



wwPDB EM Validation Summary Report ⓘ

Aug 23, 2026 – 07:23 pm BST

PDB ID : 8QRM / pdb_00008qrm
EMDB ID : EMD-18440
Title : mt-SSU assembly intermediate in GTPBP8 knock-out cells, state 3
Authors : Valentin Gese, G.; Cipullo, M.; Rorbach, J.; Hallberg, B.M.
Deposited on : 2023-10-09
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

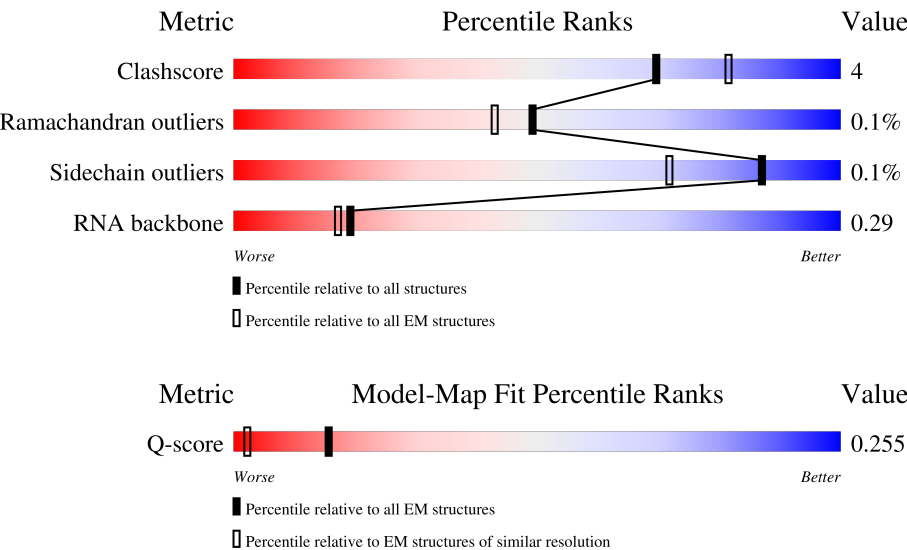
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.05 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	13971 (2.55 - 3.55)

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

Mol	Chain	Length	Quality of chain
1	A	955	12% 64% 30% 5%
2	B	296	72% 24%
3	C	167	19% 63% 16% 21%

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Mol	Chain	Length	Quality of chain
4	D	430	
5	E	125	
6	F	242	
7	G	396	
8	H	201	
9	I	194	
10	J	138	
11	K	128	
12	L	257	
13	M	137	
14	N	130	
15	O	258	
16	P	142	
17	Q	86	
18	R	360	
19	S	190	
20	T	173	
21	U	205	
22	V	414	
23	W	187	
24	X	398	
25	Y	395	
26	Z	106	
27	0	218	
28	1	323	

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Mol	Chain	Length	Quality of chain
29	2	117	89% 74% 26%
30	3	199	34% 65%
31	4	689	73% 79% 7% 15%
32	8	285	64% 59% 8% 33%

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 68726 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 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	955	Total	C	N	O	P	0	0
			20282	9098	3652	6577	955		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	709	G	A	conflict	GB OM714795.1

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	225	Total	C	N	O	S	0	0
			1828	1164	331	323	10		

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2707	1697	514	484	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	323	Total	C	N	O	S	0	0
			2657	1691	471	481	14		

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	137	Total	C	N	O	S	0	0
			1019	641	193	181	4		

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	119	Total	C	N	O	S	0	0
			942	594	185	157	6		

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	194	Total	C	N	O	S	0	0
			1599	1019	295	278	7		

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 17 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	86	Total	C	N	O	S	0	0
			744	460	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	ARG	CYS	variant	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	149	Total	C	N	O	S	0	0
			1246	801	207	234	4		

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

- Molecule 27 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	276	Total	C	N	O	S	0	0
			2238	1419	381	427	11		

- Molecule 29 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	117	Total	C	N	O	S	0	0
			935	579	182	166	8		

- Molecule 30 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

- Molecule 31 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	588	Total	C	N	O	S	0	0
			4768	3053	808	879	28		

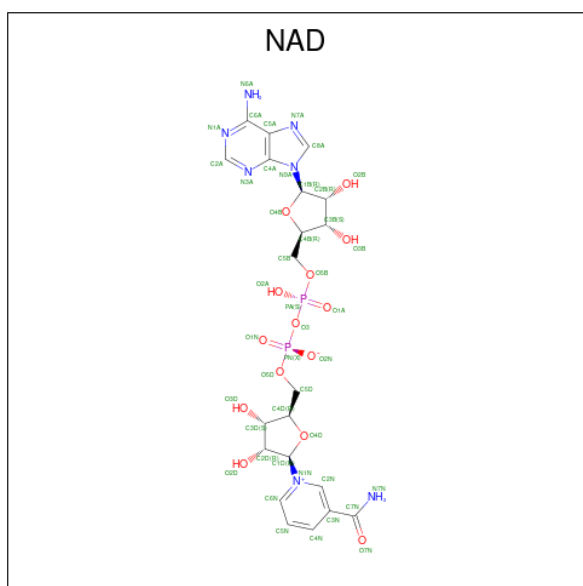
- Molecule 32 is a protein called Translation initiation factor IF-3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	191	Total	C	N	O	S	0	0
			1543	953	289	293	8		

There are 9 discrepancies between the modelled and reference sequences:

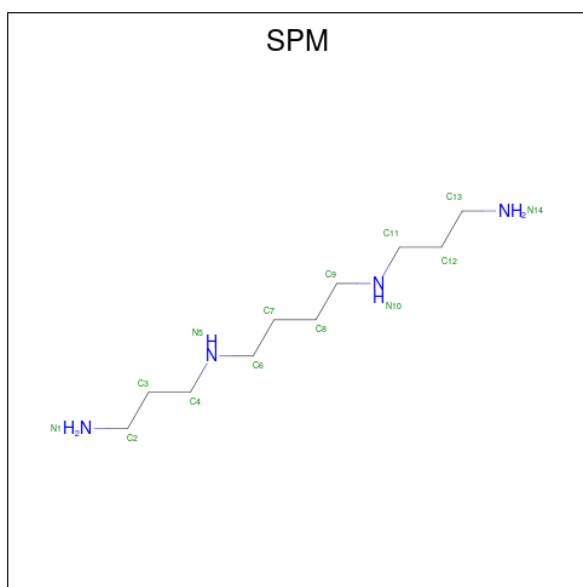
Chain	Residue	Modelled	Actual	Comment	Reference
8	68	ILE	THR	variant	UNP Q9H2K0
8	243	LEU	PHE	variant	UNP Q9H2K0
8	279	GLY	-	expression tag	UNP Q9H2K0
8	280	LEU	-	expression tag	UNP Q9H2K0
8	281	GLU	-	expression tag	UNP Q9H2K0
8	282	VAL	-	expression tag	UNP Q9H2K0
8	283	LEU	-	expression tag	UNP Q9H2K0
8	284	PHE	-	expression tag	UNP Q9H2K0
8	285	GLN	-	expression tag	UNP Q9H2K0

