



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 05:43 pm BST

PDB ID : 9H51 / pdb_00009h51
EMDB ID : EMD-51873
Title : Assembly intermediate of human mitochondrial ribosome small subunit in complex with PUS1, METTL15 and RBFA(IN conformation) (state M1)
Authors : Singh, V.; Shiriaev, D.; Khawaja, A.; Rorbach, J.
Deposited on : 2024-10-22
Resolution : 3.10 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 : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

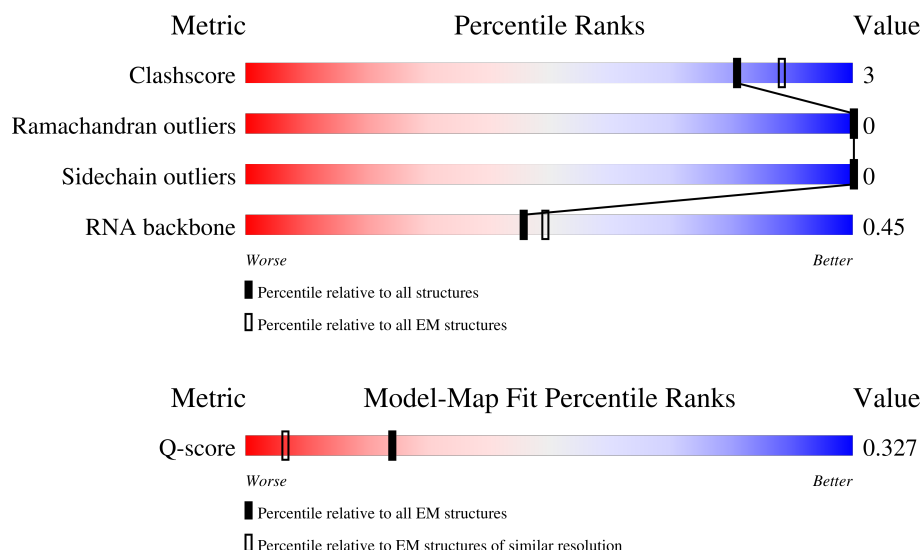
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	c	384	
2	A	959	
3	B	296	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	430	
5	E	125	
6	I	194	
7	J	138	
8	L	257	
9	M	137	
10	N	130	
11	O	258	
12	P	142	
13	Q	87	
14	R	360	
15	S	190	
16	T	173	
17	U	205	
18	V	414	
19	W	187	
20	0	215	
21	3	199	
22	b	407	
23	a	343	
24	4	689	
25	H	201	
26	1	323	
27	Z	106	
28	X	398	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	K	128	
30	Y	395	
31	G	396	
32	F	242	
33	C	167	
34	9	698	

2 Entry composition [i](#)

There are 44 unique types of molecules in this entry. The entry contains 134104 atoms, of which 62548 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 Pseudouridylate synthase 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	c	311	Total	C	H	N	O	S	0	0
			4988	1580	2493	448	451	16		

- Molecule 2 is a RNA chain called RNA (969-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	925	Total	C	H	N	O	P	0	0
			29598	8810	9952	3535	6376	925		

- Molecule 3 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	225	Total	C	H	N	O	S	0	0
			3653	1164	1825	331	323	10		

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0
			5511	1704	2794	515	485	13		

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	113	Total	C	H	N	O	S	0	0
			1806	563	914	162	163	4		

- Molecule 6 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	137	Total	C	H	N	O	S	0	0
			2077	642	1057	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 7 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	108	Total	C	H	N	O	S	0	0
			1730	521	891	169	143	6		

- Molecule 8 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	L	174	Total	C	H	N	O	S	0	0
			2997	925	1544	270	251	7		

- Molecule 9 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	M	119	Total	C	H	N	O	S	0	0
			1913	594	971	185	157	6		

- Molecule 10 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	N	110	Total	C	H	N	O	S	0	0
			1800	562	932	156	147	3		

- Molecule 11 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	O	194	Total	C	H	N	O	S	0	0
			3173	1019	1574	295	278	7		

- Molecule 12 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	P	97	Total	C	H	N	O	S	0	0
			1589	501	808	134	138	8		

- Molecule 13 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Q	87	Total	C	H	N	O	S	0	0
			1504	460	760	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	variant	UNP P82921

- Molecule 14 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	R	295	Total	C	H	N	O	S	0	0
			4844	1533	2435	413	455	8		

- Molecule 15 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	S	135	Total	C	H	N	O	S	0	0
			2227	716	1116	198	196	1		

- Molecule 16 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	T	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

- Molecule 17 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	U	176	Total	C	H	N	O	S	0	0
			2992	916	1504	301	267	4		

- Molecule 18 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	V	362	Total	C	H	N	O	S	0	0
			5939	1904	2970	495	558	12		

- Molecule 19 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	W	100	Total	C	H	N	O	S	0	0
			1594	498	805	141	146	4		

- Molecule 20 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	0	215	Total	C	H	N	O	S	0	0
			3588	1130	1801	339	313	5		

- Molecule 21 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	3	70	Total	C	H	N	O	S	0	0
			1326	401	701	134	89	1		

- Molecule 22 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	b	303	Total	C	H	N	O	S	0	0
			4796	1498	2433	421	431	13		

- Molecule 23 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	a	157	Total	C	H	N	O	S	0	0
			2500	776	1252	224	242	6		

- Molecule 24 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	4	588	Total	C	H	N	O	S	0	0
			9550	3053	4782	808	879	28		

- Molecule 25 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	H	140	Total	C	H	N	O	S	0	0
			2342	745	1190	194	210	3		

- Molecule 26 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	276	Total	C	H	N	O	S	0	0
			4512	1419	2274	381	427	11		

- Molecule 27 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Z	93	Total	C	H	N	O	S	0	0
			1593	504	805	141	139	4		

- Molecule 28 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	X	352	Total	C	H	N	O	S	0	0
			5707	1822	2858	499	517	11		

- Molecule 29 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	K	101	Total	C	H	N	O	S	0	0
			1750	537	888	179	141	5		

- Molecule 30 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	Y	149	Total	C	H	N	O	S	0	0
			2448	801	1202	207	234	4		

- Molecule 31 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	G	316	Total	C	H	N	O	S	0	0
			5202	1652	2599	463	474	14		

- Molecule 32 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	F	202	Total	C	H	N	O	S	0	0
			3397	1066	1726	303	291	11		

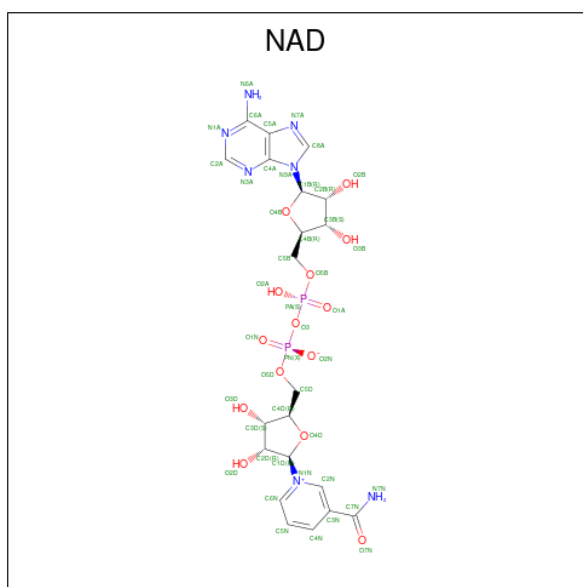
- Molecule 33 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	C	132	Total	C	H	N	O	S	0	0
			2178	699	1095	195	185	4		

- Molecule 34 is a protein called Nitric oxide-associated protein 1.

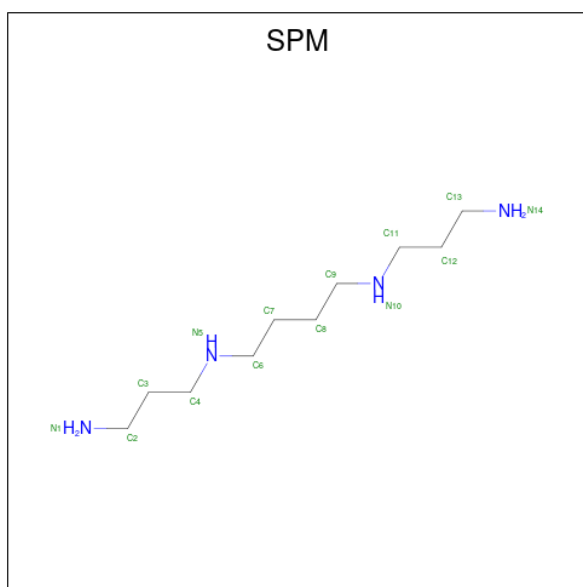
Mol	Chain	Residues	Atoms						AltConf	Trace
34	9	12	Total	C	H	N	O	S	0	0
			219	76	108	16	18	1		

- Molecule 35 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



Mol	Chain	Residues	Atoms						AltConf
35	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 36 is SPERMINE (CCD ID: SPM) (formula: $\text{C}_{10}\text{H}_{26}\text{N}_4$).



Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	H	N	0
			40	10	26	4	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	A	38	Total	Mg	0
			38	38	
37	B	1	Total	Mg	0
			1	1	
37	3	1	Total	Mg	0
			1	1	

- Molecule 38 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
38	A	6	Total	K	0
			6	6	

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

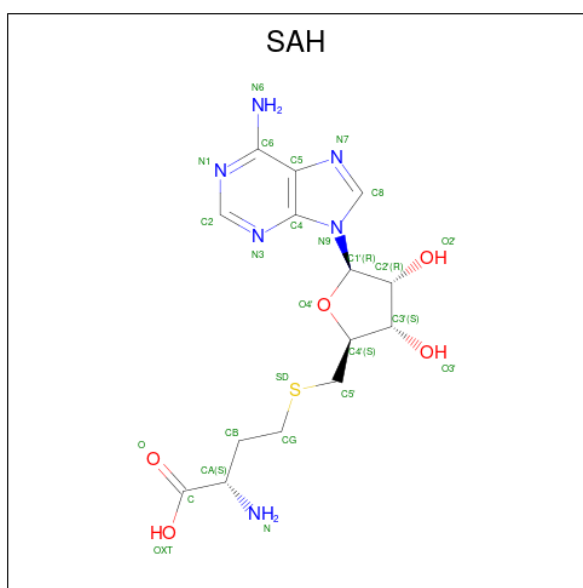
Mol	Chain	Residues	Atoms		AltConf
39	O	1	Total	Zn	0
			1	1	

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
40	P	1	Total	Fe	S	0
			4	2	2	
40	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 41 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



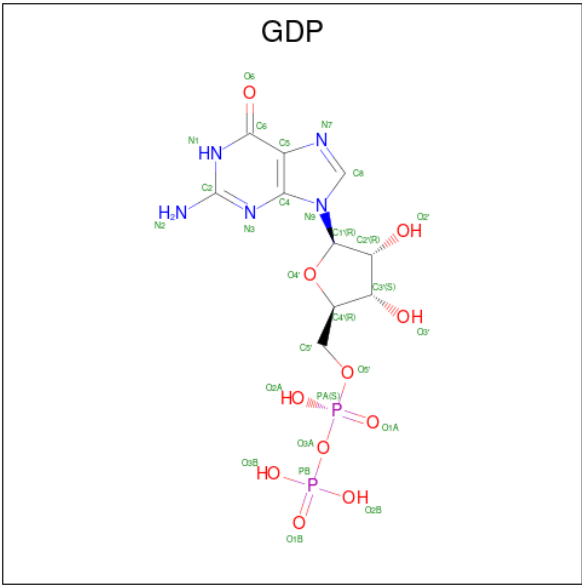
Mol	Chain	Residues	Atoms					AltConf	
41	b	1	Total	C	H	N	O	S	0
			45	14	19	6	5	1	

- Molecule 42 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 43 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						AltConf
43	X	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

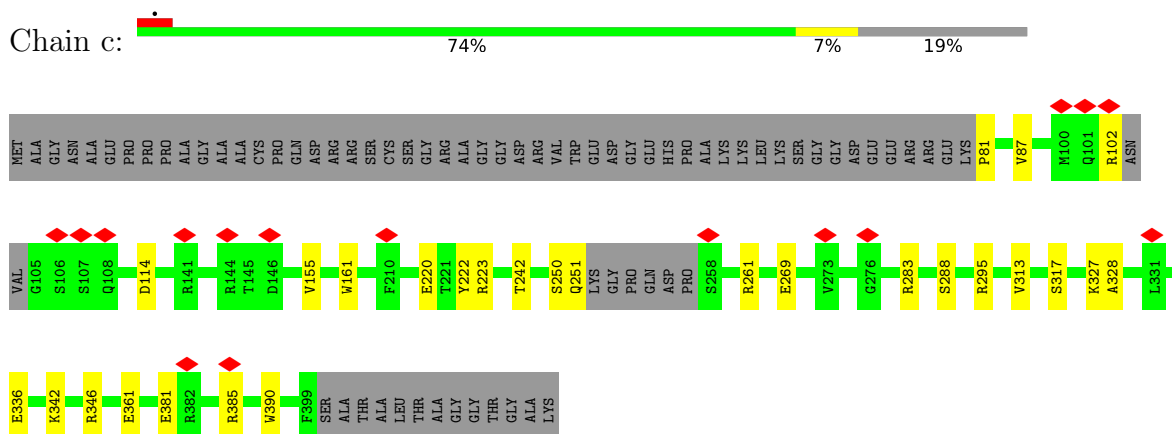
- Molecule 44 is water.

Mol	Chain	Residues	Atoms		AltConf
44	A	1	Total 1	O 1	0
44	I	1	Total 1	O 1	0
44	0	1	Total 1	O 1	0

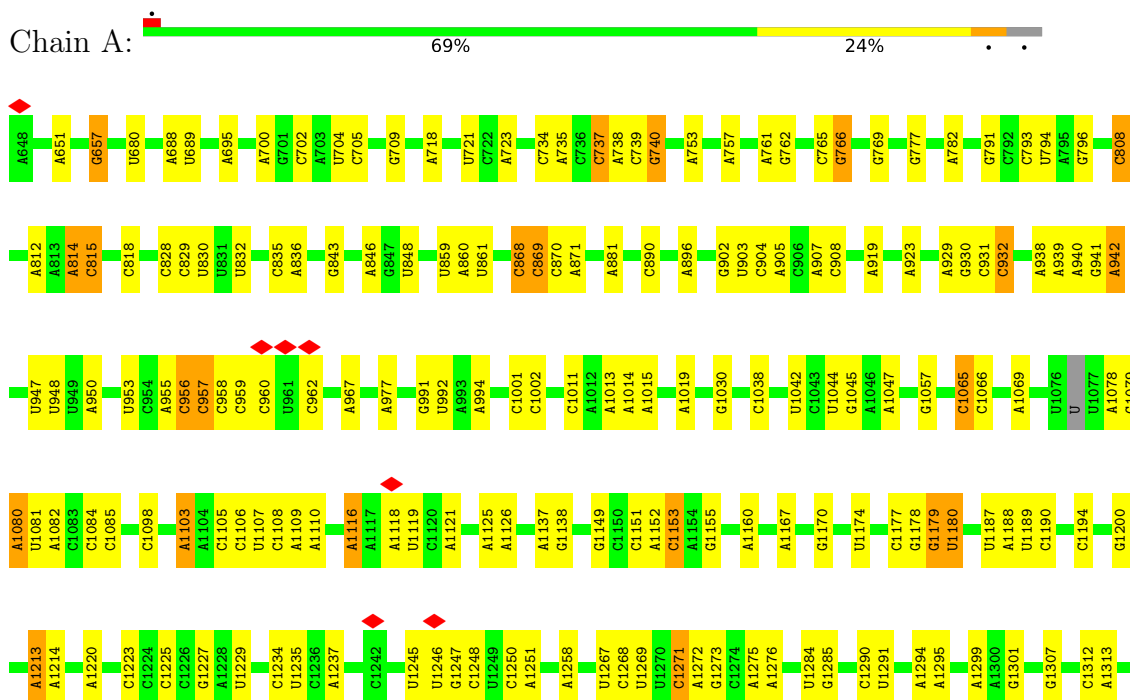
3 Residue-property plots

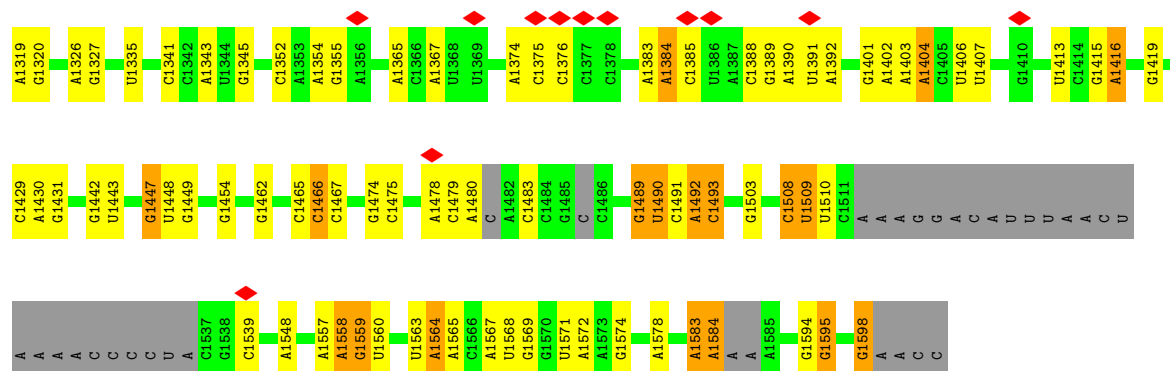
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Pseudouridylate synthase 1 homolog

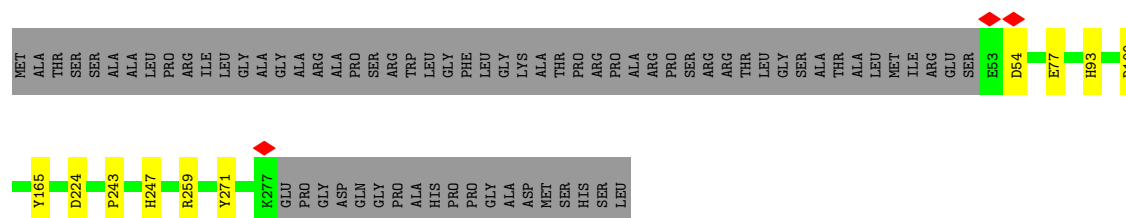


• Molecule 2: RNA (969-MER)

