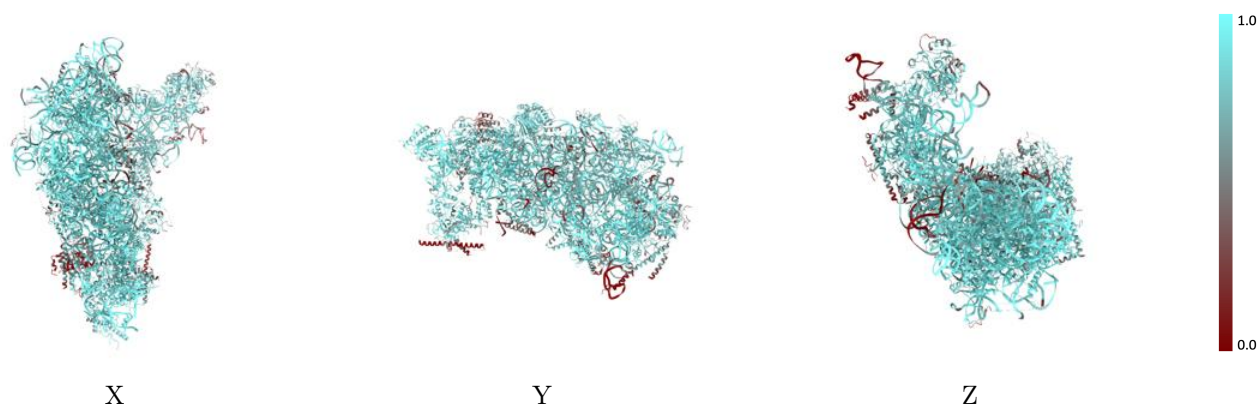
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



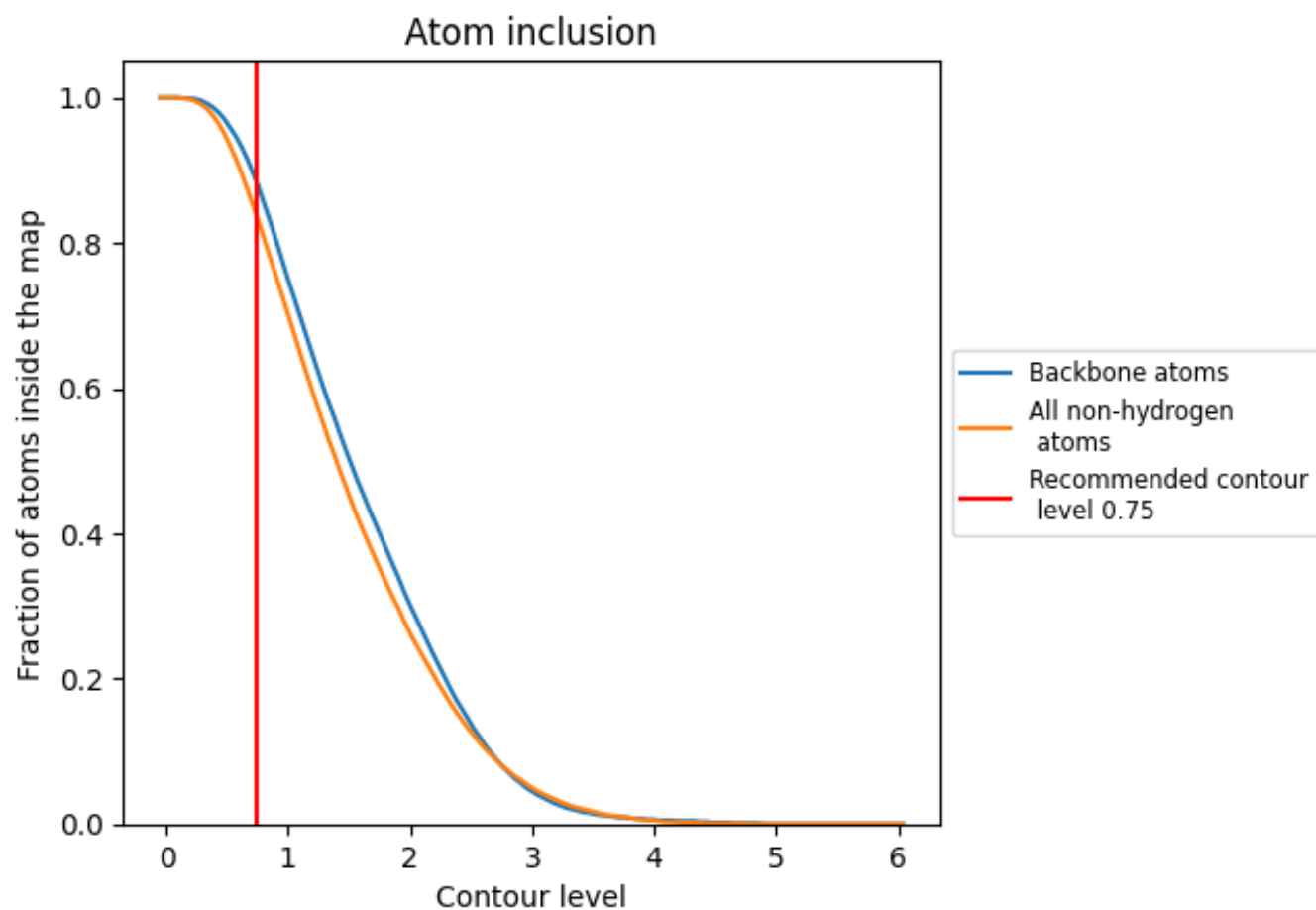
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.75).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8340	 0.5250
L1	 0.8310	 0.5210
L2	 0.9460	 0.5650
L3	 0.8780	 0.5130
L6	 0.9520	 0.6070
L7	 0.7960	 0.5040
L8	 0.8190	 0.5300
L9	 0.9660	 0.6190
LA	 0.8040	 0.5230
LB	 0.9550	 0.6180
LC	 0.8010	 0.5400
LE	 0.7100	 0.4250
LG	 0.7420	 0.4720
LH	 0.5200	 0.4810
LI	 0.8860	 0.5890
LK	 0.7910	 0.4190
LL	 0.9590	 0.6170
LN	 0.8520	 0.5470
LQ	 0.9550	 0.6230
LS	 0.6940	 0.5150
LT	 0.9640	 0.6220
LU	 0.8400	 0.5670
LW	 0.7300	 0.5510
NE	 0.6820	 0.3950
NG	 0.4440	 0.3450
NN	 0.8260	 0.5010
SA	 0.9490	 0.6140
SC	 0.8180	 0.5320
SD	 0.9520	 0.6100
SE	 0.9400	 0.5970
SH	 0.8810	 0.5730
SI	 0.8440	 0.5770
SJ	 0.6870	 0.5180
SK	 0.7200	 0.4520
SL	 0.8550	 0.5650



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SM	 0.7280	 0.5010
SN	 0.7390	 0.4810
SO	 0.7930	 0.5360
SR	 0.5470	 0.3920
SS	 0.7510	 0.5090
ST	 0.6060	 0.4910
SV	 0.6420	 0.4330
SW	 0.6170	 0.4790
SZ	 0.8540	 0.5540