- Molecule 33 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



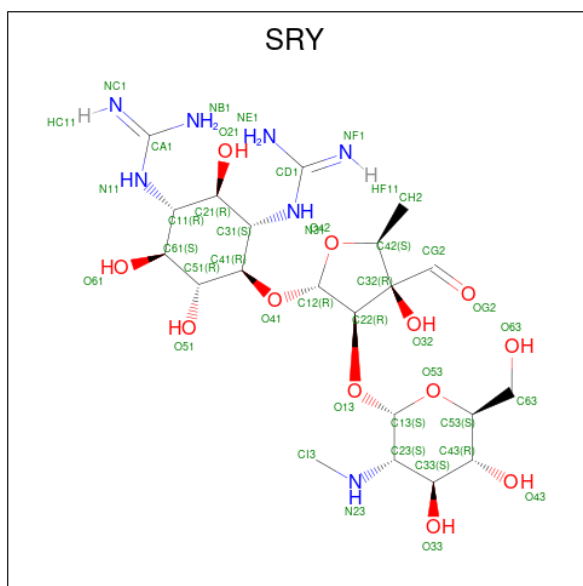
Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 34 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	N	0
			14	10	4	

- Molecule 35 is STREPTOMYCIN (CCD ID: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			40	21	7	12	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	A	56	Total	Mg	0
			56	56	
36	B	1	Total	Mg	0
			1	1	
36	X	1	Total	Mg	0
			1	1	
36	3	1	Total	Mg	0
			1	1	

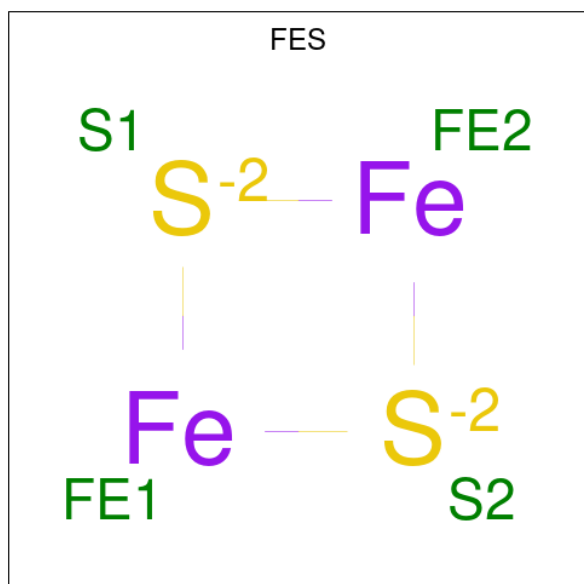
- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
37	A	17	Total	K	0
			17	17	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



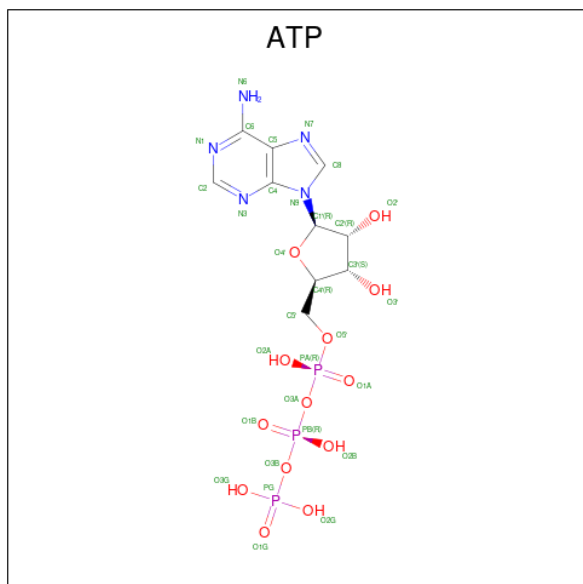
Mol	Chain	Residues	Atoms			AltConf
39	P	1	Total	Fe	S	0
			4	2	2	

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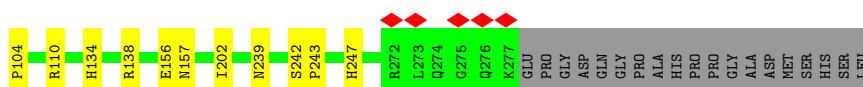
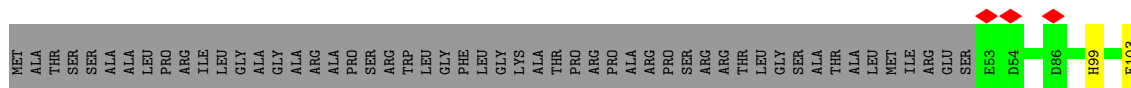
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
39	T	1	4	2	2	0

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

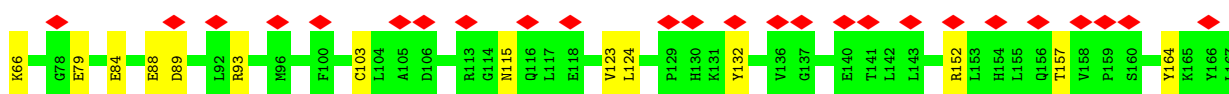
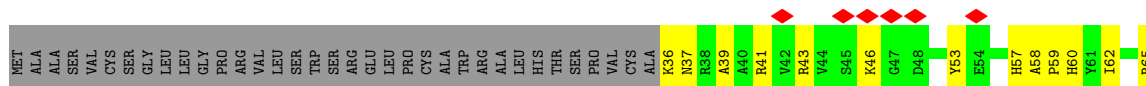


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	X	1	32	10	6	13	3	0

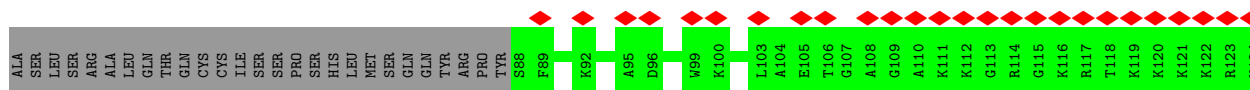
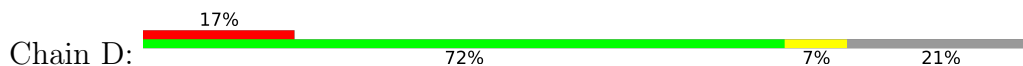
- Molecule 2: 28S ribosomal protein S2, mitochondrial



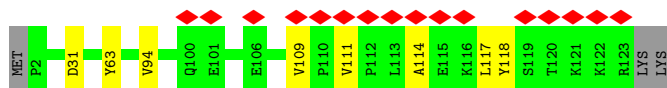
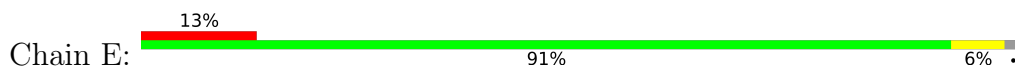
- Molecule 3: 28S ribosomal protein S24, mitochondrial