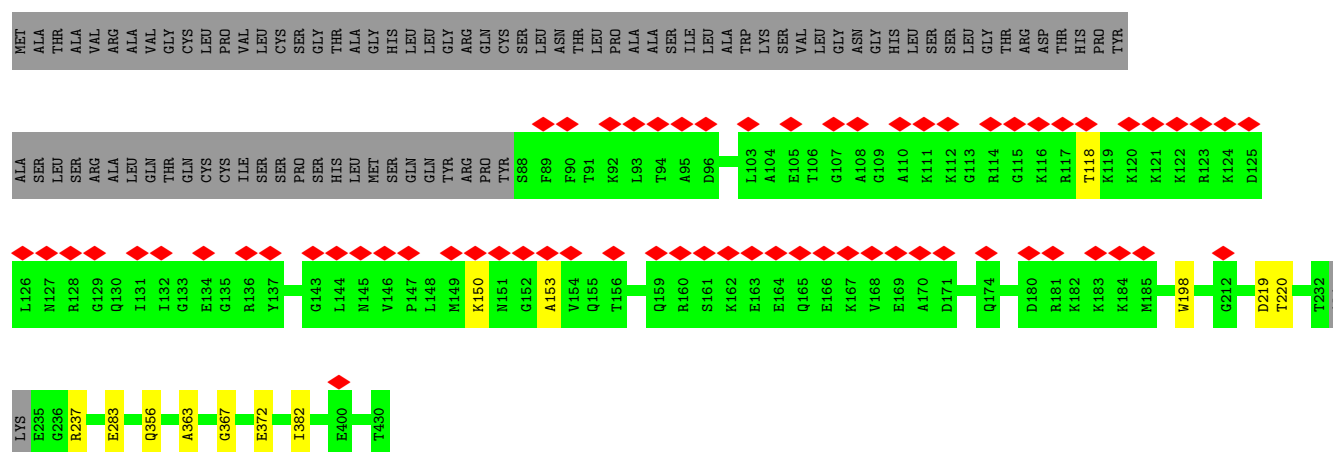
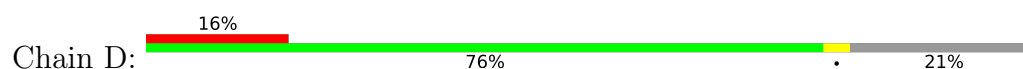




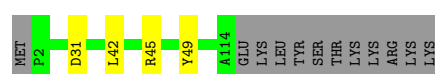
• Molecule 3: 28S ribosomal protein S2, mitochondrial



• Molecule 4: 28S ribosomal protein S5, mitochondrial

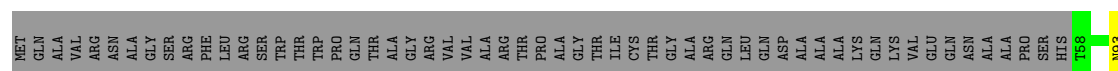


• Molecule 5: 28S ribosomal protein S6, mitochondrial

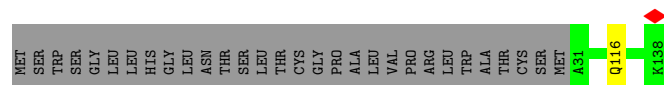
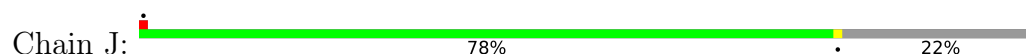


• Molecule 6: 28S ribosomal protein S11, mitochondrial

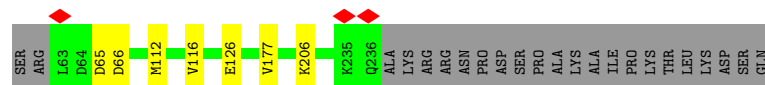
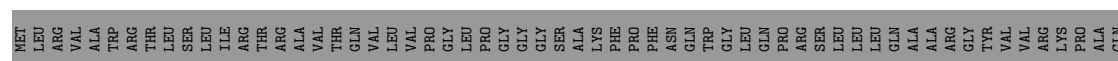




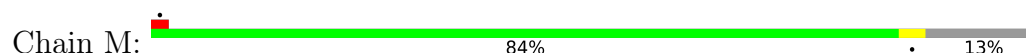
- Molecule 7: 28S ribosomal protein S12, mitochondrial



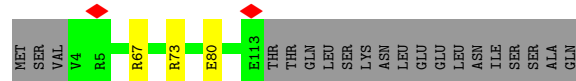
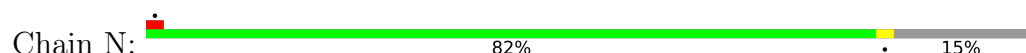
- Molecule 8: 28S ribosomal protein S15, mitochondrial



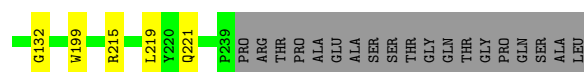
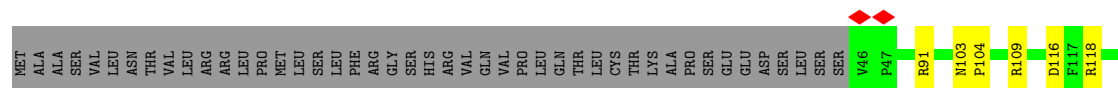
- Molecule 9: 28S ribosomal protein S16, mitochondrial



- Molecule 10: 28S ribosomal protein S17, mitochondrial

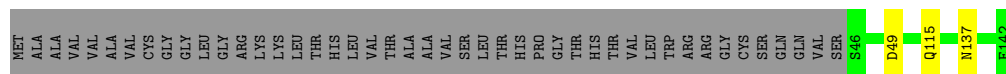


- Molecule 11: 28S ribosomal protein S18b, mitochondrial



- Molecule 12: 28S ribosomal protein S18c, mitochondrial

Chain P:  66% 32%




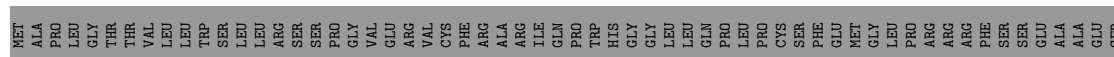
- Molecule 13: Small ribosomal subunit protein bS21m

Chain Q:  97%



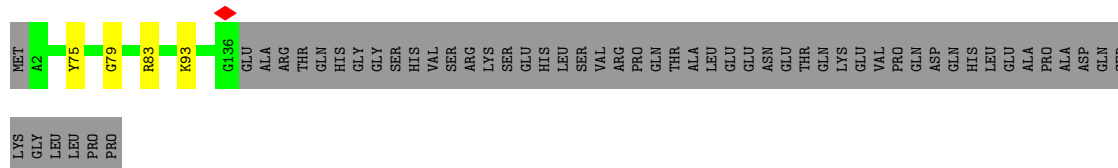
- Molecule 14: 28S ribosomal protein S22, mitochondrial

Chain R:  78% 18%



- Molecule 15: 28S ribosomal protein S23, mitochondrial

Chain S:  69% 29%




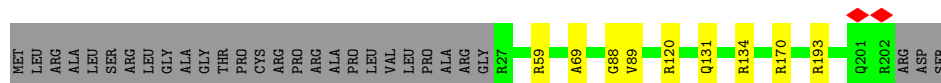
- Molecule 16: 28S ribosomal protein S25, mitochondrial

Chain T:  93%



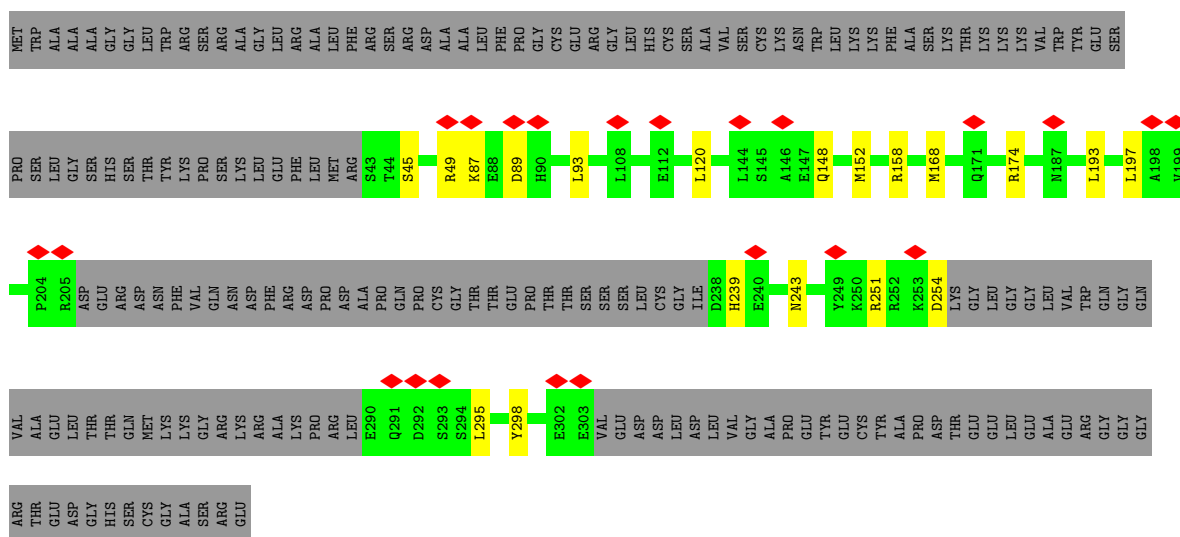
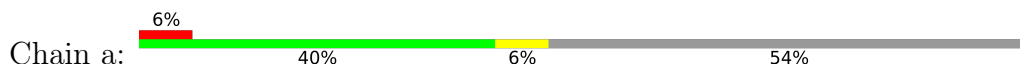
- Molecule 17: 28S ribosomal protein S26, mitochondrial

Chain U:  81% 14%

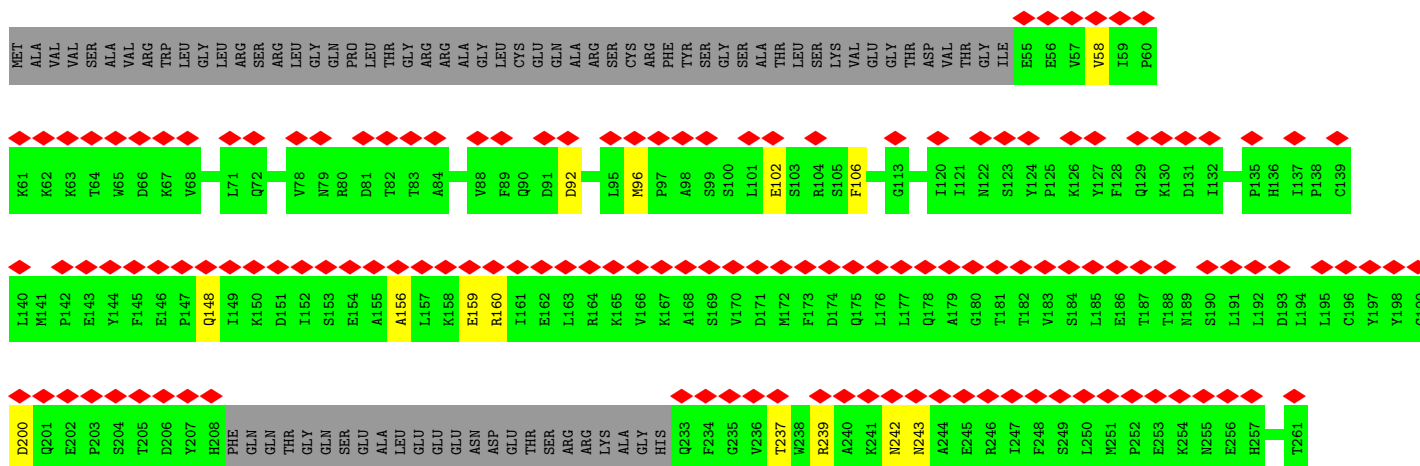
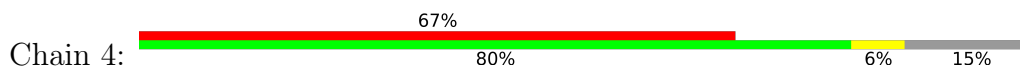


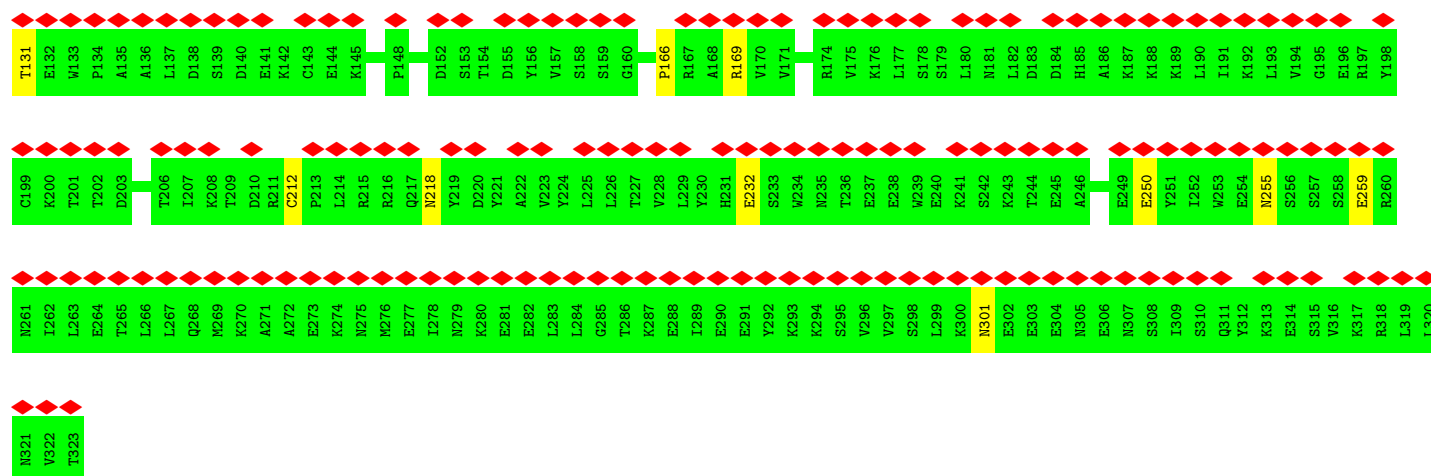
- Molecule 18: 28S ribosomal protein S27, mitochondrial

- Molecule 23: Putative ribosome-binding factor A, mitochondrial

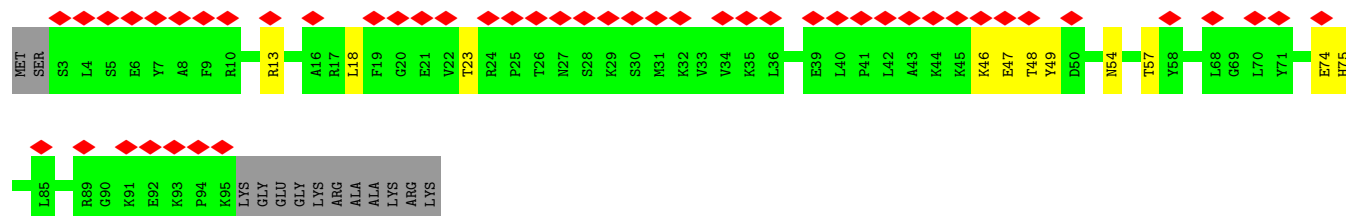


- Molecule 24: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

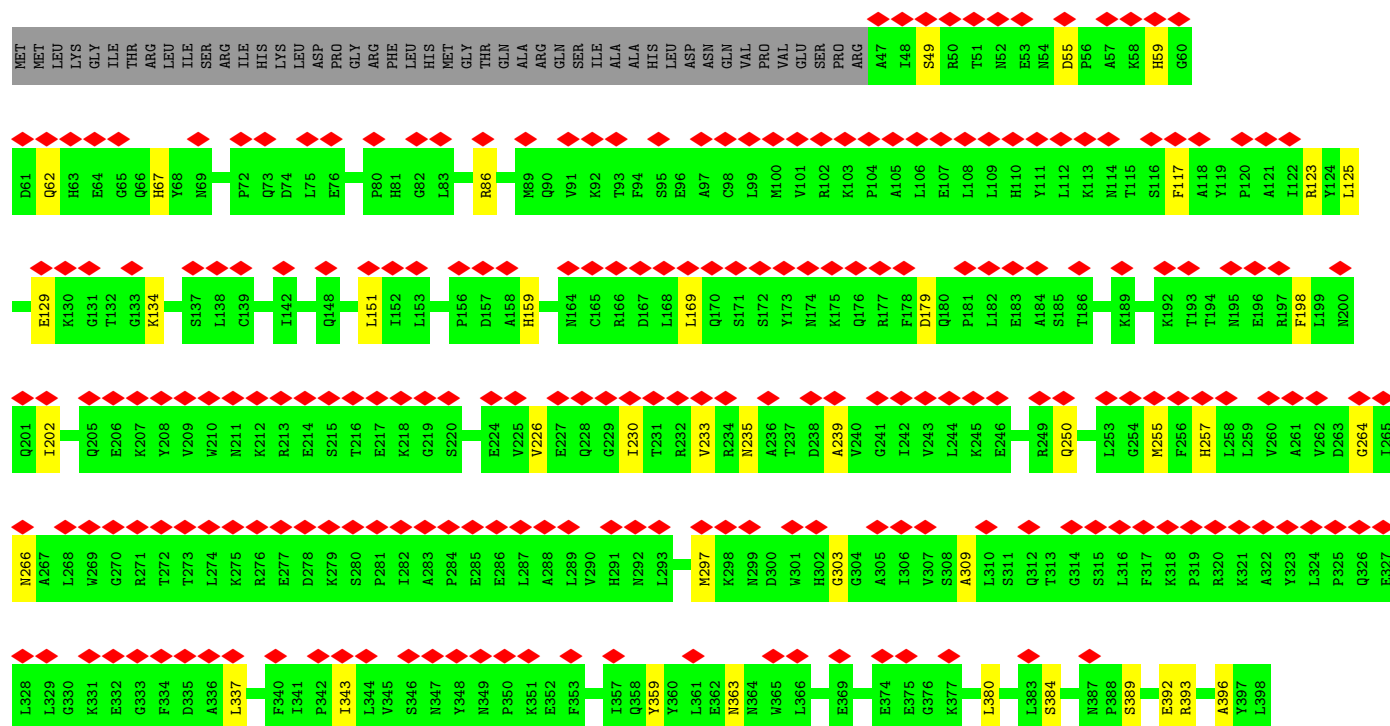
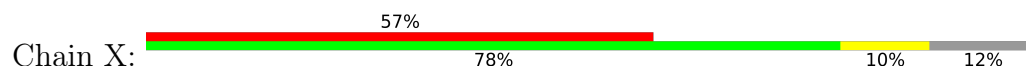