- Molecule 4: 28S ribosomal protein S5, mitochondrial

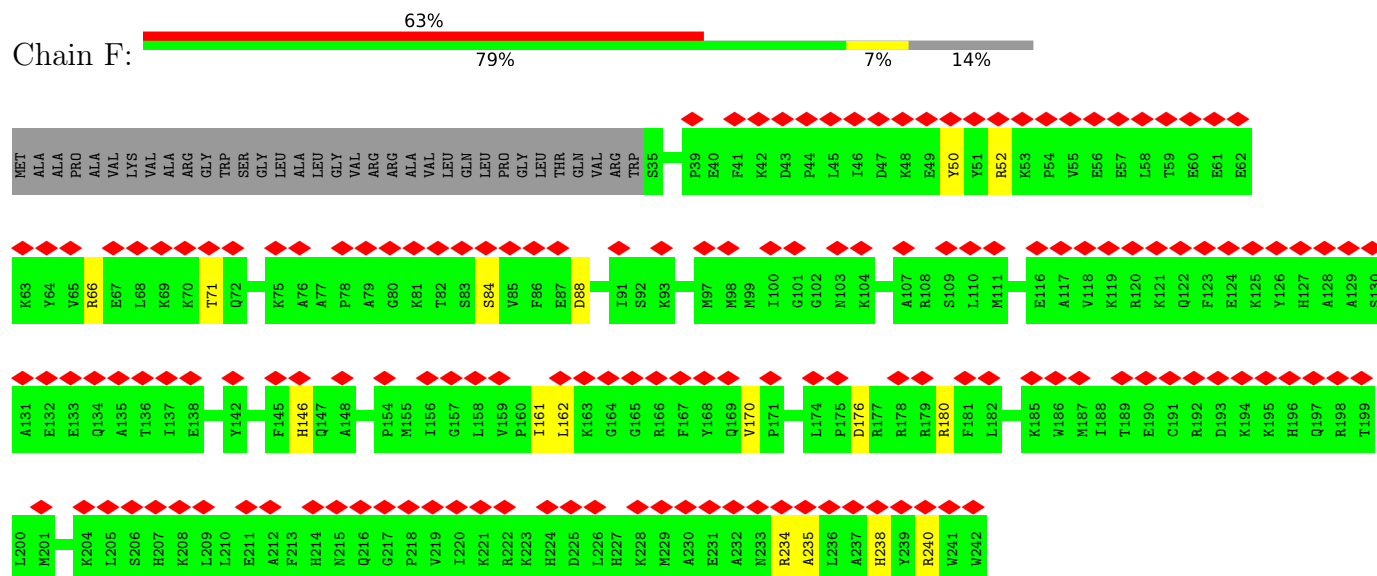


- Molecule 5: 28S ribosomal protein S6, mitochondrial



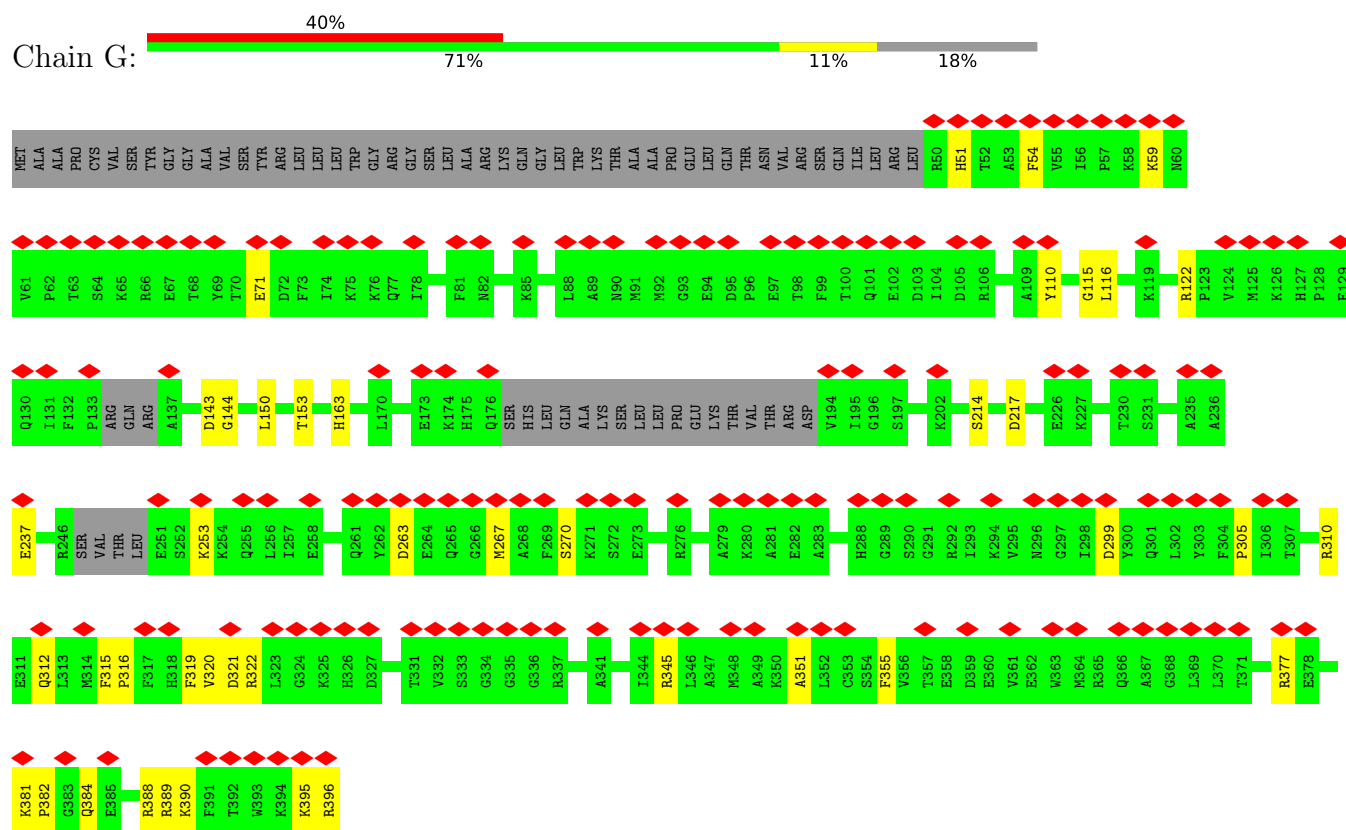
- Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F:



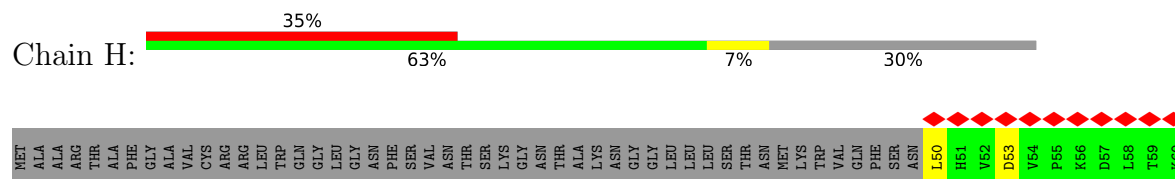
- Molecule 7: 28S ribosomal protein S9, mitochondrial

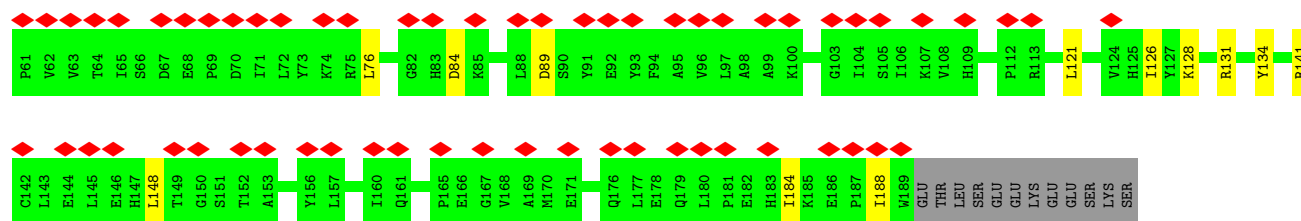
Chain G:



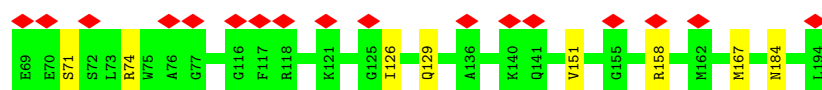
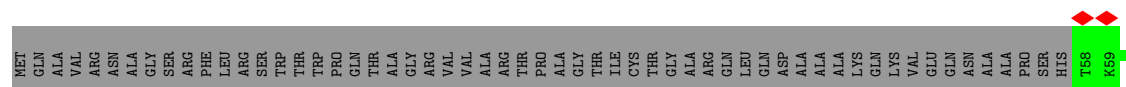
- Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:

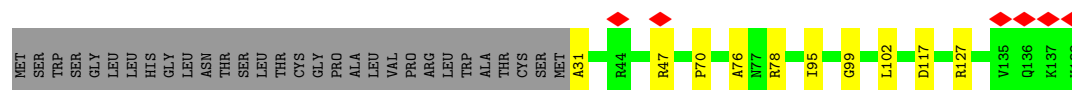




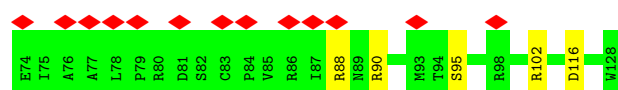
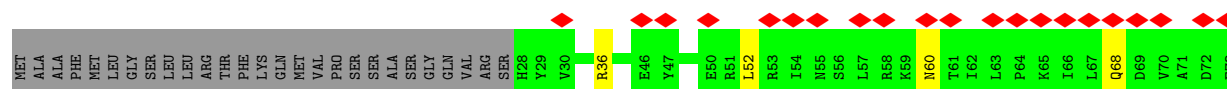
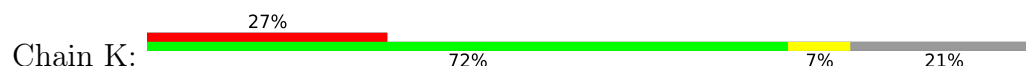
• Molecule 9: 28S ribosomal protein S11, mitochondrial



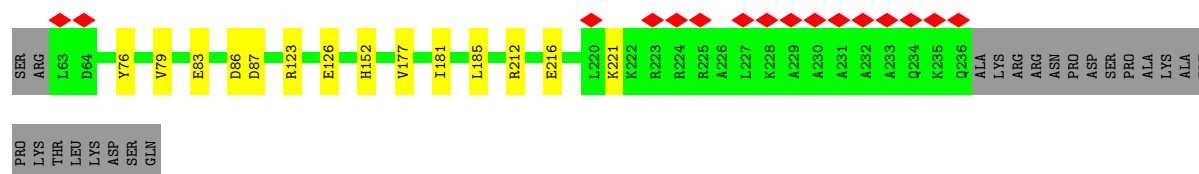
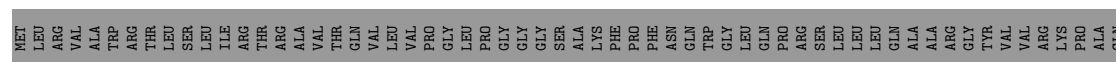
• Molecule 10: 28S ribosomal protein S12, mitochondrial



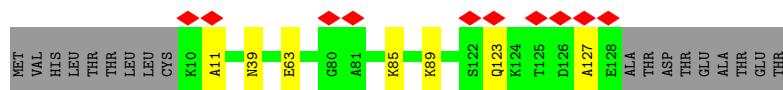
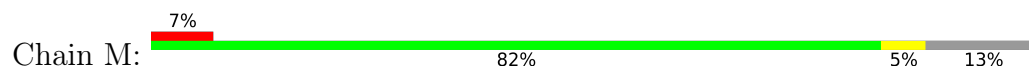
• Molecule 11: 28S ribosomal protein S14, mitochondrial



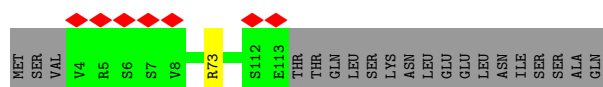
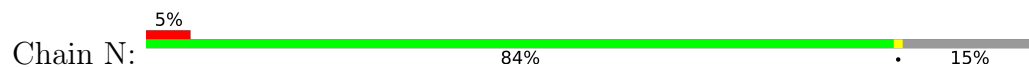
• Molecule 12: 28S ribosomal protein S15, mitochondrial



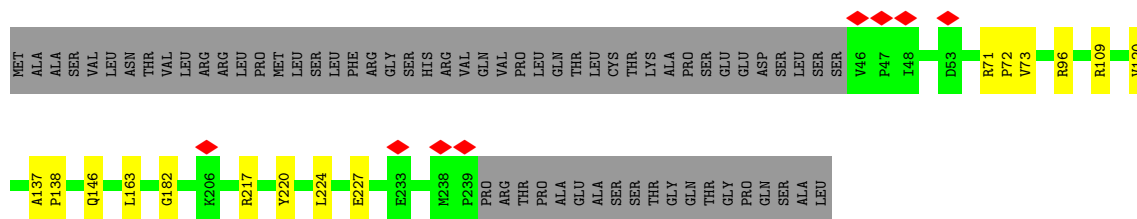
- Molecule 13: 28S ribosomal protein S16, mitochondrial



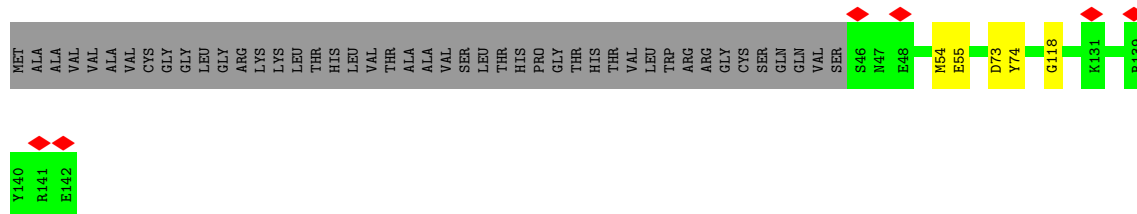
- Molecule 14: 28S ribosomal protein S17, mitochondrial



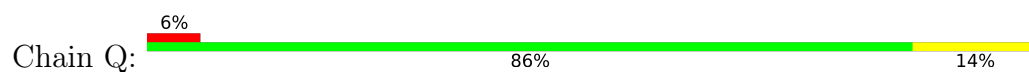
- Molecule 15: 28S ribosomal protein S18b, mitochondrial



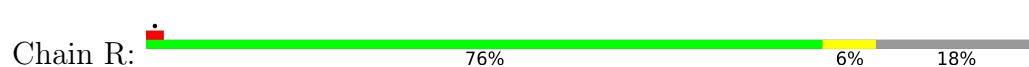
- Molecule 16: 28S ribosomal protein S18c, mitochondrial

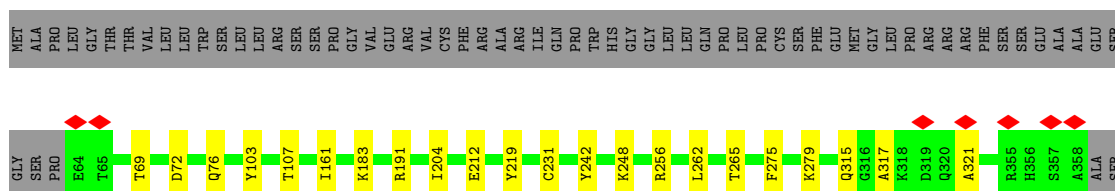


- Molecule 17: 28S ribosomal protein S21, mitochondrial

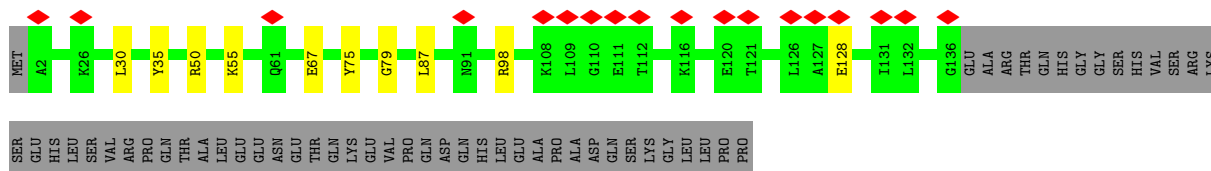


- Molecule 18: 28S ribosomal protein S22, mitochondrial

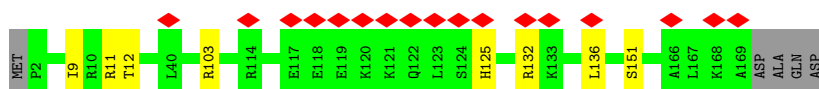




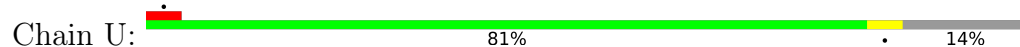
• Molecule 19: 28S ribosomal protein S23, mitochondrial