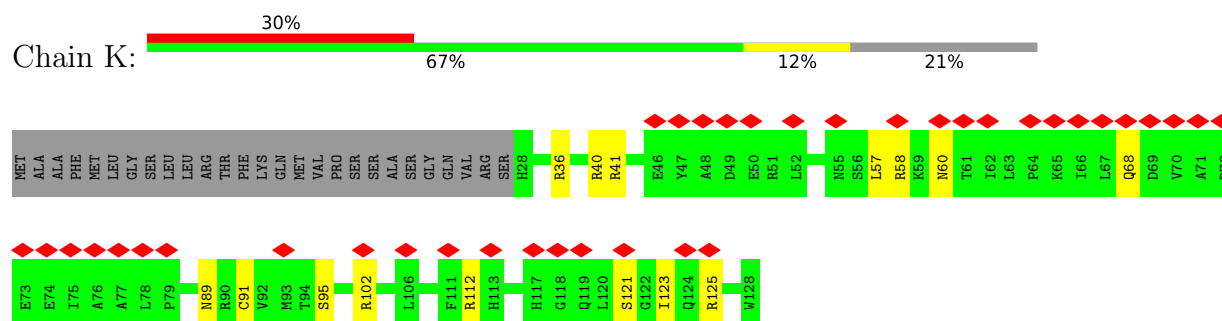
- Molecule 27: 28S ribosomal protein S33, mitochondrial



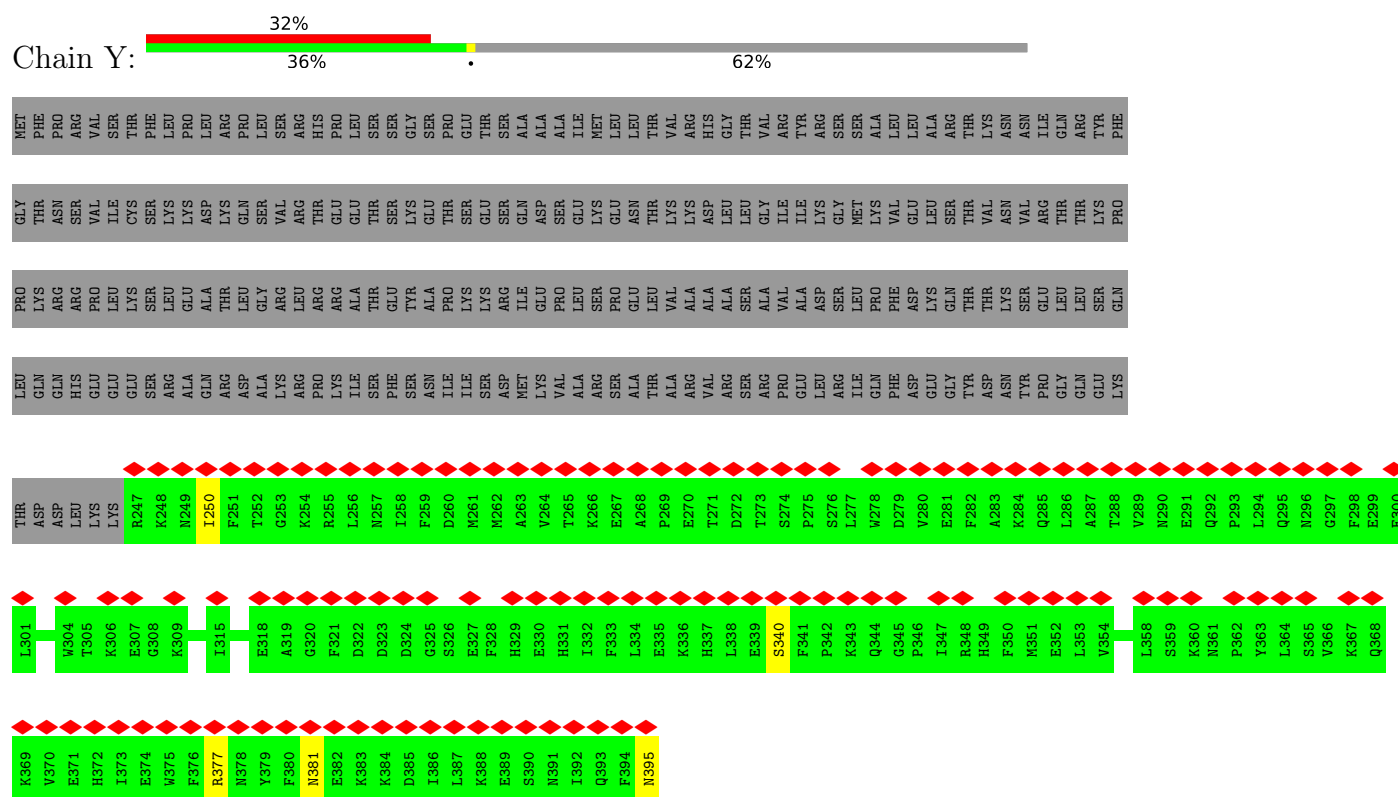
- Molecule 28: 28S ribosomal protein S29, mitochondrial



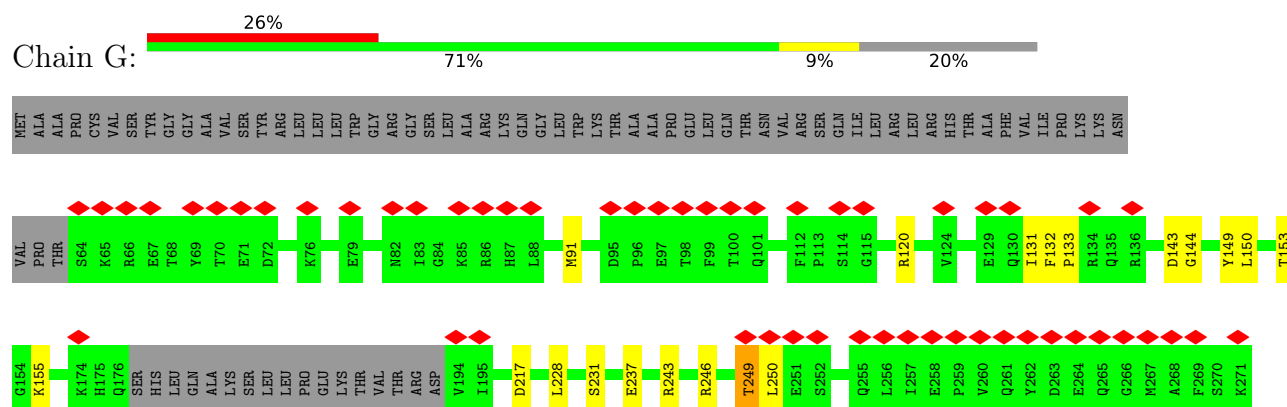
- Molecule 29: 28S ribosomal protein S14, mitochondrial

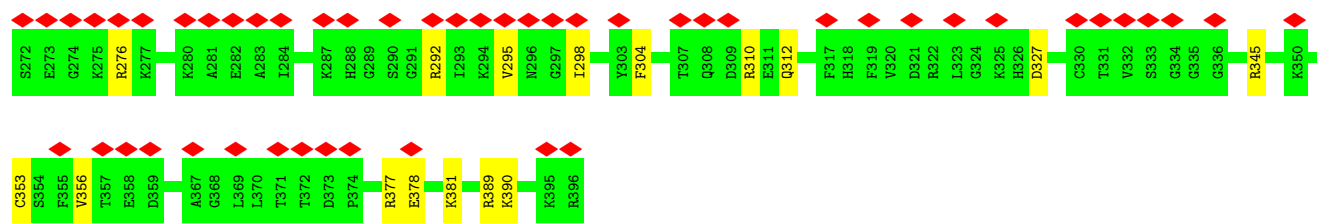


- Molecule 30: 28S ribosomal protein S31, mitochondrial



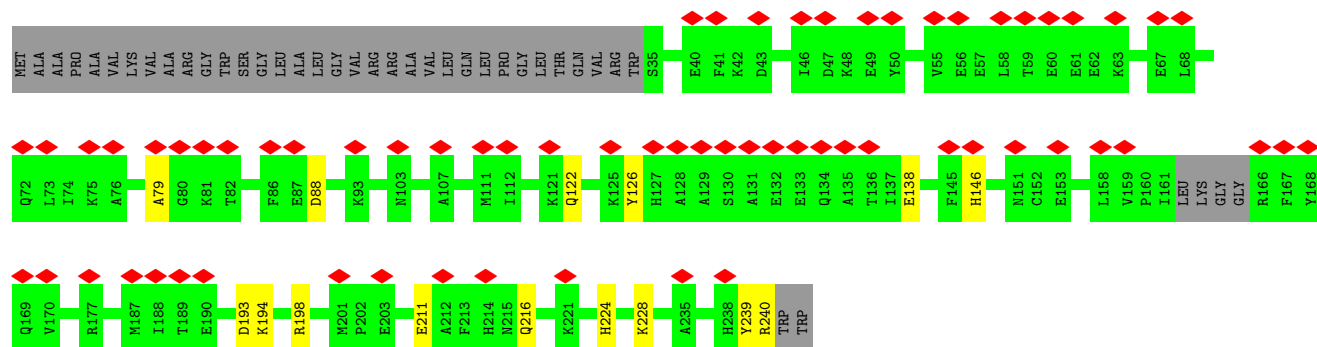
- Molecule 31: 28S ribosomal protein S9, mitochondrial





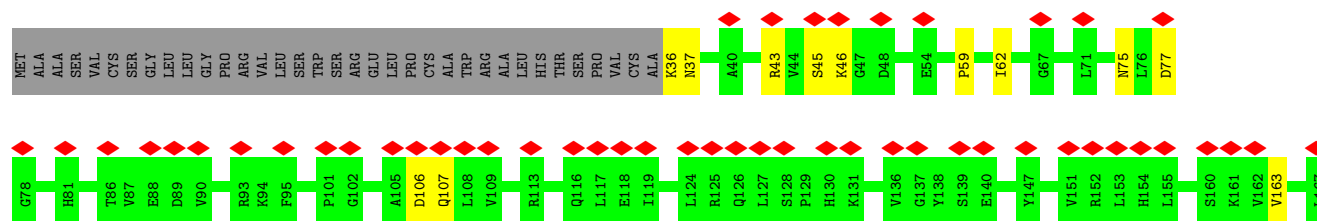
• Molecule 32: 28S ribosomal protein S7, mitochondrial

Chain F:



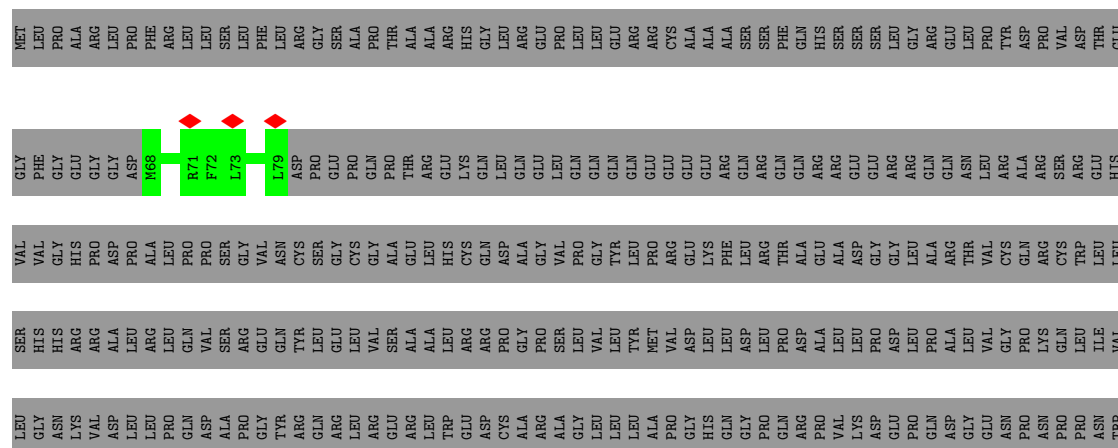
• Molecule 33: 28S ribosomal protein S24, mitochondrial

Chain C:



• Molecule 34: Nitric oxide-associated protein 1

Chain 9:



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.523	Depositor
Minimum map value	-0.582	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.24	Depositor
Map size (Å)	609.12, 609.12, 609.12	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0152, 1.0152, 1.0152	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SAH, NAD, K, 5MU, ATP, FES, 5F0, SPM, GDP, ZN, MA6, ACE

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	c	0.09	0/2549	0.23	0/3431
2	A	0.19	0/21895	0.25	0/34084
3	B	0.16	0/1871	0.26	0/2531
4	D	0.15	0/2768	0.24	0/3703
5	E	0.14	0/908	0.24	0/1229
6	I	0.12	0/1030	0.23	0/1386
7	J	0.16	0/855	0.29	0/1148
8	L	0.16	0/1477	0.27	0/1974
9	M	0.18	0/963	0.29	0/1295
10	N	0.17	0/886	0.30	0/1199
11	O	0.15	0/1655	0.25	0/2254
12	P	0.16	0/798	0.27	0/1070
13	Q	0.18	0/754	0.28	0/1003
14	R	0.14	0/2456	0.25	0/3317
15	S	0.13	0/1138	0.22	0/1533
16	T	0.16	0/1402	0.27	0/1883
17	U	0.12	0/1510	0.22	0/2025
18	V	0.08	0/3030	0.21	0/4093
19	W	0.13	0/801	0.23	0/1079
20	0	0.11	0/1834	0.27	0/2484
21	3	0.14	0/636	0.26	0/839
22	b	0.08	0/2404	0.24	0/3241
23	a	0.10	0/1264	0.24	0/1700
24	4	0.08	0/4877	0.22	0/6598
25	H	0.08	0/1178	0.25	0/1598
26	1	0.08	0/2285	0.22	0/3090
27	Z	0.07	0/806	0.20	0/1076
28	X	0.08	0/2921	0.24	0/3954
29	K	0.07	0/880	0.19	0/1182
30	Y	0.07	0/1280	0.20	0/1725
31	G	0.10	0/2658	0.28	2/3560 (0.1%)
32	F	0.08	0/1708	0.22	0/2292

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	C	0.07	0/1113	0.22	0/1505
34	9	0.09	0/114	0.28	0/152
All	All	0.14	0/74704	0.24	2/105233 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	I	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G	249	THR	CA-C-N	5.57	131.73	121.70
31	G	249	THR	C-N-CA	5.57	131.73	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	I	184	5F0	Mainchain

5.2 Too-close contacts [i](#)

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	c	2495	2493	2481	20	0
2	A	19646	9952	9985	88	0
3	B	1828	1825	1815	6	0
4	D	2717	2794	2785	8	0
5	E	892	914	910	3	0
6	I	1020	1057	1053	7	0
7	J	839	891	887	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	1453	1544	1540	6	0
9	M	942	971	965	4	0
10	N	868	932	928	2	0
11	O	1599	1574	1565	7	0
12	P	781	808	806	3	0
13	Q	744	760	758	3	0
14	R	2409	2435	2428	9	0
15	S	1111	1116	1115	2	0
16	T	1371	1396	1393	5	0
17	U	1488	1504	1499	8	0
18	V	2969	2970	2961	9	0
19	W	789	805	802	1	0
20	0	1787	1801	1796	13	0
21	3	625	701	699	4	0
22	b	2363	2433	2425	30	0
23	a	1248	1252	1247	13	0
24	4	4768	4782	4766	22	0
25	H	1152	1190	1183	10	0
26	1	2238	2274	2269	13	0
27	Z	788	805	802	8	0
28	X	2849	2858	2844	23	0
29	K	862	888	885	14	0
30	Y	1246	1202	1197	3	0
31	G	2603	2599	2591	22	0
32	F	1671	1726	1718	9	0
33	C	1083	1095	1088	9	0
34	9	111	108	108	0	0
35	A	44	26	26	0	0
36	A	14	26	26	0	0
37	3	1	0	0	0	0
37	A	38	0	0	0	0
37	B	1	0	0	0	0
38	A	6	0	0	0	0
39	O	1	0	0	0	0
40	P	4	0	0	0	0
40	T	4	0	0	0	0
41	b	26	19	19	3	0
42	X	31	12	12	0	0
43	X	28	10	12	0	0
44	0	1	0	0	1	0
44	A	1	0	0	0	0
44	I	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	71556	62548	62389	323	0