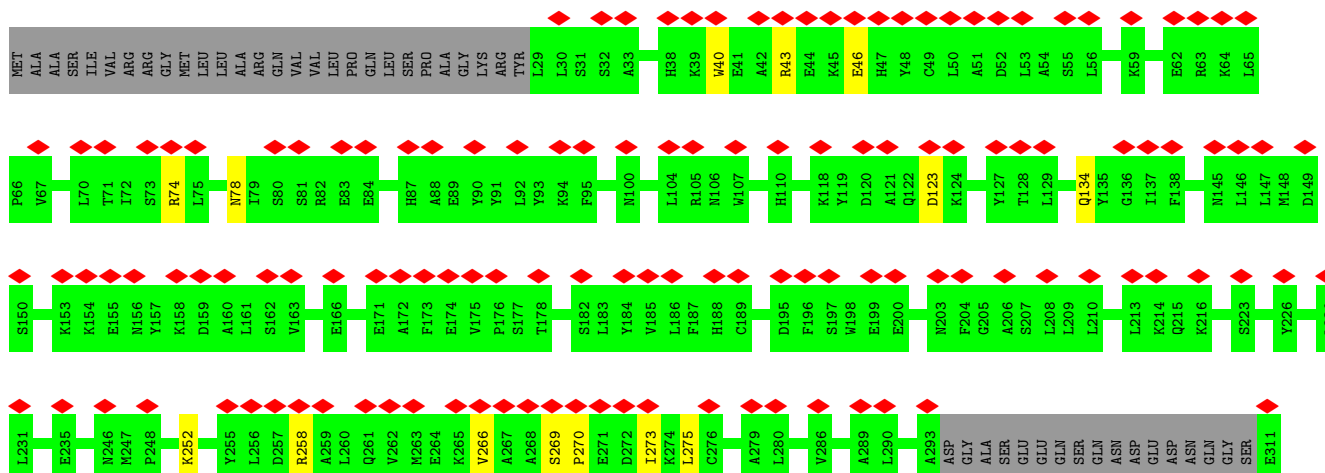
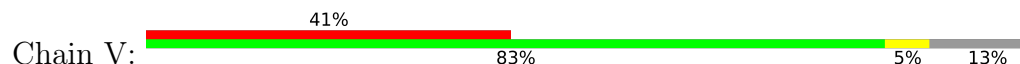
• Molecule 20: 28S ribosomal protein S25, mitochondrial

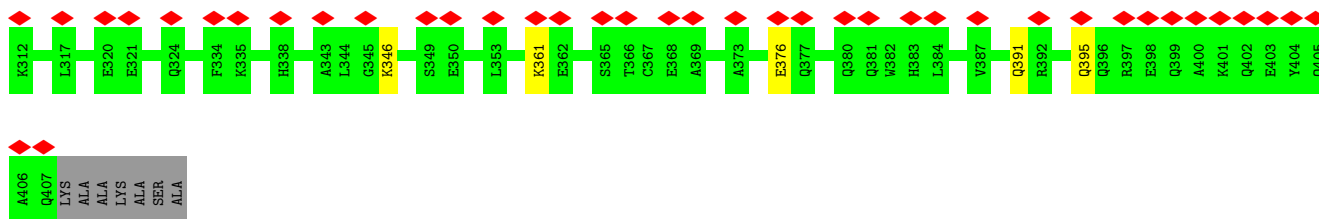


• Molecule 21: 28S ribosomal protein S26, mitochondrial



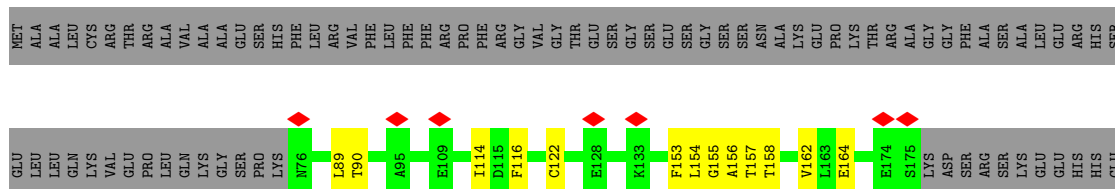
• Molecule 22: 28S ribosomal protein S27, mitochondrial





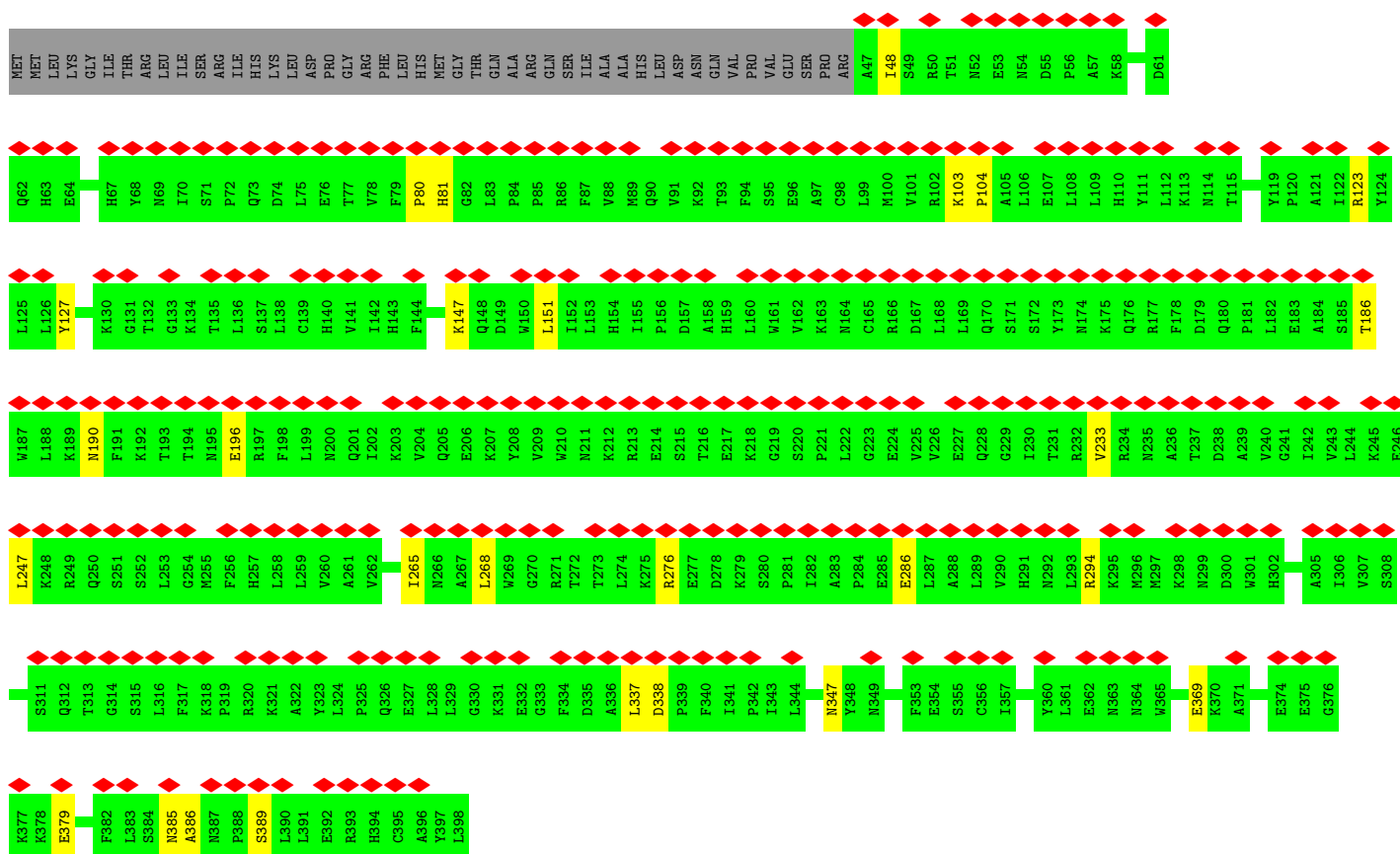
- Molecule 23: 28S ribosomal protein S28, mitochondrial

Chain W: 47% 7% 47%



- Molecule 24: 28S ribosomal protein S29, mitochondrial

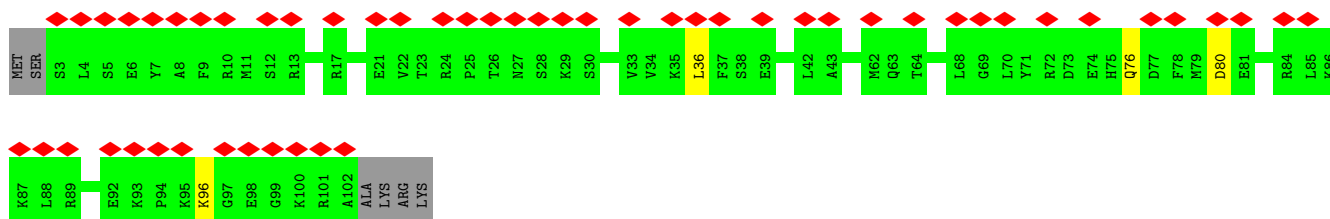
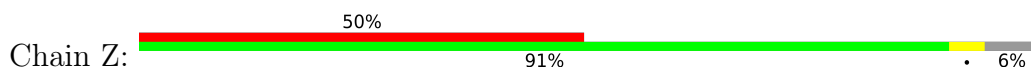
Chain X: 71% 82% 7% 12%



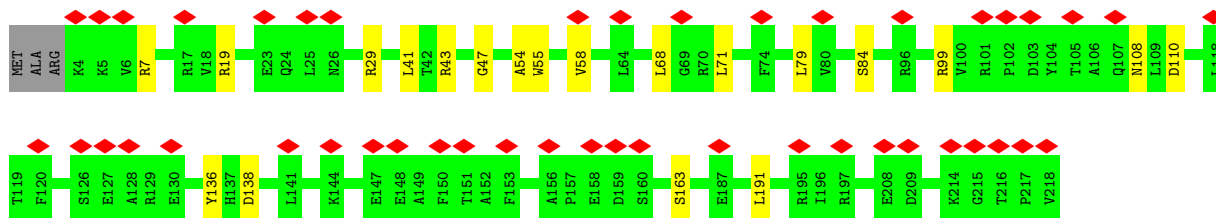
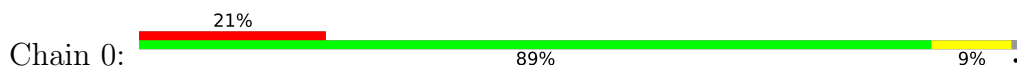
- Molecule 25: 28S ribosomal protein S31, mitochondrial

Chain Y: 26% 36% 62%

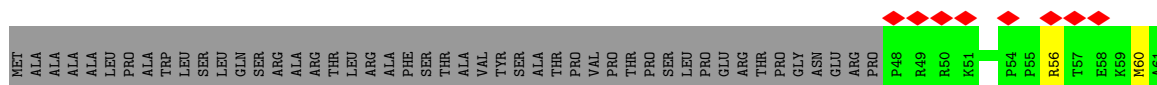
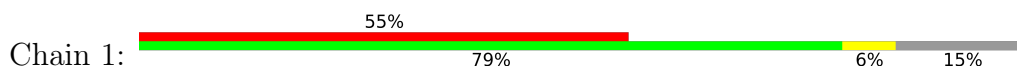
- Molecule 26: 28S ribosomal protein S33, mitochondrial

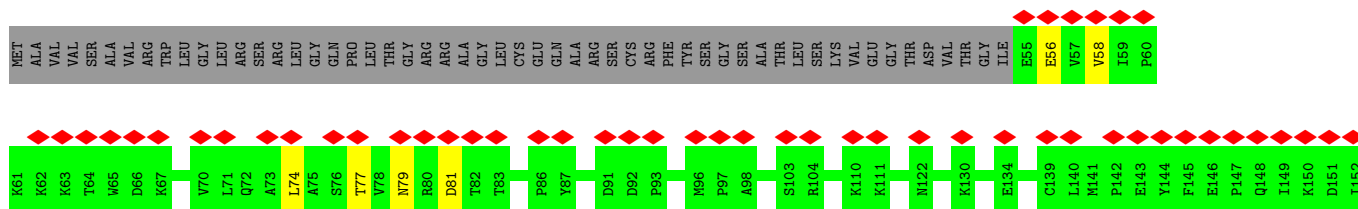


- Molecule 27: 28S ribosomal protein S34, mitochondrial



- Molecule 28: 28S ribosomal protein S35, mitochondrial





I641	C642	E643	G644	L645	T646	Q647	R648	V649	M650	S651	D652	F653	A654	T655	M656	Q657	E658	Q659	K660	E661	A662	L663	S664	M665	L666	THR	ALA	LEU	THR	SER	ASP	SER	SER	SER	ASP	SER	ASP	ASP	THR	THR	THR	GLY	LYS																
I581	L582	F583	L584	R585	A586	G587	R588	T589	Q590	E591	A592	M593	K594	M595	L596	G597	L598	F599	R600	K601	H602	N603	K604	I605	P606	R607	S608	E609	L610	L611	N612	E613	A614	M615	D616	S617	A618	K619	V620	S621	M622	S623	P624	S625	Q626	A627	I628	E629	V630	V631	E632	L633	A634	S635	A636	F637	S638	L639	P640
H521	T522	F523	R524	S525	D526	L527	R528	E529	E530	I531	L532	M533	L534	M535	A536	R537	D538	K539	H540	P541	P542	E543	L544	Q545	V546	A547	F548	A549	D550	C551	A552	A553	D554	I555	K556	S557	A558	Y559	E560	S561	Q562	P563	I564	R565	Q566	T567	A568	Q569	D570	M571	P572	A573	T574	S575	L576	N577	C578	I579	A580
S459	K460	F461	F462	D463	L464	L465	C466	L467	E469	Q470	L471	D472	V473	T474	L475	K476	V477	Y478	E479	D480	L481	L482	P483	S484	A485	Y486	F487	P488	H489	T492	M493	L496	L497	Q498	A499	L500	D501	V502	A503	N504	R505	L506	E507	V508	I509	P510	K511	I512	W513	D515	S516	K517	E518	Y519	G520				
E399	L400	M401	G402	R403	R404	F405	F406	P407	K408	D409	P410	D411	D412	K413	F415	F416	Q417	S418	A419	M420	S421	I422	C423	S424	S425	L426	R427	D428	L429	E430	L431	A432	Y433	Q434	V435	H436	Q437	L438	K440	T441	G442	D443	M444	W445	L446	F447	T448	G449	P450	D451	Q452	H453	R454	F456	Y457	Y458			
I338	L339	K340	C341	L342	R343	R344	F345	F346	V347	F348	A349	H350	S351	L354	Q355	V356	L357	K358	E359	N360	K361	A362	I363	G364	I365	E366	P367	S368	L369	A370	T371	Y372	H373	W374	H375	I376	R377	L378	F379	D380	Q381	P382	G383	D384	P385	L386	K387	R388	S389	S390	F391	I392	I393	Y394	D395	I396	N397	N398	
L276	N277	L278	Y279	T280	E281	L282	L283	N284	N285	R286	L287	H288	A289	D290	Y291	T292	T293	F294	N295	A296	A300	T301	V302	C303	A304	I305	N306	E307	K308	F309	E310	E311	K312	W313	S314	K315	I316	L317	E318	L319	L320	R321	H322	M323	V324	A325	Q326	K327	V328	K329	P330	N331	L332	Q333	T334	F335	N336	T337	
GLY	GLN	SER	GLU	ALA	LEU	GLU	GLU	ASP	ASN	ASP	GLU	THR	SER	ARG	ARG	LYS	ALA	ALA	GLY	HIS	Q233	F234	G235	V236	T237	W238	R239	A240	L241	N242	N243	A244	E245	R246	I247	F248	S249	L250	M251	P252	E253	K254	N255	E256	H257	S258	Y259	C260	T261	R264	K268	H269	R270	A271	Y272	E273	Q274	A275	
S153	E154	A155	A156	L157	K158	E159	R160	A161	E162	L163	R164	K165	V166	K167	A168	S169	V170	D171	M172	F173	D174	Q175	L176	L177	Q178	A179	G180	T181	T182	V183	S184	L185	E186	T187	T188	N189	S190	L191	L192	D193	L194	C196	Y197	Y198	G199	D200	Q201	E202	P203	S204	T205	D206	Y207	H208	PHE	GLN	GLN	THR	