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

All (323) 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)
2:A:942:A:N6	2:A:1047:A:OP2	2.11	0.82
9:M:63:GLU:OE2	14:R:191:ARG:NH2	2.14	0.80
2:A:1085:C:OP1	6:I:192:ARG:NH1	2.17	0.77
27:Z:47:GLU:OE1	29:K:102:ARG:NH2	2.19	0.75
22:b:298:GLU:OE1	41:b:501:SAH:N6	2.21	0.74
24:4:480:ASP:O	24:4:484:SER:OG	2.07	0.73
6:I:129:GLN:NE2	6:I:167:MET:SD	2.63	0.72
22:b:339:THR:O	23:a:87:LYS:NZ	2.22	0.72
24:4:295:ASN:OD1	24:4:296:ALA:N	2.23	0.71
33:C:37:ASN:O	33:C:43:ARG:NH2	2.24	0.70
27:Z:48:THR:O	29:K:41:ARG:NH1	2.25	0.70
24:4:397:MET:O	24:4:401:MET:N	2.24	0.69
22:b:174:SER:O	22:b:178:ASP:N	2.25	0.69
2:A:808:C:OP1	20:0:19:ARG:NH1	2.26	0.69
22:b:321:PHE:N	22:b:325:GLU:OE1	2.27	0.68
2:A:1595:G:O6	13:Q:50:ARG:NH2	2.27	0.67
1:c:346:ARG:NH1	2:A:1152:A:OP1	2.27	0.67
2:A:932:C:N3	16:T:11:ARG:NH2	2.42	0.67
2:A:1401:G:N1	2:A:1404:A:OP2	2.26	0.67
2:A:1267:U:O4	33:C:36:LYS:N	2.28	0.67
12:P:49:ASP:OD2	19:W:82:SER:OG	2.09	0.66
28:X:359:TYR:O	28:X:363:ASN:ND2	2.29	0.66
2:A:1235:U:OP1	29:K:36:ARG:NH1	2.29	0.66
17:U:131:GLN:OE1	17:U:134:ARG:NH2	2.30	0.65
28:X:49:SER:O	28:X:67:HIS:N	2.29	0.65
25:H:71:ILE:O	25:H:150:GLY:N	2.28	0.65
27:Z:74:GLU:OE1	27:Z:74:GLU:N	2.30	0.64
18:V:46:GLU:OE2	18:V:74:ARG:NE	2.31	0.64
6:I:94:ASN:OD1	6:I:95:THR:N	2.30	0.64
1:c:361:GLU:OE1	1:c:361:GLU:N	2.31	0.64
1:c:261:ARG:NH1	1:c:288:SER:OG	2.29	0.63
22:b:182:ARG:NH2	22:b:195:ARG:O	2.31	0.63
2:A:1598:G:O6	13:Q:61:ARG:NH1	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1598:G:N2	23:a:158:ARG:O	2.32	0.62
2:A:1307:G:O2'	31:G:120:ARG:NH2	2.32	0.62
2:A:1583:MA6:H102	2:A:1584:MA6:H103	1.81	0.62
29:K:57:LEU:O	29:K:60:ASN:ND2	2.33	0.62
4:D:283:GLU:O	4:D:356:GLN:NE2	2.32	0.61
29:K:60:ASN:O	29:K:68:GLN:NE2	2.33	0.61
2:A:947:U:P	2:A:1045:G:O6	2.58	0.61
18:V:43:ARG:NH2	18:V:77:ASP:OD1	2.33	0.61
2:A:815:C:O2	2:A:818:C:N4	2.33	0.61
2:A:1454:G:OP2	31:G:377:ARG:NH1	2.32	0.61
18:V:270:PRO:O	18:V:346:LYS:NZ	2.35	0.60
18:V:74:ARG:O	18:V:78:ASN:ND2	2.35	0.60
1:c:220:GLU:N	1:c:220:GLU:OE1	2.34	0.60
18:V:174:GLU:OE1	18:V:214:LYS:NZ	2.35	0.59
22:b:85:SER:OG	22:b:315:ARG:NH1	2.36	0.59
11:O:91:ARG:NH1	11:O:103:ASN:O	2.35	0.59
2:A:1583:MA6:H93	2:A:1584:MA6:N1	2.17	0.59
14:R:69:THR:N	14:R:72:ASP:OD2	2.33	0.59
1:c:102:ARG:NE	1:c:114:ASP:OD1	2.24	0.58
20:0:78:ARG:NH2	20:0:142:VAL:O	2.36	0.58
31:G:312:GLN:NE2	32:F:79:ALA:O	2.37	0.58
23:a:148:GLN:O	23:a:152:MET:N	2.32	0.58
2:A:1583:MA6:H102	2:A:1584:MA6:C10	2.34	0.58
26:1:255:ASN:N	26:1:259:GLU:OE1	2.35	0.57
20:0:132:GLU:O	44:0:301:HOH:O	2.17	0.57
20:0:178:ARG:NH1	20:0:187:GLU:O	2.33	0.57
24:4:156:ALA:O	24:4:160:ARG:NH1	2.37	0.57
24:4:433:TYR:OH	24:4:469:GLU:OE1	2.21	0.57
33:C:106:ASP:OD1	33:C:107:GLN:N	2.36	0.56
22:b:229:GLU:OE2	22:b:231:HIS:N	2.35	0.56
24:4:200:ASP:OD2	24:4:243:ASN:N	2.38	0.56
2:A:1275:A:O2'	2:A:1276:A:O4'	2.23	0.56
2:A:1229:U:O2'	2:A:1442:G:O4'	2.24	0.56
4:D:363:ALA:O	4:D:367:GLY:N	2.39	0.56
31:G:150:LEU:O	31:G:153:THR:OG1	2.24	0.55
3:B:243:PRO:O	3:B:247:HIS:ND1	2.34	0.55
22:b:214:LEU:O	22:b:243:ARG:NH1	2.38	0.55
2:A:904:C:N3	4:D:118:THR:OG1	2.37	0.55
2:A:762:G:OP1	8:L:206:LYS:NZ	2.35	0.54
23:a:89:ASP:O	23:a:93:LEU:N	2.34	0.54
24:4:237:THR:O	24:4:237:THR:HG22	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:91:ILE:O	22:b:164:ASP:N	2.40	0.54
2:A:1384:A:OP1	32:F:198:ARG:NH1	2.40	0.54
2:A:769:G:OP2	10:N:73:ARG:NH2	2.39	0.53
26:1:212:CYS:O	26:1:218:ASN:ND2	2.41	0.53
31:G:292:ARG:NH1	31:G:327:ASP:OD2	2.41	0.53
26:1:115:THR:OG1	31:G:91:MET:O	2.25	0.53
2:A:812:A:O2'	2:A:814:A:N1	2.41	0.53
28:X:264:GLY:N	28:X:309:ALA:O	2.41	0.53
2:A:1044:U:OP1	2:A:1110:A:O2'	2.27	0.52
31:G:155:LYS:NZ	31:G:217:ASP:OD2	2.42	0.52
2:A:846:A:OP1	9:M:85:LYS:NZ	2.41	0.52
22:b:176:GLN:NE2	41:b:501:SAH:O2'	2.38	0.52
29:K:41:ARG:NH2	29:K:89:ASN:OD1	2.41	0.52
22:b:187:ARG:O	22:b:252:GLN:NE2	2.42	0.52
28:X:159:HIS:NE2	28:X:266:ASN:OD1	2.43	0.52
29:K:121:SER:O	33:C:75:ASN:ND2	2.41	0.52
2:A:1080:A:H1'	2:A:1081:U:C6	2.45	0.52
2:A:1320:G:OP2	33:C:37:ASN:ND2	2.43	0.52
25:H:152:THR:OG1	26:1:131:THR:O	2.28	0.51
26:1:115:THR:HG23	26:1:118:ALA:H	1.75	0.51
22:b:150:GLU:O	22:b:154:MET:N	2.39	0.51
18:V:80:SER:N	18:V:84:GLU:OE1	2.44	0.51
24:4:599:PHE:O	24:4:604:LYS:N	2.42	0.51
2:A:1272:A:N6	2:A:1320:G:O2'	2.38	0.51
17:U:69:ALA:HB3	20:0:191:LEU:HD21	1.93	0.51
26:1:250:GLU:OE2	26:1:301:ASN:ND2	2.44	0.51
31:G:249:THR:HA	31:G:250:LEU:HB3	1.92	0.51
24:4:239:ARG:O	24:4:242:ASN:ND2	2.44	0.51
31:G:389:ARG:NH1	31:G:390:LYS:O	2.44	0.51
1:c:381:GLU:O	1:c:385:ARG:N	2.39	0.51
18:V:277:ARG:N	18:V:348:GLU:O	2.40	0.51
4:D:372:GLU:N	4:D:382:ILE:O	2.42	0.51
2:A:947:U:OP2	2:A:1045:G:O6	2.28	0.50
2:A:843:G:N2	2:A:846:A:OP2	2.38	0.50
22:b:128:ALA:O	22:b:132:SER:N	2.39	0.50
2:A:1367:A:OP2	2:A:1384:A:N6	2.37	0.50
26:1:166:PRO:O	26:1:169:ARG:NH1	2.43	0.50
31:G:378:GLU:OE2	31:G:381:LYS:NZ	2.45	0.50
23:a:45:SER:O	23:a:49:ARG:HG3	2.12	0.49
28:X:55:ASP:O	28:X:59:HIS:ND1	2.45	0.49
33:C:45:SER:OG	33:C:46:LYS:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:705:C:H2'	20:0:136:TYR:CE1	2.47	0.49
2:A:1177:C:N4	2:A:1178:G:O6	2.45	0.49
24:4:400:LEU:HD22	24:4:405:PHE:CE1	2.48	0.49
31:G:228:LEU:O	31:G:231:SER:OG	2.26	0.49
28:X:86:ARG:NE	28:X:392:GLU:OE1	2.40	0.49
1:c:269:GLU:OE2	1:c:283:ARG:NH1	2.45	0.49
26:1:232:GLU:HG3	27:Z:18:LEU:HD21	1.93	0.49
15:S:83:ARG:NH1	15:S:93:LYS:O	2.46	0.49
2:A:1558:A:O2'	2:A:1559:G:P	2.70	0.49
5:E:49:TYR:OH	12:P:115:GLN:O	2.27	0.49
2:A:657:G:O3'	4:D:237:ARG:NH2	2.42	0.48
24:4:369:LEU:HD22	24:4:415:PHE:CD2	2.48	0.48
28:X:198:PHE:O	28:X:202:ILE:N	2.42	0.48
31:G:304:PHE:O	31:G:310:ARG:NH1	2.46	0.48
2:A:1584:MA6:O5'	2:A:1584:MA6:H8	2.14	0.48
4:D:219:ASP:OD1	4:D:220:THR:N	2.47	0.48
11:O:116:ASP:OD2	11:O:118:ARG:NH2	2.40	0.48
16:T:89:ASP:OD2	17:U:120:ARG:NH2	2.37	0.48
2:A:1508:C:O2'	2:A:1509:U:OP1	2.24	0.48
9:M:108:GLU:OE2	17:U:59:ARG:NH2	2.42	0.48
27:Z:54:ASN:ND2	27:Z:57:THR:OG1	2.47	0.48
22:b:164:ASP:OD1	22:b:311:ARG:NH1	2.47	0.47
23:a:120:LEU:HD22	23:a:152:MET:SD	2.53	0.47
28:X:123:ARG:NH2	28:X:337:LEU:O	2.46	0.47
28:X:151:LEU:N	28:X:257:HIS:O	2.47	0.47
24:4:491:GLN:O	24:4:495:HIS:ND1	2.46	0.47
32:F:122:GLN:NE2	32:F:138:GLU:O	2.42	0.47
2:A:1084:C:O3'	6:I:192:ARG:NH2	2.47	0.47
2:A:1116:A:P	3:B:100:ARG:HH22	2.37	0.47
31:G:295:VAL:N	31:G:298:ILE:O	2.45	0.47
2:A:1492:A:H4'	2:A:1493:C:OP1	2.15	0.47
28:X:123:ARG:NH1	28:X:297:MET:SD	2.88	0.47
2:A:1271:C:N4	2:A:1320:G:O2'	2.47	0.47
2:A:1431:G:O6	31:G:276:ARG:NH2	2.48	0.47
15:S:75:TYR:O	15:S:79:GLY:N	2.48	0.47
1:c:222:TYR:O	1:c:223:ARG:NH1	2.46	0.46
6:I:146:HIS:NE2	6:I:171:GLU:OE1	2.48	0.46
8:L:112:MET:O	8:L:116:VAL:HG12	2.15	0.46
1:c:342:LYS:NZ	2:A:1153:C:O2'	2.37	0.46
22:b:115:LEU:N	22:b:138:GLN:O	2.45	0.46
5:E:42:LEU:O	5:E:45:ARG:NH2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:92:THR:O	16:T:92:THR:HG22	2.16	0.46
23:a:193:LEU:O	23:a:197:LEU:N	2.40	0.46
2:A:1491:C:H3'	2:A:1492:A:H5''	1.96	0.46
14:R:357:SER:O	14:R:358:ALA:C	2.58	0.46
22:b:326:ASP:OD2	22:b:402:ARG:NH2	2.47	0.46
2:A:1170:G:OP1	21:3:129:ASN:ND2	2.49	0.46
2:A:1489:G:H3'	2:A:1490:U:O4'	2.15	0.46
28:X:250:GLN:NE2	28:X:255:MET:SD	2.88	0.46
32:F:239:TYR:O	32:F:240:ARG:C	2.59	0.46
2:A:1019:A:O4'	13:Q:62:ARG:NH1	2.49	0.46
3:B:77:GLU:OE2	3:B:259:ARG:NH1	2.46	0.46
20:0:41:LEU:HD13	20:0:55:TRP:CG	2.50	0.46
23:a:239:HIS:O	23:a:243:ASN:N	2.41	0.46
1:c:295:ARG:NE	1:c:328:ALA:O	2.47	0.46
9:M:64:LYS:HD2	14:R:156:TYR:CE1	2.51	0.46
2:A:948:U:OP2	2:A:1045:G:N2	2.38	0.46
2:A:1179:G:O5'	2:A:1180:U:OP1	2.34	0.46
25:H:76:LEU:N	25:H:145:LEU:O	2.49	0.46
2:A:738:A:H2'	2:A:739:C:O4'	2.16	0.45
23:a:251:ARG:NH2	23:a:254:ASP:OD2	2.48	0.45
24:4:428:ASP:OD1	24:4:431:LEU:N	2.39	0.45
1:c:283:ARG:NH2	1:c:336:GLU:OE2	2.48	0.45
22:b:96:THR:O	41:b:501:SAH:N	2.49	0.45
2:A:1415:G:H4'	2:A:1416:A:H5'	1.99	0.45
14:R:312:GLN:O	14:R:316:GLY:N	2.42	0.45
24:4:102:GLU:O	24:4:106:PHE:N	2.41	0.45
25:H:81:LYS:NZ	33:C:77:ASP:O	2.28	0.45
31:G:243:ARG:O	31:G:246:ARG:NH1	2.48	0.45
21:3:150:THR:HG22	21:3:150:THR:O	2.17	0.45
7:J:116:GLN:OE1	7:J:116:GLN:N	2.46	0.45
1:c:242:THR:OG1	2:A:1548:A:N3	2.49	0.45
2:A:1388:C:O2	2:A:1419:G:N2	2.49	0.45
1:c:261:ARG:NH1	1:c:288:SER:O	2.50	0.45
2:A:1170:G:OP1	21:3:129:ASN:CG	2.60	0.45
22:b:272:ASP:CG	22:b:273:LEU:N	2.75	0.45
31:G:237:GLU:OE1	31:G:237:GLU:N	2.47	0.45
22:b:138:GLN:OE1	22:b:138:GLN:N	2.39	0.44
22:b:158:VAL:HG23	22:b:158:VAL:O	2.16	0.44
2:A:739:C:H2'	2:A:740:G:C1'	2.47	0.44
23:a:148:GLN:O	23:a:152:MET:HG2	2.18	0.44
20:0:37:ASP:O	20:0:41:LEU:N	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:376:GLU:N	22:b:405:ILE:O	2.50	0.44
25:H:67:ASP:OD1	25:H:68:GLU:N	2.51	0.44
31:G:131:ILE:HG23	31:G:132:PHE:N	2.32	0.44
2:A:702:C:OP1	2:A:848:U:O2'	2.31	0.44
32:F:224:HIS:O	32:F:228:LYS:N	2.45	0.44
22:b:119:ASP:OD1	22:b:120:ARG:N	2.51	0.44
28:X:392:GLU:O	28:X:396:ALA:N	2.51	0.44
33:C:59:PRO:O	33:C:62:ILE:HG13	2.17	0.44
17:U:69:ALA:CB	20:O:191:LEU:HD21	2.48	0.44
24:4:148:GLN:N	24:4:159:GLU:OE2	2.45	0.44
4:D:198:TRP:CD2	23:a:295:LEU:HD21	2.53	0.44
14:R:212:GLU:OE2	14:R:216:ARG:NH1	2.51	0.43
1:c:81:PRO:O	1:c:161:TRP:NE1	2.51	0.43
5:E:31:ASP:OD1	17:U:170:ARG:NH2	2.47	0.43
12:P:137:ASN:OD1	17:U:193:ARG:NH2	2.40	0.43
22:b:181:GLU:OE1	22:b:181:GLU:N	2.43	0.43
28:X:233:VAL:HG12	28:X:233:VAL:O	2.18	0.43
3:B:165:TYR:HD1	31:G:149:TYR:HA	1.83	0.43
28:X:129:GLU:O	28:X:134:LYS:NZ	2.43	0.43
2:A:991:G:OP2	6:I:93:ASN:ND2	2.50	0.43
2:A:1335:U:OP1	27:Z:75:HIS:NE2	2.52	0.43
8:L:65:ASP:OD1	8:L:65:ASP:N	2.51	0.43
28:X:235:ASN:O	28:X:239:ALA:N	2.42	0.43
29:K:91:CYS:O	29:K:95:SER:N	2.49	0.43
32:F:193:ASP:OD1	32:F:194:LYS:N	2.52	0.43
2:A:734:C:H3'	2:A:735:A:C5'	2.49	0.43
2:A:1491:C:C3'	2:A:1492:A:H5''	2.49	0.43
24:4:58:VAL:HG23	24:4:58:VAL:O	2.18	0.43
24:4:92:ASP:O	24:4:96:MET:N	2.51	0.43
31:G:143:ASP:OD1	31:G:144:GLY:N	2.52	0.43
14:R:82:MET:HE1	14:R:300:LEU:HA	2.00	0.43
22:b:92:PHE:CD1	22:b:113:ILE:HD11	2.54	0.43
25:H:122:GLN:O	29:K:112:ARG:NH1	2.52	0.43
2:A:1563:U:H4'	2:A:1564:A:O5'	2.19	0.43
2:A:977:A:H4'	6:I:180:PRO:HB2	2.01	0.43
11:O:215:ARG:O	11:O:219:LEU:N	2.44	0.43
11:O:104:PRO:HB2	11:O:109:ARG:HB3	2.01	0.42
28:X:226:VAL:HG12	28:X:230:ILE:HD12	2.01	0.42
30:Y:340:SER:O	30:Y:395:ASN:ND2	2.46	0.42
31:G:353:CYS:HA	31:G:356:VAL:HG22	2.01	0.42
28:X:169:LEU:O	28:X:179:ASP:N	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:297:MET:SD	28:X:297:MET:C	3.02	0.42
32:F:88:ASP:OD2	32:F:146:HIS:NE2	2.52	0.42
2:A:1057:G:H4'	2:A:1578:A:H4'	2.01	0.42
18:V:103:TYR:O	18:V:104:LEU:C	2.62	0.42
26:1:86:ARG:HG2	26:1:96:PRO:HB2	2.02	0.42
26:1:91:VAL:O	26:1:94:GLY:N	2.52	0.42
28:X:62:GLN:OE1	28:X:62:GLN:N	2.47	0.42
2:A:1403:A:OP1	29:K:58:ARG:NH2	2.52	0.42
23:a:295:LEU:O	23:a:298:TYR:N	2.52	0.42
20:0:34:TYR:O	20:0:43:ARG:NH1	2.52	0.42
2:A:1079:G:H2'	2:A:1080:A:H5'	2.02	0.42
3:B:54:ASP:OD1	3:B:271:TYR:OH	2.37	0.42
11:O:221:GLN:NE2	18:V:314:VAL:O	2.47	0.42
24:4:306:ASN:OD1	24:4:344:ARG:NH2	2.52	0.42
24:4:358:ARG:NE	30:Y:250:ILE:O	2.53	0.42
28:X:380:LEU:O	28:X:384:SER:OG	2.36	0.42
30:Y:377:ARG:O	30:Y:381:ASN:ND2	2.53	0.42
31:G:312:GLN:OE1	31:G:345:ARG:NH1	2.53	0.42
8:L:206:LYS:HE3	21:3:176:ILE:HD11	2.02	0.42
16:T:43:GLY:HA3	16:T:93:LYS:O	2.20	0.42
22:b:145:GLN:O	22:b:149:ALA:N	2.53	0.42
2:A:1234:C:O3'	29:K:40:ARG:NH2	2.52	0.42
20:0:91:GLU:OE1	20:0:91:GLU:N	2.51	0.42
22:b:103:THR:HG23	22:b:115:LEU:HD21	2.01	0.42
25:H:136:MET:HG2	29:K:123:ILE:HD13	2.02	0.42
27:Z:13:ARG:NH1	27:Z:23:THR:O	2.53	0.42
2:A:765:C:H5'	2:A:766:G:OP2	2.19	0.42
3:B:93:HIS:CD2	3:B:224:ASP:OD2	2.71	0.42
32:F:211:GLU:O	32:F:216:GLN:N	2.51	0.42
2:A:868:C:H2'	2:A:869:C:O4'	2.19	0.42
2:A:1079:G:C6	2:A:1080:A:N7	2.88	0.42
2:A:1103:A:N7	2:A:1574:G:O2'	2.44	0.42
32:F:122:GLN:O	32:F:126:TYR:N	2.48	0.42
2:A:1237:A:OP1	29:K:36:ARG:NH2	2.53	0.41
31:G:132:PHE:HB2	31:G:133:PRO:HD3	2.02	0.41
2:A:1558:A:H4'	2:A:1559:G:C8	2.55	0.41
22:b:274:LEU:HG	22:b:274:LEU:O	2.20	0.41
22:b:331:ARG:O	22:b:335:GLY:N	2.53	0.41
25:H:80:VAL:HG23	25:H:80:VAL:O	2.20	0.41
2:A:1319:A:OP1	29:K:125:ARG:NH1	2.53	0.41
28:X:125:LEU:O	28:X:343:ILE:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:C:163:VAL:HG13	33:C:163:VAL:O	2.20	0.41
2:A:1492:A:H8	2:A:1492:A:OP1	2.03	0.41
1:c:295:ARG:NH2	1:c:328:ALA:O	2.53	0.41
1:c:327:LYS:O	1:c:390:TRP:NE1	2.53	0.41
2:A:1564:A:OP2	2:A:1564:A:H3'	2.21	0.41
22:b:94:ASP:OD2	22:b:103:THR:OG1	2.36	0.41
24:4:493:MET:HA	24:4:493:MET:HE2	2.03	0.41
2:A:956:C:H2'	2:A:957:C:O4'	2.21	0.41
2:A:1365:A:H4'	2:A:1389:G:H4'	2.03	0.41
14:R:317:ALA:O	14:R:321:ALA:N	2.53	0.41
2:A:1108:C:C4	2:A:1125:A:C5	3.09	0.41
8:L:66:ASP:OD1	8:L:66:ASP:N	2.53	0.41
28:X:117:PHE:O	28:X:303:GLY:N	2.54	0.41
2:A:737:C:H2'	2:A:738:A:O4'	2.20	0.41
2:A:1065:C:H2'	2:A:1066:C:O4'	2.21	0.41
10:N:67:ARG:NH2	10:N:80:GLU:OE2	2.53	0.41
1:c:313:VAL:O	1:c:317:SER:N	2.47	0.41
2:A:700:A:N1	2:A:709:G:O2'	2.48	0.41
2:A:1078:A:O2'	22:b:326:ASP:OD2	2.33	0.41
14:R:187:GLU:OE1	14:R:187:GLU:N	2.54	0.41
26:1:87:MET:HB3	26:1:102:ASN:HD21	1.86	0.41
11:O:128:CYS:O	11:O:132:GLY:N	2.50	0.41
24:4:423:CYS:O	24:4:427:ARG:N	2.54	0.41
25:H:123:SER:HB3	25:H:127:TYR:HB2	2.03	0.41
1:c:87:VAL:HG13	1:c:155:VAL:HG13	2.03	0.40
8:L:126:GLU:HG2	8:L:177:VAL:HG21	2.03	0.40
20:0:103:ASP:N	20:0:111:HIS:O	2.42	0.40
25:H:166:GLU:OE1	25:H:166:GLU:N	2.49	0.40
27:Z:46:LYS:HA	27:Z:49:TYR:CE2	2.56	0.40
1:c:250:SER:O	1:c:251:GLN:HB2	2.21	0.40
2:A:1447:G:C6	2:A:1449:G:C2	3.09	0.40
4:D:150:LYS:N	4:D:153:ALA:O	2.53	0.40
26:1:66:TRP:N	26:1:67:PRO:CD	2.85	0.40
28:X:389:SER:OG	28:X:393:ARG:NE	2.44	0.40
2:A:1466:C:H2'	2:A:1467:C:O4'	2.21	0.40
11:O:199:TRP:NE1	20:0:166:TYR:O	2.50	0.40
23:a:168:MET:HE1	23:a:174:ARG:O	2.21	0.40
1:c:283:ARG:NE	1:c:336:GLU:OE1	2.48	0.40
2:A:1374:A:H2'	2:A:1375:C:O4'	2.22	0.40
16:T:105:ILE:HG13	16:T:106:LEU:N	2.37	0.40
17:U:88:GLY:O	17:U:89:VAL:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:4:400:LEU:HD22	24:4:405:PHE:HE1	1.86	0.40
2:A:1213:A:N6	2:A:1214:A:N1	2.69	0.40
26:1:65:ASP:OD2	26:1:68:SER:OG	2.37	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	
1	c	305/384 (79%)	297 (97%)	8 (3%)	0	100	100
3	B	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
4	D	337/430 (78%)	335 (99%)	2 (1%)	0	100	100
5	E	111/125 (89%)	108 (97%)	3 (3%)	0	100	100
6	I	134/194 (69%)	132 (98%)	2 (2%)	0	100	100
7	J	106/138 (77%)	100 (94%)	6 (6%)	0	100	100
8	L	172/257 (67%)	171 (99%)	1 (1%)	0	100	100
9	M	117/137 (85%)	114 (97%)	3 (3%)	0	100	100
10	N	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
11	O	192/258 (74%)	188 (98%)	4 (2%)	0	100	100
12	P	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
13	Q	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
14	R	293/360 (81%)	290 (99%)	3 (1%)	0	100	100
15	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
16	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
17	U	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
18	V	358/414 (86%)	356 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	W	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
20	0	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
21	3	68/199 (34%)	68 (100%)	0	0	100	100
22	b	297/407 (73%)	289 (97%)	8 (3%)	0	100	100
23	a	149/343 (43%)	146 (98%)	3 (2%)	0	100	100
24	4	584/689 (85%)	573 (98%)	11 (2%)	0	100	100
25	H	138/201 (69%)	135 (98%)	3 (2%)	0	100	100
26	1	274/323 (85%)	268 (98%)	6 (2%)	0	100	100
27	Z	91/106 (86%)	89 (98%)	2 (2%)	0	100	100
28	X	350/398 (88%)	345 (99%)	5 (1%)	0	100	100
29	K	99/128 (77%)	99 (100%)	0	0	100	100
30	Y	147/395 (37%)	147 (100%)	0	0	100	100
31	G	312/396 (79%)	304 (97%)	8 (3%)	0	100	100
32	F	198/242 (82%)	196 (99%)	2 (1%)	0	100	100
33	C	130/167 (78%)	130 (100%)	0	0	100	100
34	9	10/698 (1%)	10 (100%)	0	0	100	100
All	All	6267/9014 (70%)	6165 (98%)	102 (2%)	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	c	269/319 (84%)	269 (100%)	0	100	100
3	B	198/249 (80%)	198 (100%)	0	100	100
4	D	285/357 (80%)	285 (100%)	0	100	100
5	E	95/107 (89%)	95 (100%)	0	100	100
6	I	104/146 (71%)	104 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	J	93/118 (79%)	93 (100%)	0	100	100
8	L	158/226 (70%)	158 (100%)	0	100	100
9	M	97/113 (86%)	97 (100%)	0	100	100
10	N	96/115 (84%)	96 (100%)	0	100	100
11	O	175/230 (76%)	175 (100%)	0	100	100
12	P	88/123 (72%)	88 (100%)	0	100	100
13	Q	78/78 (100%)	78 (100%)	0	100	100
14	R	264/318 (83%)	264 (100%)	0	100	100
15	S	116/164 (71%)	116 (100%)	0	100	100
16	T	153/157 (98%)	153 (100%)	0	100	100
17	U	152/174 (87%)	152 (100%)	0	100	100
18	V	325/364 (89%)	325 (100%)	0	100	100
19	W	87/158 (55%)	87 (100%)	0	100	100
20	0	188/188 (100%)	188 (100%)	0	100	100
21	3	65/166 (39%)	65 (100%)	0	100	100
22	b	253/350 (72%)	253 (100%)	0	100	100
23	a	137/288 (48%)	137 (100%)	0	100	100
24	4	526/609 (86%)	526 (100%)	0	100	100
25	H	130/180 (72%)	130 (100%)	0	100	100
26	1	254/291 (87%)	254 (100%)	0	100	100
27	Z	86/95 (90%)	86 (100%)	0	100	100
28	X	311/351 (89%)	311 (100%)	0	100	100
29	K	91/113 (80%)	91 (100%)	0	100	100
30	Y	137/357 (38%)	137 (100%)	0	100	100
31	G	275/342 (80%)	275 (100%)	0	100	100
32	F	181/209 (87%)	181 (100%)	0	100	100
33	C	115/143 (80%)	115 (100%)	0	100	100
34	9	12/600 (2%)	12 (100%)	0	100	100
All	All	5594/7798 (72%)	5594 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49)

such sidechains are listed below:

Mol	Chain	Res	Type
1	c	194	ASN
1	c	353	HIS
1	c	397	HIS
3	B	64	ASN
3	B	167	HIS
3	B	201	ASN
5	E	58	HIS
6	I	87	HIS
7	J	37	HIS
9	M	82	HIS
9	M	106	ASN
10	N	52	HIS
11	O	130	HIS
11	O	160	HIS
11	O	169	GLN
11	O	207	GLN
13	Q	27	ASN
13	Q	73	ASN
14	R	139	ASN
15	S	66	HIS
16	T	14	GLN
16	T	33	ASN
16	T	63	GLN
18	V	134	GLN
18	V	141	ASN
18	V	395	GLN
20	0	26	ASN
20	0	108	ASN
20	0	145	HIS
21	3	140	HIS
23	a	151	HIS
23	a	239	HIS
24	4	122	ASN
24	4	373	HIS
24	4	540	HIS
24	4	577	ASN
25	H	83	HIS
26	1	279	ASN
27	Z	54	ASN
28	X	154	HIS
28	X	190	ASN
28	X	257	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	X	291	HIS
28	X	385	ASN
29	K	28	HIS
30	Y	337	HIS
30	Y	349	HIS
31	G	101	GLN
32	F	207	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	922/959 (96%)	194 (21%)	2 (0%)

All (194) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	651	A
2	A	657	G
2	A	680	U
2	A	688	A
2	A	689	U
2	A	695	A
2	A	704	U
2	A	718	A
2	A	721	U
2	A	723	A
2	A	737	C
2	A	740	G
2	A	753	A
2	A	757	A
2	A	761	A
2	A	766	G
2	A	777	G
2	A	782	A
2	A	791	G
2	A	793	C
2	A	794	U
2	A	796	G
2	A	808	C
2	A	814	A
2	A	815	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	828	C
2	A	829	C
2	A	830	U
2	A	832	U
2	A	835	C
2	A	836	A
2	A	859	U
2	A	860	A
2	A	861	U
2	A	868	C
2	A	869	C
2	A	870	C
2	A	871	A
2	A	881	A
2	A	890	C
2	A	896	A
2	A	902	G
2	A	903	U
2	A	905	A
2	A	907	A
2	A	908	C
2	A	919	A
2	A	923	A
2	A	929	A
2	A	930	G
2	A	931	C
2	A	932	C
2	A	938	A
2	A	939	A
2	A	940	A
2	A	941	G
2	A	942	A
2	A	950	A
2	A	953	U
2	A	955	A
2	A	956	C
2	A	957	C
2	A	958	C
2	A	959	C
2	A	960	C
2	A	962	C
2	A	967	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	992	U
2	A	994	A
2	A	1001	C
2	A	1002	C
2	A	1011	C
2	A	1013	A
2	A	1014	A
2	A	1015	A
2	A	1030	G
2	A	1038	C
2	A	1042	U
2	A	1065	C
2	A	1069	A
2	A	1080	A
2	A	1082	A
2	A	1098	C
2	A	1103	A
2	A	1105	C
2	A	1106	C
2	A	1107	U
2	A	1109	A
2	A	1116	A
2	A	1118	A
2	A	1119	U
2	A	1121	A
2	A	1126	A
2	A	1137	A
2	A	1138	G
2	A	1149	G
2	A	1151	C
2	A	1153	C
2	A	1155	G
2	A	1160	A
2	A	1167	A
2	A	1174	U
2	A	1179	G
2	A	1180	U
2	A	1187	U
2	A	1188	A
2	A	1189	U
2	A	1190	C
2	A	1194	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1200	G
2	A	1213	A
2	A	1220	A
2	A	1223	C
2	A	1225	C
2	A	1227	G
2	A	1245	U
2	A	1246	U
2	A	1247	G
2	A	1248	C
2	A	1250	C
2	A	1251	A
2	A	1258	A
2	A	1268	C
2	A	1269	U
2	A	1271	C
2	A	1273	G
2	A	1284	U
2	A	1285	G
2	A	1290	C
2	A	1291	U
2	A	1294	A
2	A	1295	A
2	A	1299	A
2	A	1301	G
2	A	1312	C
2	A	1313	A
2	A	1326	A
2	A	1327	G
2	A	1341	C
2	A	1343	A
2	A	1345	G
2	A	1352	C
2	A	1354	A
2	A	1355	G
2	A	1376	C
2	A	1383	A
2	A	1384	A
2	A	1385	C
2	A	1390	A
2	A	1391	U
2	A	1392	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1402	A
2	A	1404	A
2	A	1406	U
2	A	1407	U
2	A	1413	U
2	A	1416	A
2	A	1429	C
2	A	1430	A
2	A	1443	U
2	A	1447	G
2	A	1448	U
2	A	1462	G
2	A	1465	C
2	A	1466	C
2	A	1474	G
2	A	1475	C
2	A	1478	A
2	A	1479	C
2	A	1480	A
2	A	1483	C
2	A	1489	G
2	A	1490	U
2	A	1492	A
2	A	1493	C
2	A	1503	G
2	A	1508	C
2	A	1509	U
2	A	1510	U
2	A	1539	C
2	A	1557	A
2	A	1558	A
2	A	1559	G
2	A	1560	U
2	A	1564	A
2	A	1565	A
2	A	1567	A
2	A	1568	U
2	A	1569	G
2	A	1571	U
2	A	1572	A
2	A	1594	G
2	A	1595	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1598	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	1492	A
2	A	1508	C

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	5MU	A	1076	2	19,22,23	0.32	0	28,32,35	0.35	0
2	MA6	A	1584	2	23,26,27	1.46	4 (17%)	34,38,41	3.43	12 (35%)
6	5F0	I	184	6	8,8,9	0.56	0	7,9,11	1.17	1 (14%)
2	MA6	A	1583	2	23,26,27	1.46	4 (17%)	34,38,41	3.49	12 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MU	A	1076	2	-	0/7/25/26	0/2/2/2
2	MA6	A	1584	2	-	0/11/29/30	0/3/3/3
6	5F0	I	184	6	-	0/9/9/10	-
2	MA6	A	1583	2	-	2/11/29/30	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1584	MA6	C6-N6	4.61	1.50	1.36
2	A	1583	MA6	C6-N6	4.57	1.50	1.36
2	A	1583	MA6	C5-C4	-2.77	1.33	1.39
2	A	1584	MA6	C5-C4	-2.64	1.34	1.39
2	A	1584	MA6	C5-N7	-2.27	1.34	1.39
2	A	1583	MA6	C5-N7	-2.17	1.34	1.39
2	A	1584	MA6	C8-N9	-2.11	1.33	1.37
2	A	1583	MA6	C8-N9	-2.01	1.33	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1583	MA6	N1-C6-N6	-14.27	101.48	117.08
2	A	1584	MA6	N1-C6-N6	-13.74	102.06	117.08
2	A	1583	MA6	C5-C6-N6	7.54	138.44	125.30
2	A	1584	MA6	C5-C6-N6	7.37	138.13	125.30
2	A	1583	MA6	N1-C2-N3	-5.55	119.92	128.60
2	A	1584	MA6	N1-C2-N3	-5.40	120.16	128.60
2	A	1584	MA6	C5-C4-N3	-5.29	119.85	126.75
2	A	1583	MA6	C5-C4-N3	-4.95	120.29	126.75
2	A	1583	MA6	N9-C8-N7	-4.70	107.48	113.91
2	A	1584	MA6	N9-C8-N7	-4.50	107.76	113.91
2	A	1584	MA6	C4-C5-C6	3.87	120.21	115.88
2	A	1583	MA6	C2-N3-C4	3.51	120.04	111.75
2	A	1583	MA6	C2-N1-C6	3.51	120.04	111.75
2	A	1584	MA6	C2-N3-C4	3.50	120.01	111.75
2	A	1584	MA6	C2-N1-C6	3.48	119.97	111.75
2	A	1583	MA6	C4-C5-C6	3.35	119.63	115.88
2	A	1584	MA6	N3-C4-N9	3.34	132.59	127.08
2	A	1583	MA6	C5-N7-C8	3.24	108.11	103.51
2	A	1584	MA6	C5-N7-C8	3.21	108.07	103.51
2	A	1583	MA6	N3-C4-N9	2.97	131.97	127.08
6	I	184	5F0	O-C-CB	-2.73	117.46	125.43
2	A	1583	MA6	C4-N9-C8	2.68	108.63	105.73
2	A	1584	MA6	C4-N9-C8	2.52	108.46	105.73
2	A	1583	MA6	C4-C5-N7	-2.11	108.05	110.62
2	A	1584	MA6	C4-C5-N7	-2.03	108.15	110.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1583	MA6	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1583	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1584	MA6	4	0
2	A	1583	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 47 are monoatomic - leaving 7 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	$\# Z > 2$
40	FES	P	201	5,12	0,4,4	-	-	-		
36	SPM	A	1702	-	13,13,13	0.28	0	12,12,12	0.95	0
41	SAH	b	501	-	27,28,28	1.07	4 (14%)	38,40,40	1.96	9 (23%)
42	ATP	X	501	-	29,33,33	0.48	0	44,52,52	0.51	0
35	NAD	A	1701	37	45,48,48	0.41	0	63,73,73	0.44	0
43	GDP	X	502	-	28,30,30	0.43	0	44,47,47	0.48	0
40	FES	T	201	9,16	0,4,4	-	-	-		

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
40	FES	P	201	5,12	-	-	0/1/1/1
36	SPM	A	1702	-	-	2/11/11/11	-
41	SAH	b	501	-	-	4/15/31/31	0/3/3/3
42	ATP	X	501	-	-	6/22/38/38	0/3/3/3
35	NAD	A	1701	37	-	2/30/62/62	0/5/5/5
43	GDP	X	502	-	-	2/16/32/32	0/3/3/3
40	FES	T	201	9,16	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	b	501	SAH	C2-N3	2.45	1.38	1.33
41	b	501	SAH	C2-N1	2.45	1.38	1.33
41	b	501	SAH	OXT-C	-2.12	1.23	1.30
41	b	501	SAH	C8-N7	2.02	1.35	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	b	501	SAH	N3-C2-N1	-5.39	120.17	128.60
41	b	501	SAH	C5-C4-N3	-4.90	120.35	126.75
41	b	501	SAH	N9-C8-N7	-3.99	108.46	113.91
41	b	501	SAH	C5-N7-C8	3.73	108.81	103.51
41	b	501	SAH	C2-N3-C4	3.58	120.21	111.75
41	b	501	SAH	N3-C4-N9	3.27	132.48	127.08
41	b	501	SAH	OXT-C-O	-2.74	117.87	124.09
41	b	501	SAH	OXT-C-CA	2.26	121.07	113.38
41	b	501	SAH	C4-C5-N7	-2.14	108.01	110.62