● Molecule 32: Translation initiation factor IF-3, mitochondrial



MET	ALA	ALA	LEU	PHE	LEU	LYS	ARG	LEU	THR	LEU	GLN	THR	THR	VAL	LYS	SER	GLU	ASN	SER	CYS	ILE	ARG	CYS	PHE	GLY	LYS	HIS	ILE	LEU	GLN	LYS	THR	ALA	ALA	PRO	L89	F90	D91	E92	K93	Q94	N95	D96	L97	G98	N99	M100	H101	E102	A103	M104	V105	P106	S107	R107	L108	M109	D110	E111	R112	L113	L114	R115	L116	V117	Q118	R119	I179	Q180	R241
T121	S122	T123	E124	P125	A126	E127	Y128	Y129	L130	M131	T132	G133	L134	Q135	I136	E139	R140	Q141	S83	R142	L143	R144	E145	M146	E147	K148	A149	M150	P151	K152	T153	G154	P155	T156	L157	R158	K159	I220	E160	L161	I162	L163	S164	S165	M166	I167	G168	Q169	H170	D171	L172	D173	T174	K175	K177	Q178	C238	V239	L240											
W182	I183	K184	K185	K186	H187	L188	V189	Q190	I191	T192	I193	K194	K195	G196	K197	N198	V199	D200	V201	S202	E203	N204	E205	M206	E207	E208	I209	F210	H211	Q212	I213	L214	Q215	T216	M217	P218	G219	I220	A221	F223	S224	S225	R226	P227	Q228	A229	V230	Q231	G232	K234	A235	L236	M237	C238	V239	L240														

A242	L243	S244	K245	N246	E247	E248	K249	A250	Y251	K252	E253	T254	Q255	E256	T257	Q258	E259	R260	D261	T262	LEU	ASN	LYS	ASP	HIS	GLY	ASN	ASP	LYS	GLU	SER	ASN	VAL	LEU	HIS	GLN	GLY	LEU	GLU	VAL	LEU	PHE	GLN
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73449	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.134	Depositor
Minimum map value	-0.377	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	517.12, 517.12, 517.12	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SPM, 5MC, AYA, SRY, B8T, 5MU, MA6, FES, ATP, ZN, GNP, NAD, K, 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	A	0.31	0/22562	0.36	0/35124
2	B	0.32	0/1871	0.38	0/2531
3	C	0.40	0/1113	0.41	0/1505
4	D	0.31	0/2758	0.37	0/3690
5	E	0.27	0/989	0.36	0/1335
6	F	0.26	0/1767	0.35	0/2373
7	G	0.29	0/2714	0.36	0/3635
8	H	0.36	0/1178	0.37	0/1598
9	I	0.26	0/1039	0.35	0/1400
10	J	0.35	0/855	0.38	0/1148
11	K	0.40	0/880	0.41	0/1182
12	L	0.30	0/1477	0.36	0/1974
13	M	0.34	0/963	0.41	0/1295
14	N	0.32	0/886	0.33	0/1199
15	O	0.31	0/1655	0.36	0/2254
16	P	0.32	0/798	0.36	0/1070
17	Q	0.33	0/748	0.44	0/994
18	R	0.26	0/2456	0.33	0/3317
19	S	0.26	0/1138	0.33	0/1533
20	T	0.32	0/1402	0.38	0/1883
21	U	0.24	0/1510	0.37	0/2025
22	V	0.19	0/3030	0.32	0/4093
23	W	0.27	0/801	0.33	0/1079
24	X	0.26	0/2921	0.35	0/3954
25	Y	0.27	0/1280	0.32	0/1725
26	Z	0.30	0/857	0.36	0/1141
27	0	0.26	0/1834	0.39	0/2484
28	1	0.30	0/2285	0.35	0/3090
29	2	0.29	0/941	0.42	0/1257
30	3	0.30	0/636	0.45	0/839
31	4	0.21	0/4877	0.34	0/6598
32	8	0.16	0/1560	0.35	0/2089

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.29	0/71781	0.36	0/101414

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
29	2	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	2	37	ARG	Sidechain

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	A	20282	0	10297	101	0
2	B	1828	0	1815	10	0
3	C	1083	0	1088	18	0
4	D	2707	0	2771	48	0
5	E	972	0	1000	32	0
6	F	1725	0	1769	13	0
7	G	2657	0	2646	59	0
8	H	1152	0	1183	10	0
9	I	1019	0	1059	5	0
10	J	839	0	887	7	0
11	K	862	0	885	7	0
12	L	1453	0	1540	9	0
13	M	942	0	965	5	0
14	N	868	0	928	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	1599	0	1565	9	0
16	P	781	0	806	3	0
17	Q	744	0	758	31	0
18	R	2409	0	2428	16	0
19	S	1111	0	1115	9	0
20	T	1371	0	1393	7	0
21	U	1488	0	1499	6	0
22	V	2969	0	2961	13	0
23	W	789	0	802	42	0
24	X	2849	0	2843	19	0
25	Y	1246	0	1197	5	0
26	Z	839	0	858	3	0
27	0	1787	0	1796	13	0
28	1	2238	0	2269	15	0
29	2	935	0	968	112	0
30	3	625	0	699	2	0
31	4	4768	0	4766	27	0
32	8	1543	0	1587	17	0
33	A	44	0	26	1	0
34	A	14	0	26	0	0
35	A	40	0	39	0	0
36	3	1	0	0	0	0
36	A	56	0	0	0	0
36	B	1	0	0	0	0
36	X	1	0	0	0	0
37	A	17	0	0	1	0
38	O	1	0	0	0	0
39	P	4	0	0	0	0
39	T	4	0	0	0	0
40	X	31	0	12	0	0
41	X	32	0	13	0	0
All	All	68726	0	59259	460	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 4.