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	A	1702	SPM	C7-C8-C9-N10
42	X	501	ATP	O4'-C4'-C5'-O5'
42	X	501	ATP	PB-O3B-PG-O1G
41	b	501	SAH	C2'-C1'-N9-C8
42	X	501	ATP	C3'-C4'-C5'-O5'
35	A	1701	NAD	PA-O3-PN-O2N
42	X	501	ATP	C4'-C5'-O5'-PA
43	X	502	GDP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

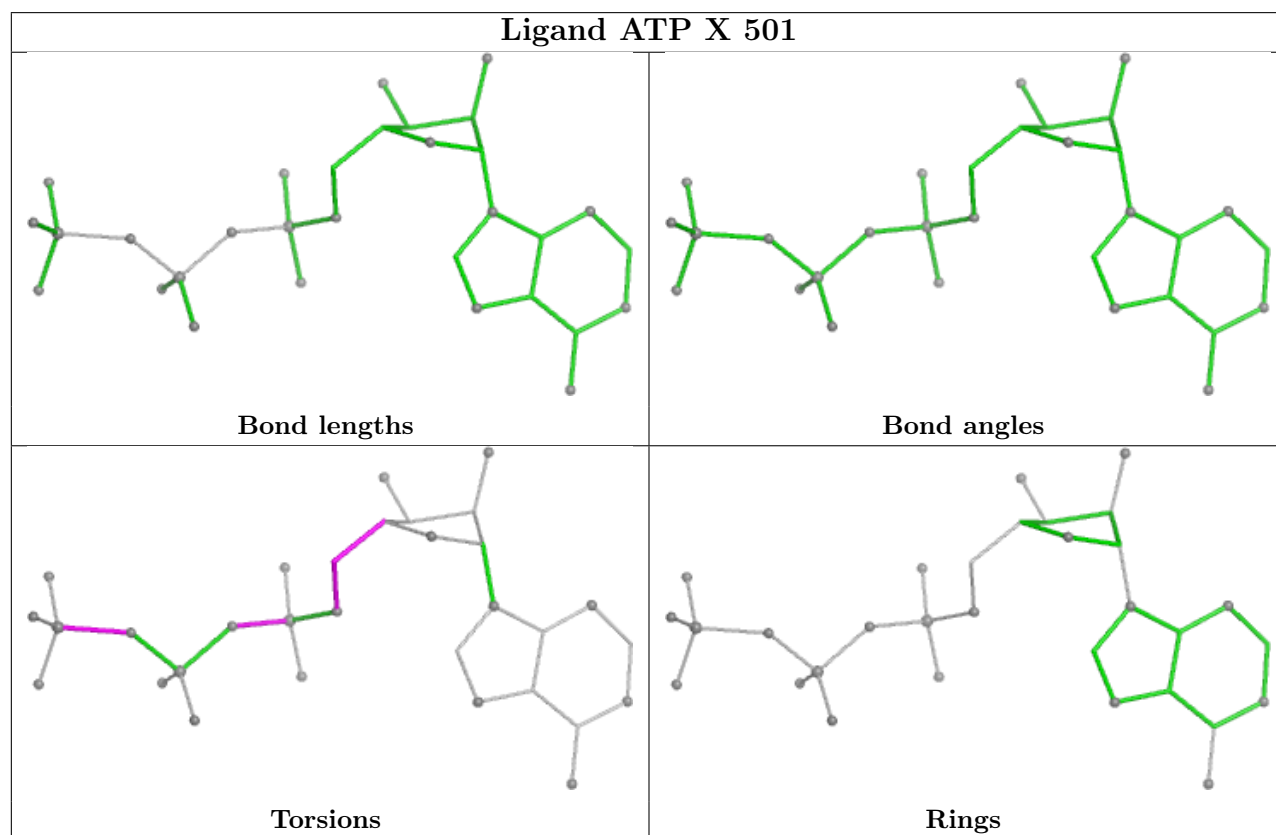
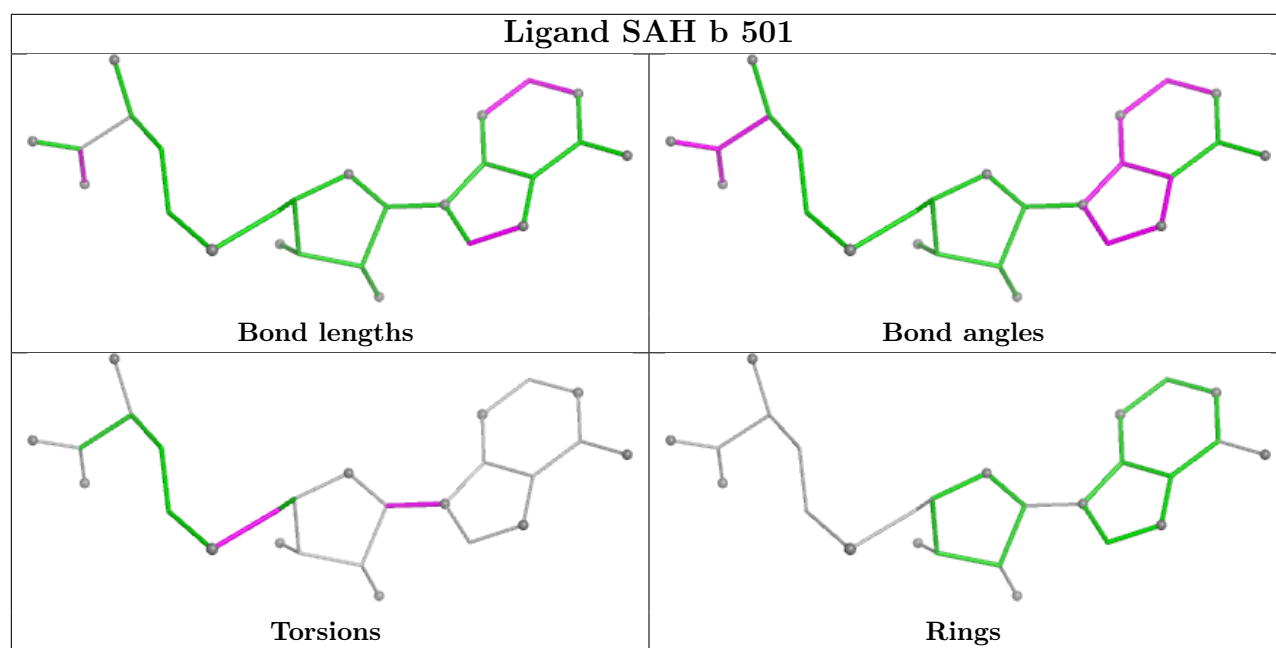
Mol	Chain	Res	Type	Atoms
41	b	501	SAH	O4'-C1'-N9-C8
42	X	501	ATP	PB-O3A-PA-O1A
36	A	1702	SPM	C6-C7-C8-C9
41	b	501	SAH	C4'-C5'-SD-CG
43	X	502	GDP	O4'-C4'-C5'-O5'
35	A	1701	NAD	C2B-C1B-N9A-C8A
42	X	501	ATP	PB-O3A-PA-O2A
41	b	501	SAH	C2'-C1'-N9-C4

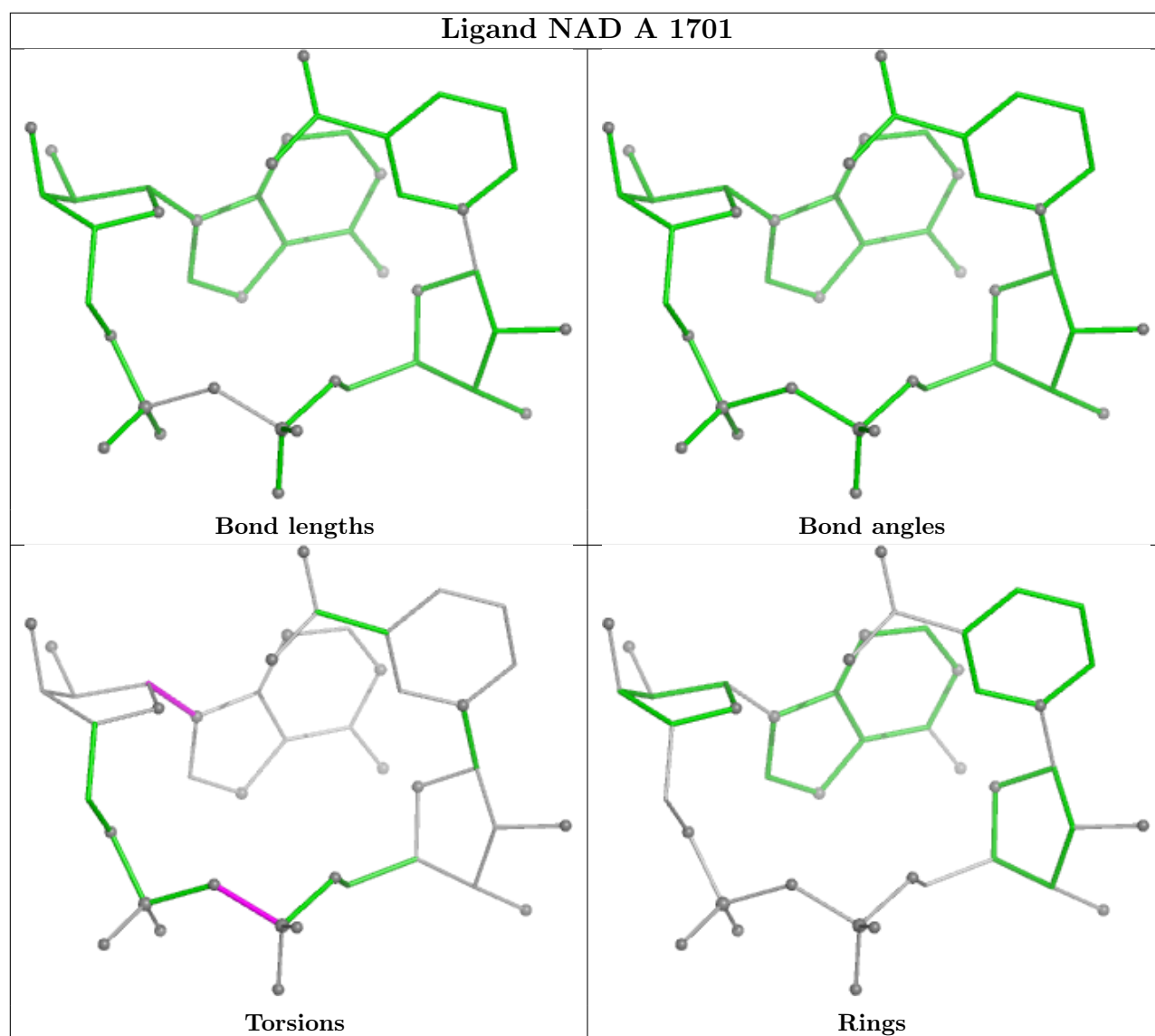
There are no ring outliers.

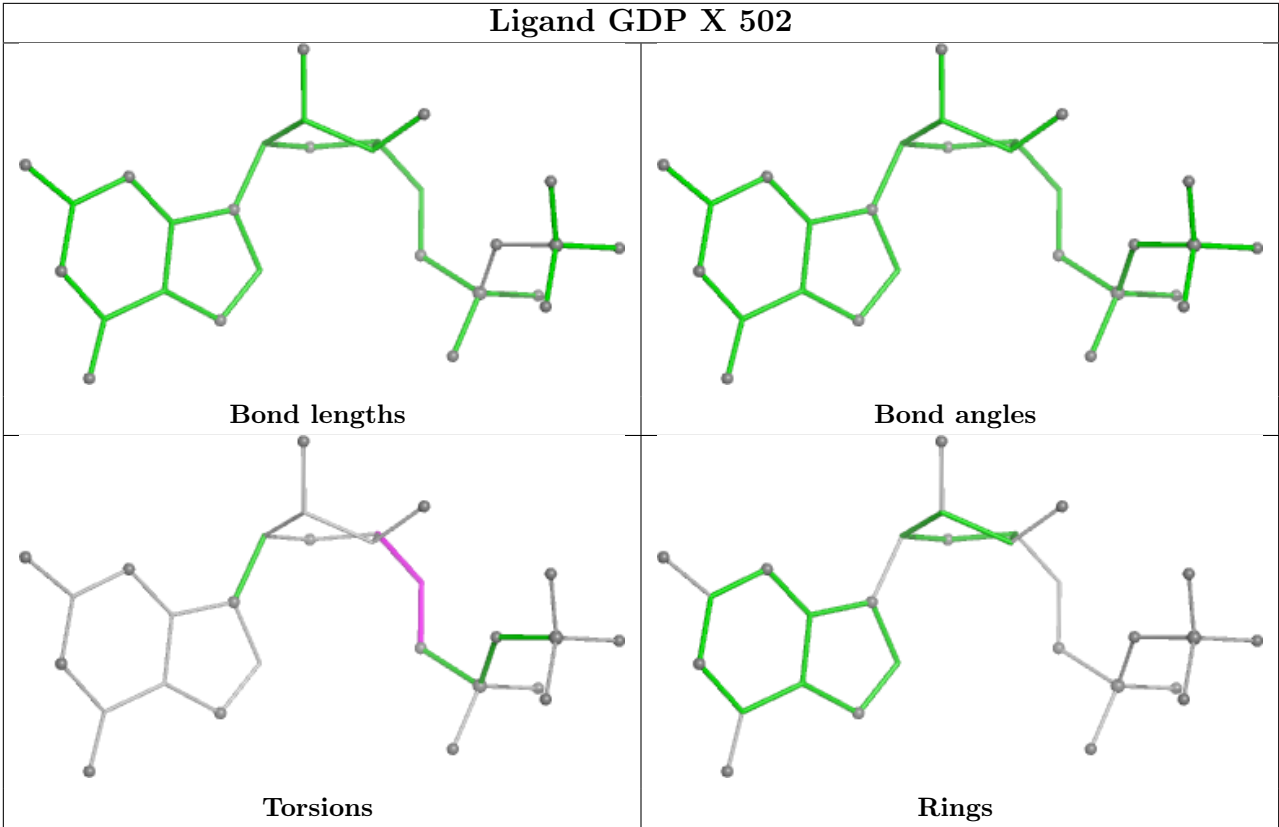
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	b	501	SAH	3	0

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







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	49:ARG	C	87:LYS	N	39.97

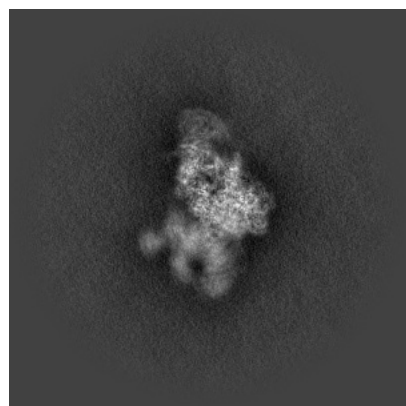
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51873. These allow visual inspection of the internal detail of the map and identification of artifacts.

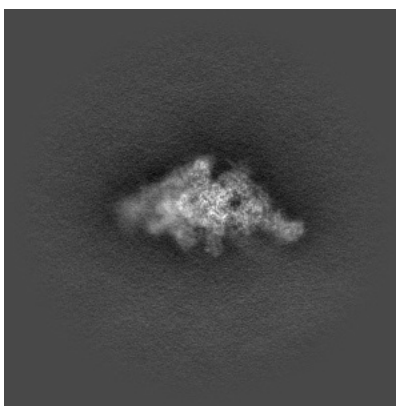
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

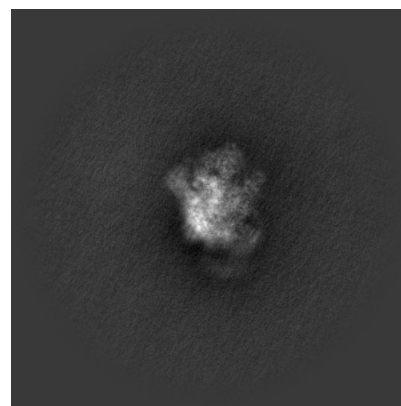
6.1.1 Primary map



X

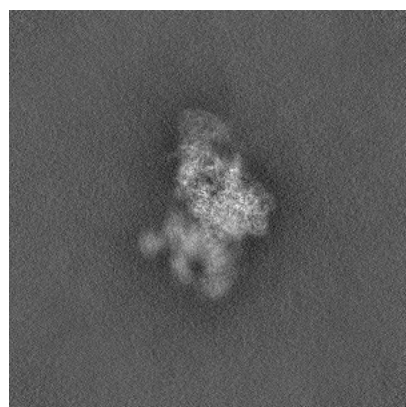


Y

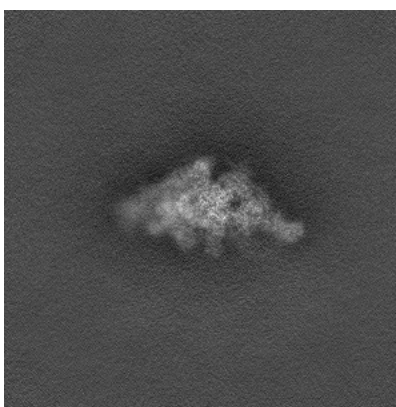


Z

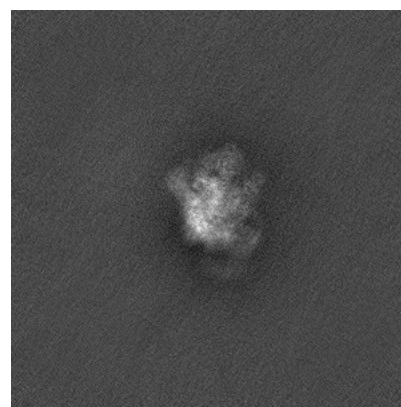
6.1.2 Raw map



X



Y

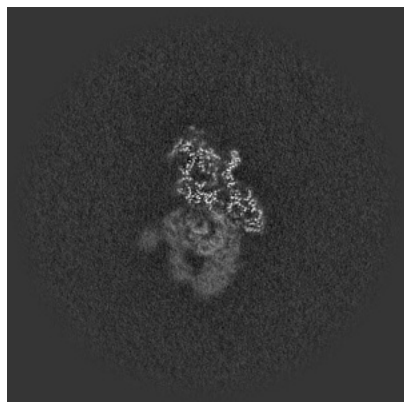


Z

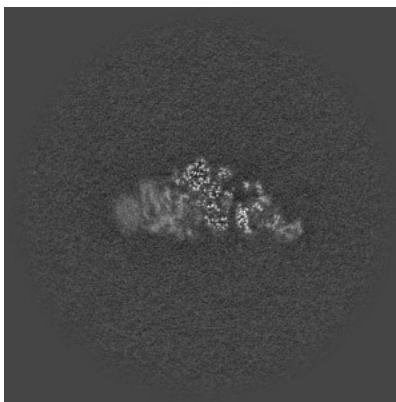
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

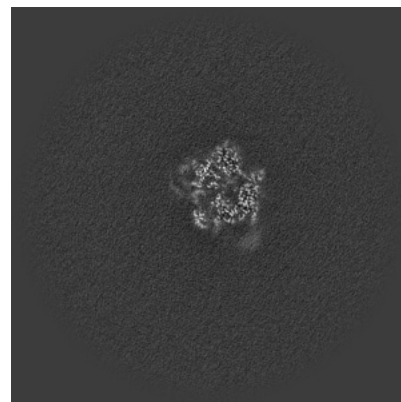
6.2.1 Primary map



X Index: 300

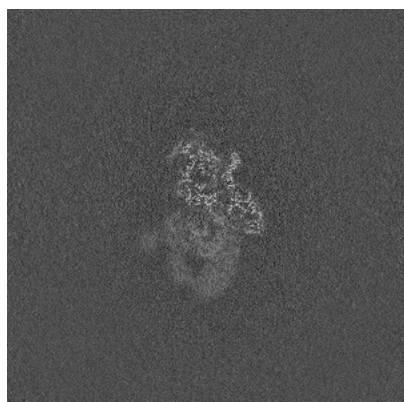


Y Index: 300

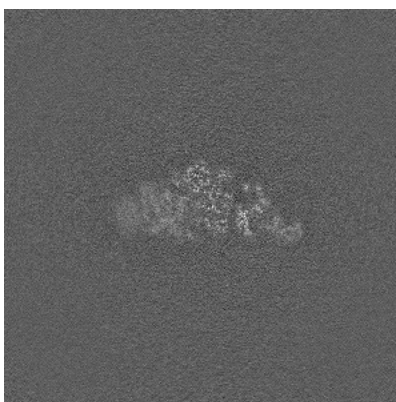


Z Index: 300

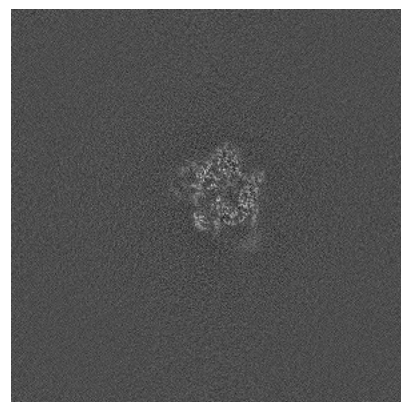
6.2.2 Raw map



X Index: 300



Y Index: 300

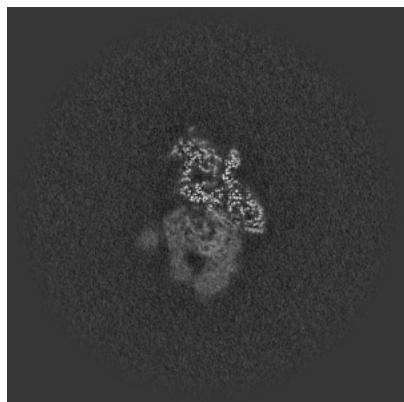


Z Index: 300

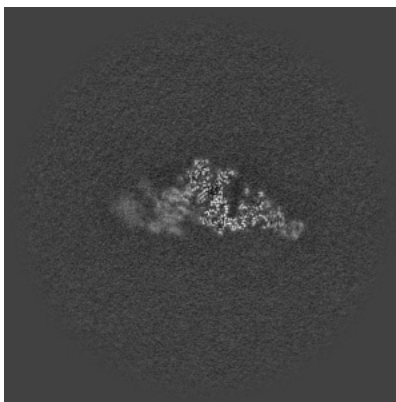
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

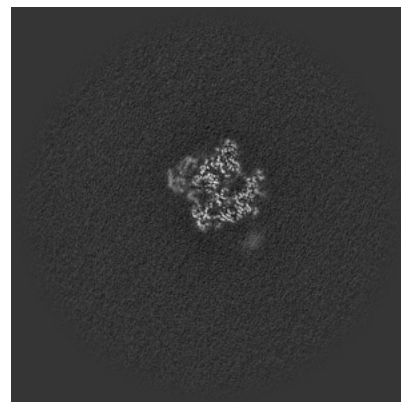
6.3.1 Primary map



X Index: 302

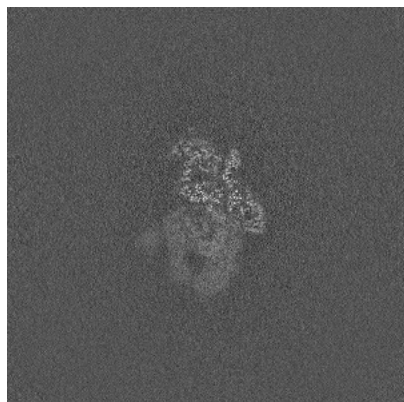


Y Index: 293

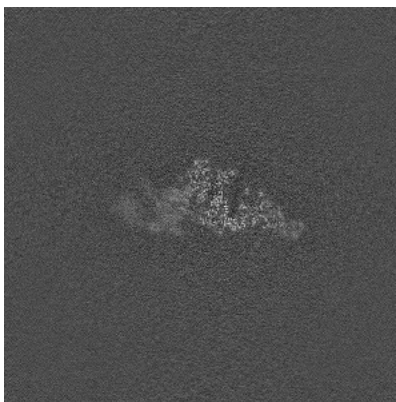


Z Index: 305

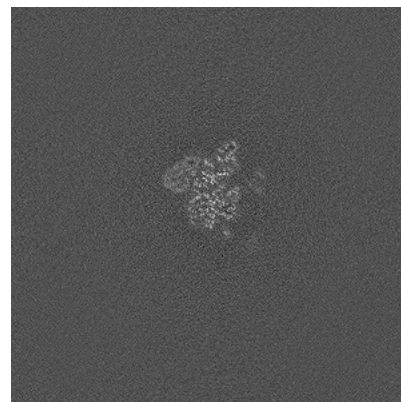
6.3.2 Raw map



X Index: 302



Y Index: 293

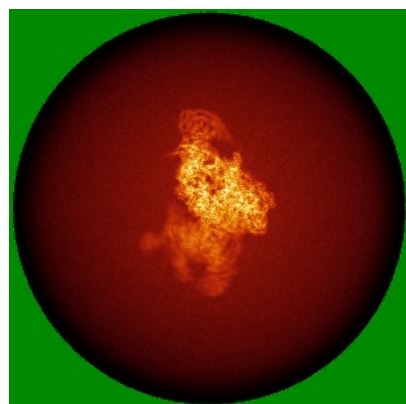


Z Index: 314

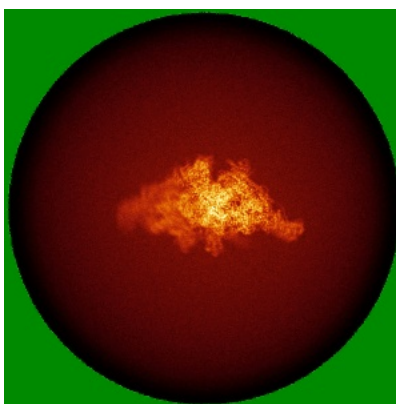
The images above show the largest variance slices of the map in three orthogonal directions.

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

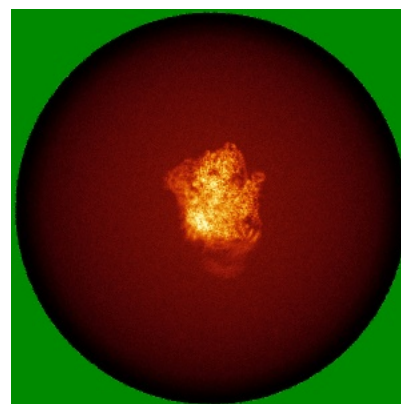
6.4.1 Primary map



X

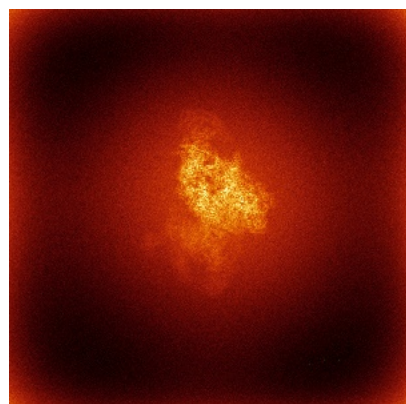


Y

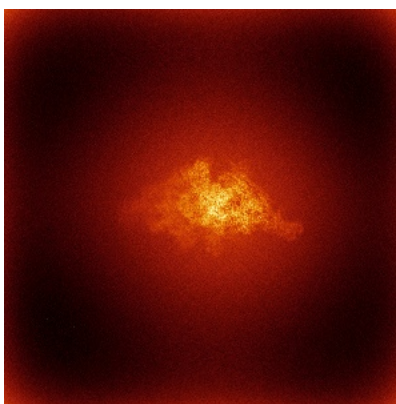


Z

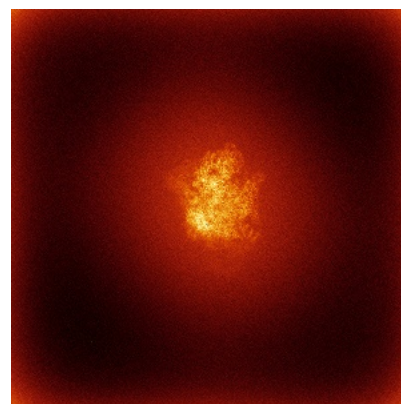
6.4.2 Raw map



X



Y

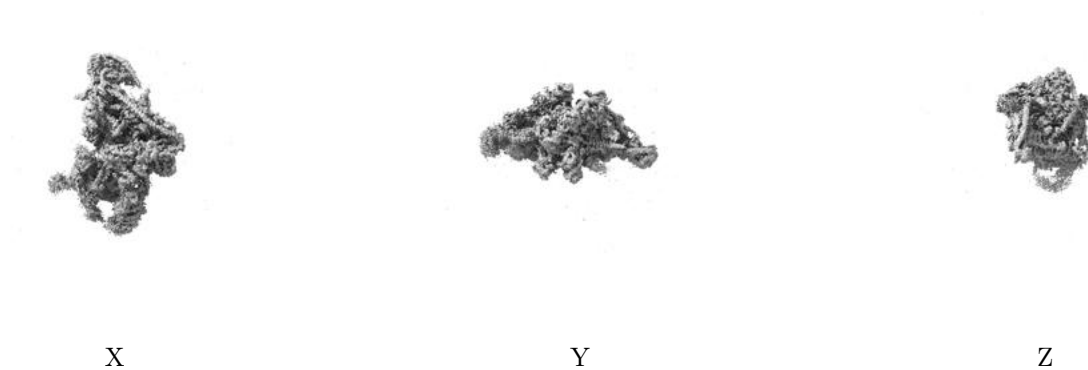


Z

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

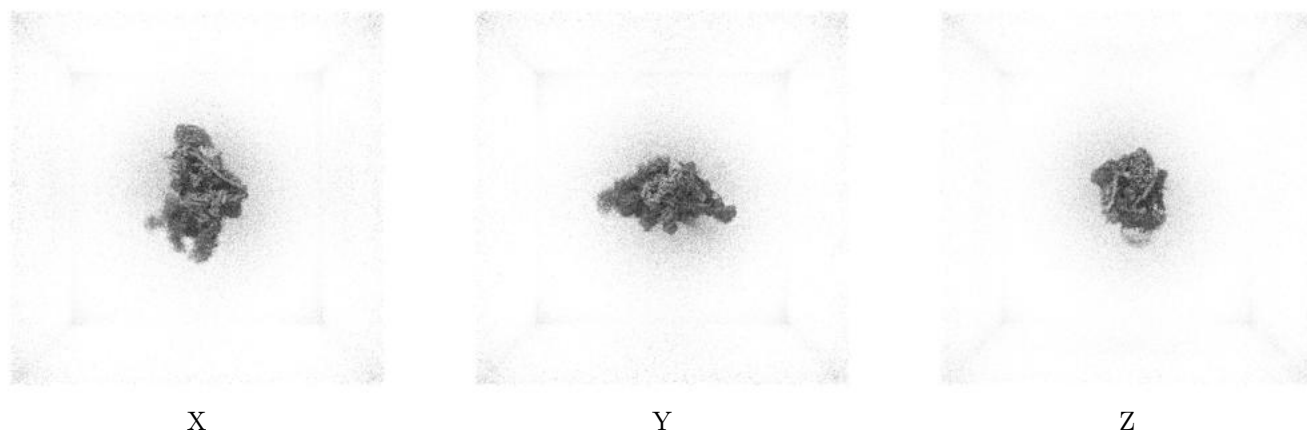
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

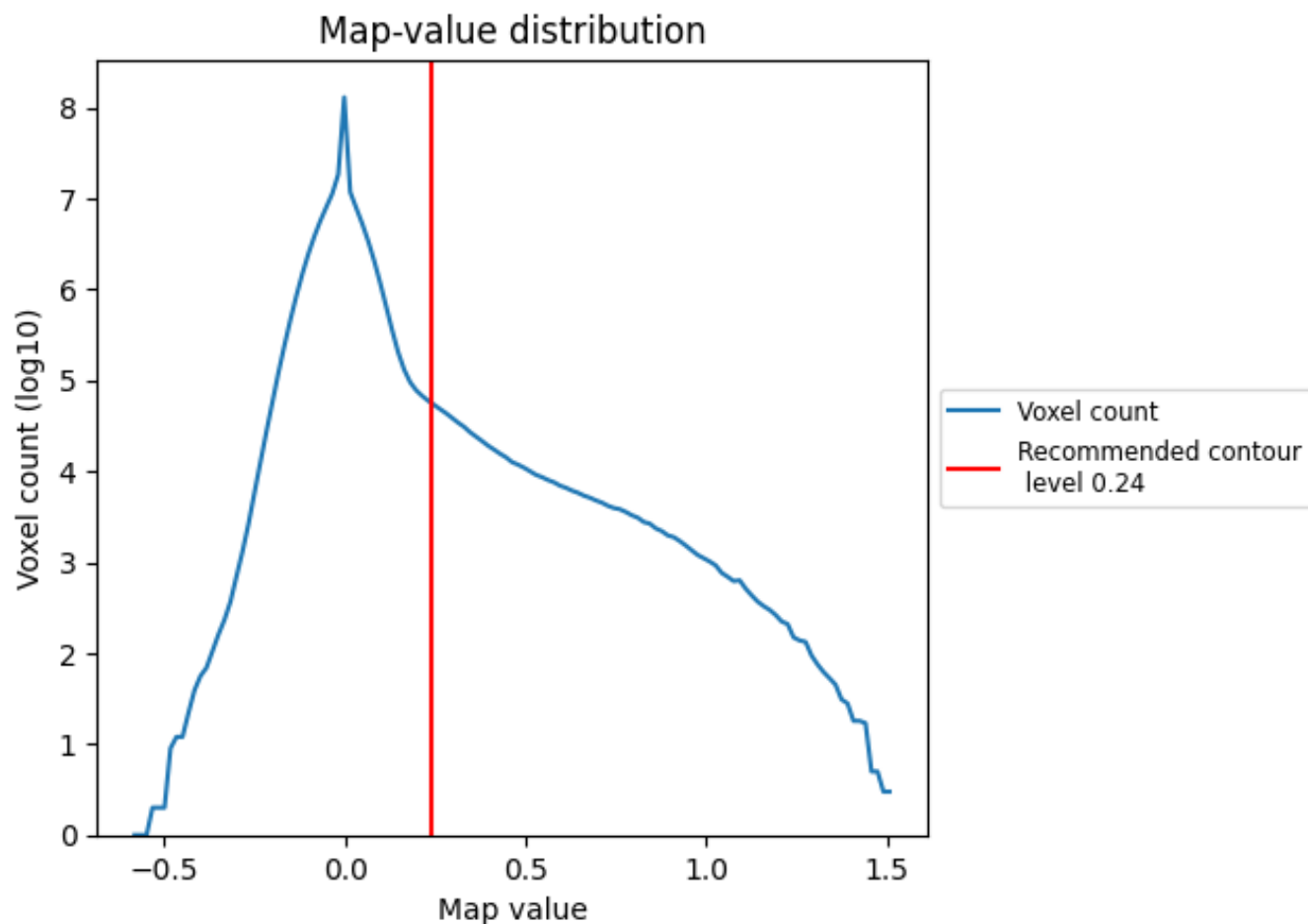
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

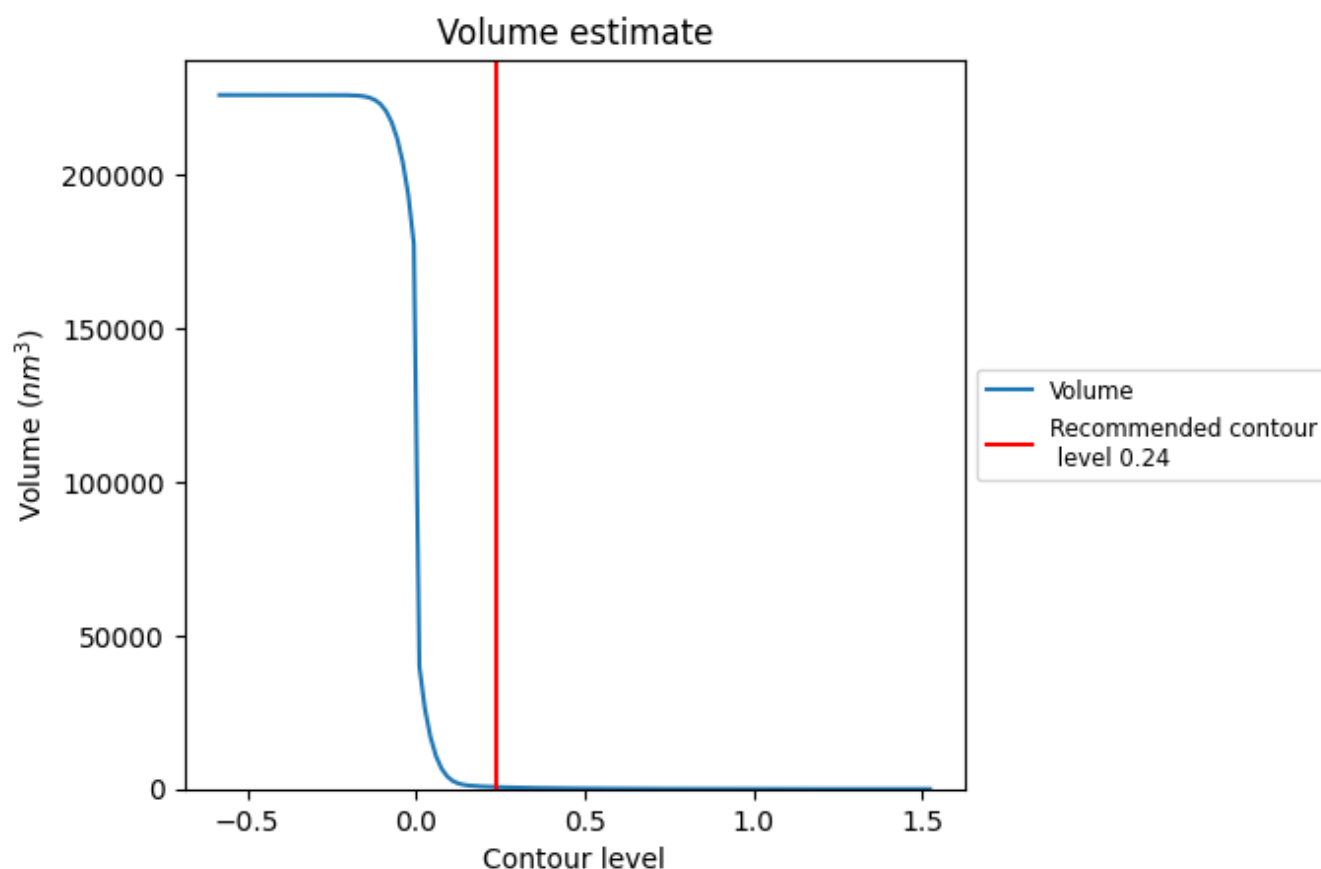
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

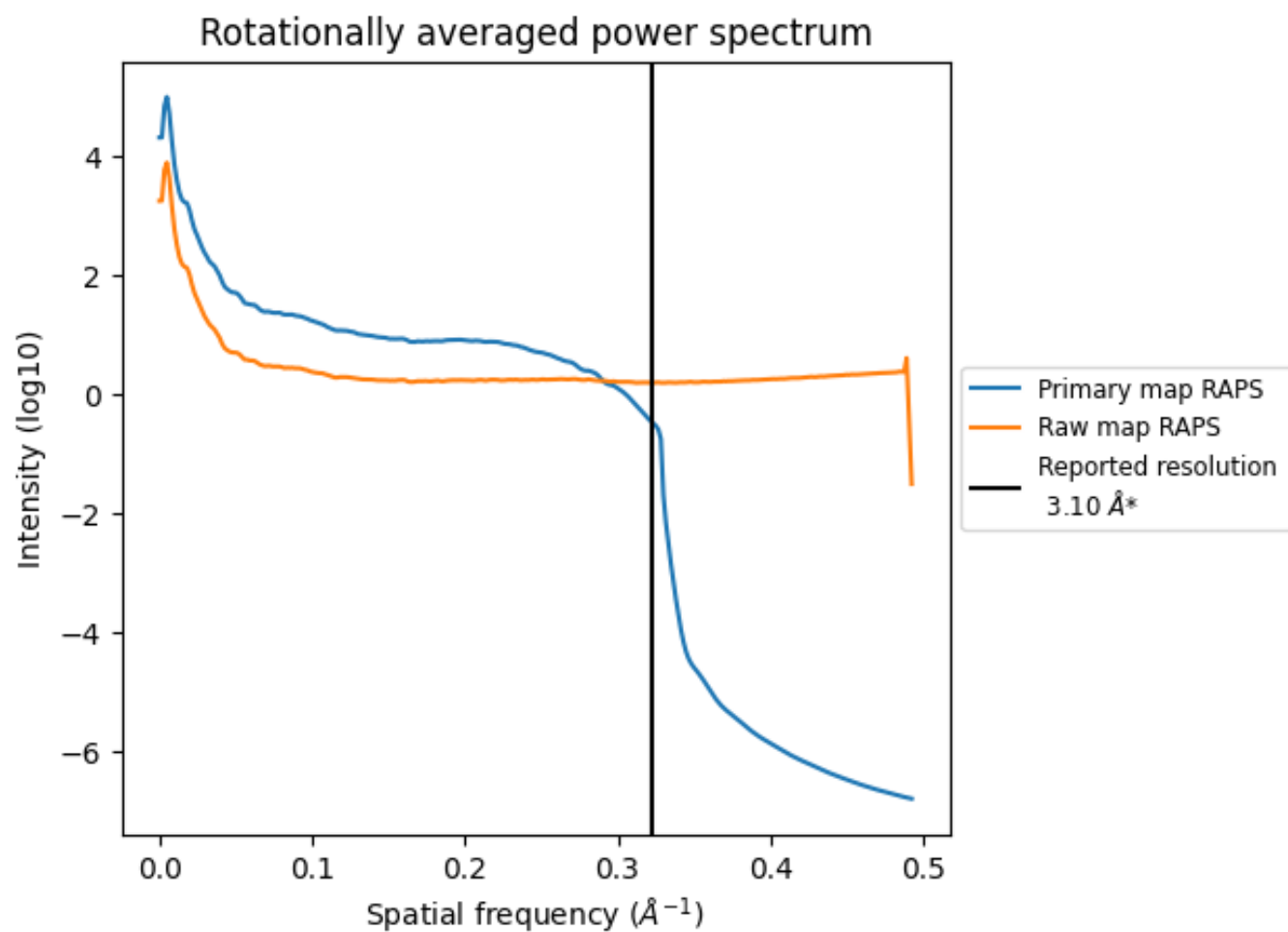
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 613 nm³; this corresponds to an approximate mass of 554 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 ⓘ

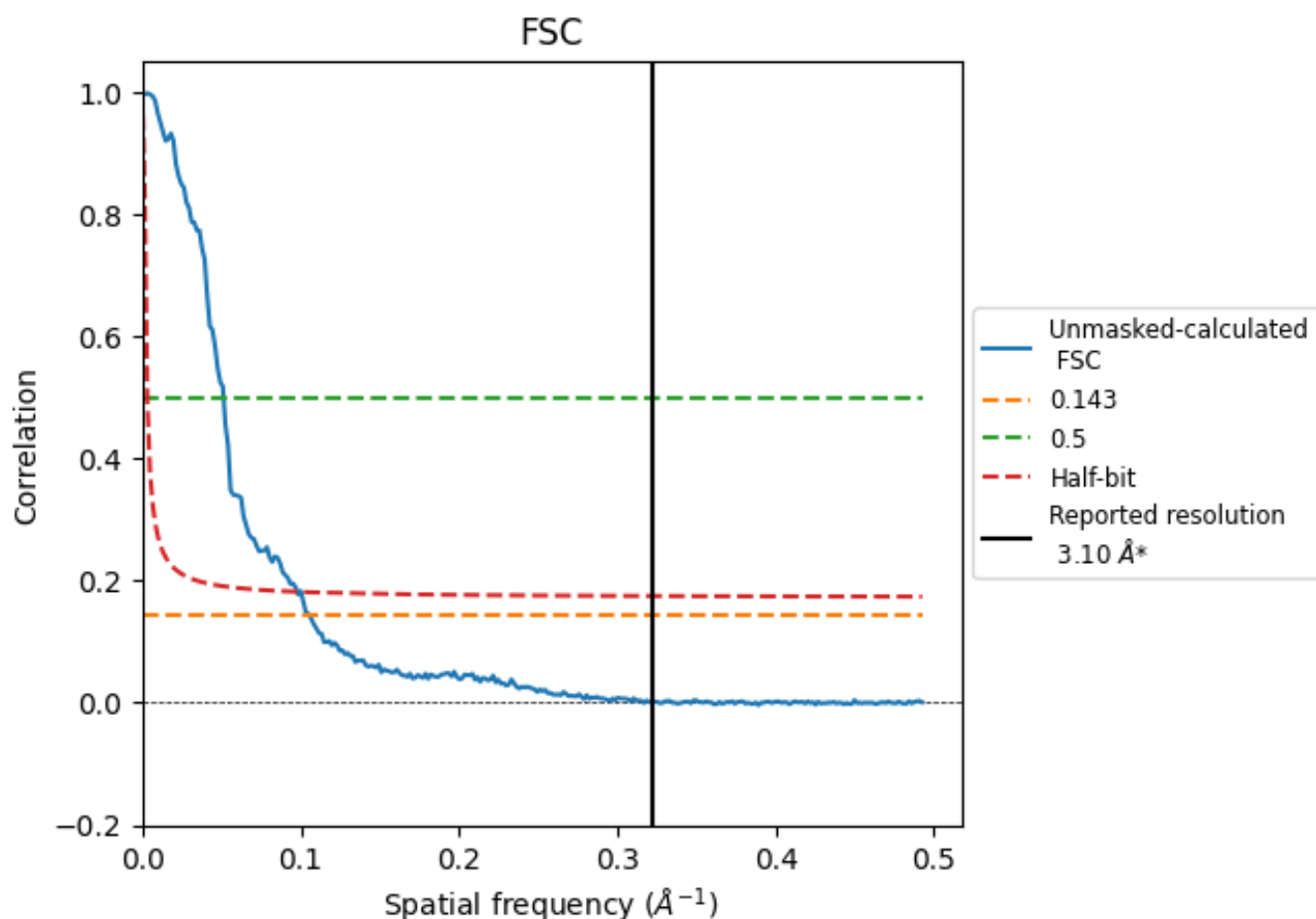


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

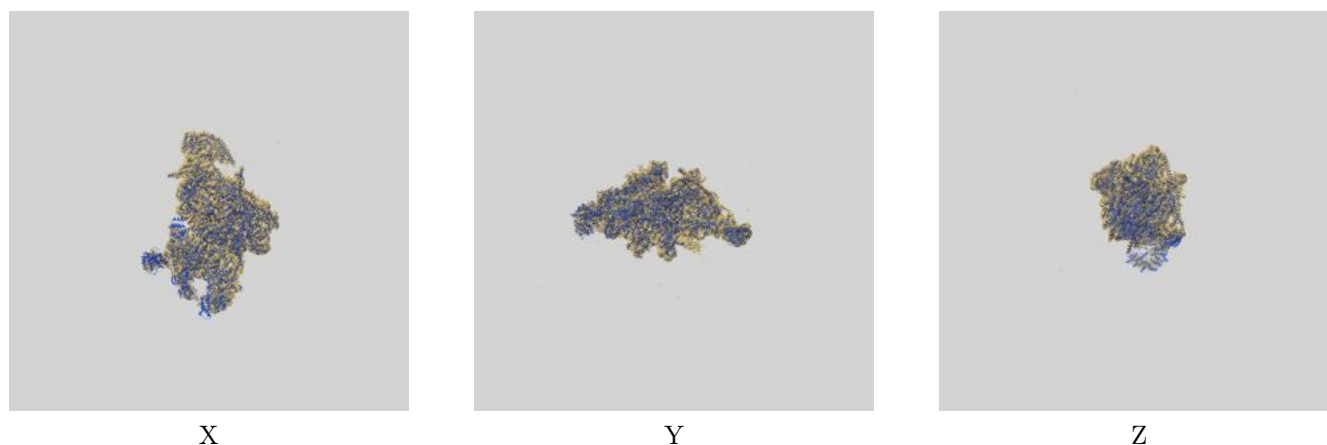
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.47	19.46	10.21

*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 9.47 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

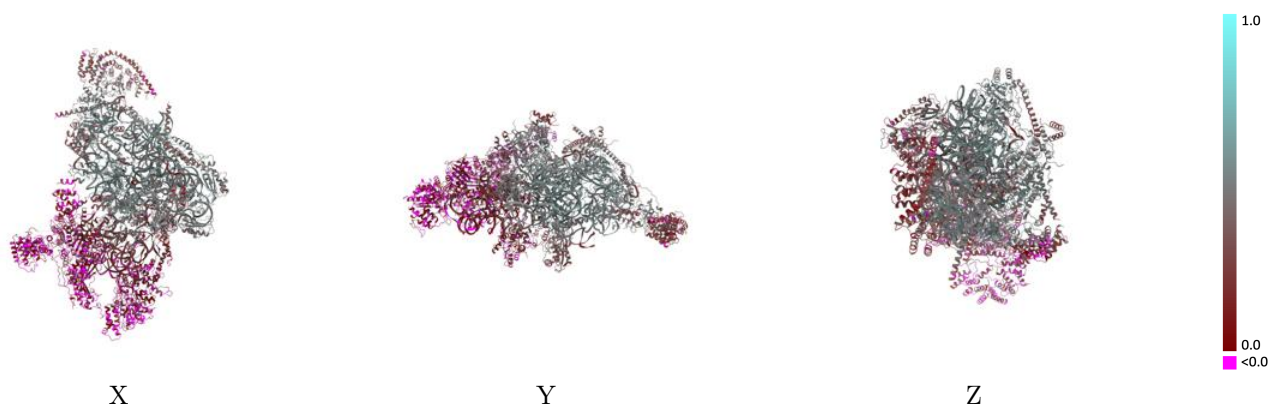
This section contains information regarding the fit between EMDB map EMD-51873 and PDB model 9H51. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



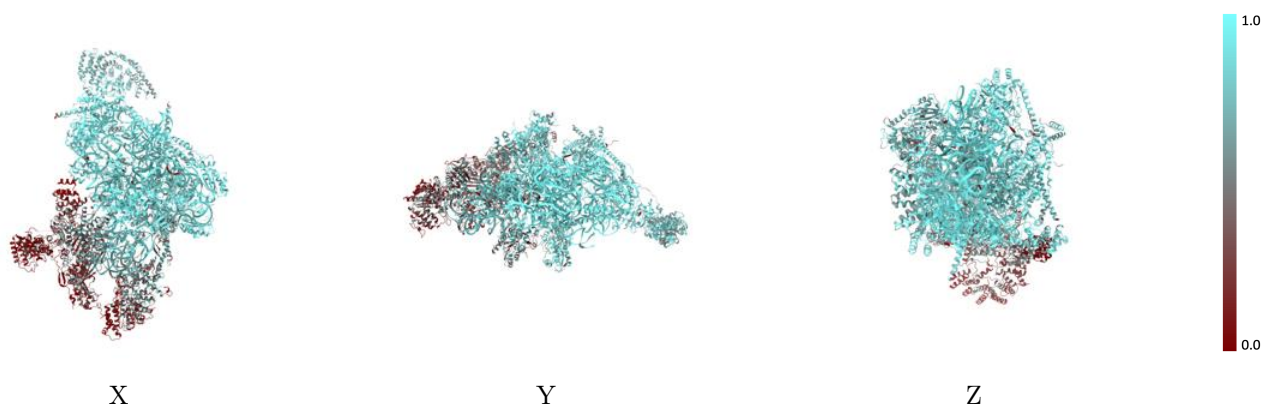
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



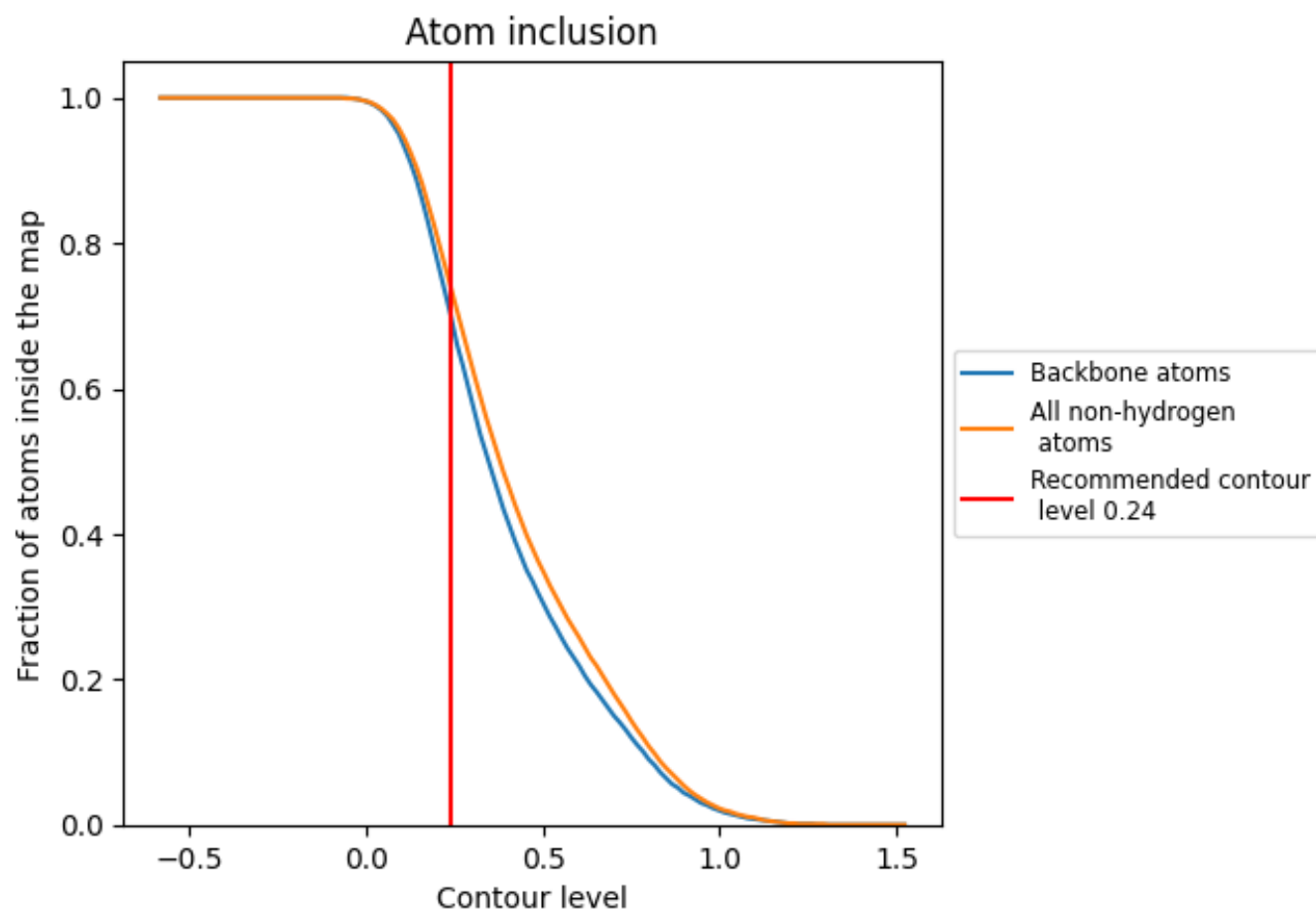
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 74% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7380	 0.3270
0	 0.8390	 0.4300
1	 0.2230	 0.0510
3	 0.8440	 0.4810
4	 0.2070	 0.0580
9	 0.6300	 0.1870
A	 0.9290	 0.4070
B	 0.9000	 0.4950
C	 0.5170	 0.1890
D	 0.7180	 0.4100
E	 0.8660	 0.4900
F	 0.5440	 0.1410
G	 0.5520	 0.2000
H	 0.3550	 0.0940
I	 0.8950	 0.4780
J	 0.9010	 0.5150
K	 0.5450	 0.1400
L	 0.8690	 0.4840
M	 0.9080	 0.5140
N	 0.9120	 0.5300
O	 0.9130	 0.4980
P	 0.8990	 0.4980
Q	 0.8900	 0.5030
R	 0.8700	 0.4600
S	 0.8530	 0.4230
T	 0.8890	 0.5040
U	 0.8520	 0.4370
V	 0.7180	 0.2560
W	 0.8560	 0.4670
X	 0.3260	 0.0470
Y	 0.1530	 0.0600
Z	 0.4120	 0.1080
a	 0.6260	 0.3160
b	 0.5980	 0.1910
c	 0.7550	 0.3740