The worst 5 of 460 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)
17:Q:75:LEU:O	29:2:107:LEU:HD21	1.10	1.28
5:E:117:LEU:O	29:2:12:ARG:NH1	1.66	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:207:ASP:OD1	7:G:59:LYS:NZ	1.70	1.21
5:E:117:LEU:HD22	29:2:10:LEU:HD12	1.24	1.19
1:A:1292:A:OP1	29:2:106:LYS:NZ	1.80	1.15

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	
2	B	223/296 (75%)	212 (95%)	11 (5%)	0	100	100
3	C	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
4	D	336/430 (78%)	324 (96%)	12 (4%)	0	100	100
5	E	120/125 (96%)	116 (97%)	4 (3%)	0	100	100
6	F	206/242 (85%)	202 (98%)	4 (2%)	0	100	100
7	G	315/396 (80%)	303 (96%)	12 (4%)	0	100	100
8	H	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	18	45
9	I	135/194 (70%)	126 (93%)	8 (6%)	1 (1%)	18	45
10	J	106/138 (77%)	100 (94%)	6 (6%)	0	100	100
11	K	99/128 (77%)	99 (100%)	0	0	100	100
12	L	172/257 (67%)	168 (98%)	4 (2%)	0	100	100
13	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
14	N	108/130 (83%)	101 (94%)	7 (6%)	0	100	100
15	O	192/258 (74%)	184 (96%)	8 (4%)	0	100	100
16	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
17	Q	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
18	R	293/360 (81%)	287 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
20	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	U	174/205 (85%)	171 (98%)	3 (2%)	0	100	100
22	V	358/414 (86%)	350 (98%)	8 (2%)	0	100	100
23	W	98/187 (52%)	93 (95%)	5 (5%)	0	100	100
24	X	350/398 (88%)	344 (98%)	6 (2%)	0	100	100
25	Y	147/395 (37%)	145 (99%)	2 (1%)	0	100	100
26	Z	98/106 (92%)	94 (96%)	4 (4%)	0	100	100
27	0	213/218 (98%)	207 (97%)	6 (3%)	0	100	100
28	1	274/323 (85%)	260 (95%)	14 (5%)	0	100	100
29	2	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
30	3	68/199 (34%)	65 (96%)	3 (4%)	0	100	100
31	4	584/689 (85%)	563 (96%)	21 (4%)	0	100	100
32	8	189/285 (66%)	184 (97%)	4 (2%)	1 (0%)	24	52
All	All	5836/7586 (77%)	5659 (97%)	174 (3%)	3 (0%)	49	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	184	ASN
8	H	126	ILE
32	8	218	PRO

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	
2	B	198/249 (80%)	198 (100%)	0	100	100
3	C	115/143 (80%)	115 (100%)	0	100	100
4	D	283/357 (79%)	283 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	104/107 (97%)	104 (100%)	0	100	100
6	F	185/209 (88%)	185 (100%)	0	100	100
7	G	281/342 (82%)	281 (100%)	0	100	100
8	H	130/180 (72%)	130 (100%)	0	100	100
9	I	105/147 (71%)	105 (100%)	0	100	100
10	J	93/118 (79%)	93 (100%)	0	100	100
11	K	91/113 (80%)	91 (100%)	0	100	100
12	L	158/226 (70%)	158 (100%)	0	100	100
13	M	97/113 (86%)	97 (100%)	0	100	100
14	N	96/115 (84%)	96 (100%)	0	100	100
15	O	175/230 (76%)	175 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100
17	Q	78/78 (100%)	78 (100%)	0	100	100
18	R	264/318 (83%)	264 (100%)	0	100	100
19	S	116/164 (71%)	116 (100%)	0	100	100
20	T	153/157 (98%)	153 (100%)	0	100	100
21	U	152/174 (87%)	152 (100%)	0	100	100
22	V	325/364 (89%)	325 (100%)	0	100	100
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	311/351 (89%)	310 (100%)	1 (0%)	86	85
25	Y	137/357 (38%)	137 (100%)	0	100	100
26	Z	90/95 (95%)	90 (100%)	0	100	100
27	0	188/190 (99%)	187 (100%)	1 (0%)	81	82
28	1	254/291 (87%)	253 (100%)	1 (0%)	84	84
29	2	100/100 (100%)	100 (100%)	0	100	100
30	3	65/166 (39%)	65 (100%)	0	100	100
31	4	526/609 (86%)	525 (100%)	1 (0%)	87	87
32	8	172/253 (68%)	171 (99%)	1 (1%)	78	81
All	All	5217/6597 (79%)	5212 (100%)	5 (0%)	87	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	X	81	HIS
27	0	79	LEU
28	1	307	ASN
31	4	577	ASN
32	8	238	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	162	GLN
27	0	145	HIS
18	R	214	ASN
31	4	489	HIS
23	W	106	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	954/955 (99%)	280 (29%)	11 (1%)

5 of 280 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	649	A
1	A	657	G
1	A	676	G
1	A	680	U
1	A	688	A

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1512	A
1	A	1531	C
1	A	1557	A
1	A	1532	C
1	A	1246	U

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

7 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
1	5MC	A	1488	1	18,22,23	1.23	2 (11%)	26,32,35	1.92	8 (30%)
17	AYA	Q	2	17	6,7,8	1.43	1 (16%)	5,8,10	1.19	0
1	MA6	A	1583	1	23,26,27	0.81	0	34,38,41	2.12	9 (26%)
1	5MU	A	1076	1	19,22,23	1.12	3 (15%)	28,32,35	2.14	8 (28%)
1	B8T	A	1486	1	19,22,23	0.88	2 (10%)	26,31,34	0.98	1 (3%)
1	MA6	A	1584	1	23,26,27	0.82	1 (4%)	34,38,41	2.13	9 (26%)
29	AYA	2	2	29	6,7,8	1.37	1 (16%)	5,8,10	1.33	1 (20%)

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
1	5MC	A	1488	1	-	0/7/25/26	0/2/2/2
17	AYA	Q	2	17	-	1/4/6/8	-
1	MA6	A	1583	1	-	0/11/29/30	0/3/3/3
1	5MU	A	1076	1	-	0/7/25/26	0/2/2/2
1	B8T	A	1486	1	-	0/7/27/28	0/2/2/2
1	MA6	A	1584	1	-	1/11/29/30	0/3/3/3
29	AYA	2	2	29	-	0/4/6/8	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	2	AYA	CA-N	-3.05	1.43	1.46
29	2	2	AYA	CA-N	-2.81	1.43	1.46
1	A	1488	5MC	C2-N1	-2.67	1.34	1.40
1	A	1076	5MU	C4-C5	-2.62	1.40	1.44
1	A	1076	5MU	C2-N1	-2.61	1.34	1.38

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1076	5MU	C4-N3-C2	-5.59	120.12	127.35
1	A	1584	MA6	C5-C4-N3	-5.38	119.73	126.75
1	A	1583	MA6	C5-C4-N3	-4.87	120.40	126.75
1	A	1583	MA6	N1-C2-N3	-4.73	121.20	128.60
1	A	1583	MA6	C2-N1-C6	4.67	122.79	111.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	Q	2	AYA	C-CA-N-CT
1	A	1584	MA6	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1488	5MC	1	0
1	A	1583	MA6	3	0
1	A	1584	MA6	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 84 ligands modelled in this entry, 77 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	$\# Z > 2$
39	FES	T	201	13,20	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	SRY	A	1703	-	40,42,42	0.78	2 (5%)	49,63,63	1.32	6 (12%)
41	GNP	X	403	-	33,34,34	1.28	5 (15%)	46,54,54	0.95	1 (2%)
34	SPM	A	1702	-	13,13,13	0.15	0	12,12,12	1.15	0
39	FES	P	201	16,5	0,4,4	-	-	-	-	-
33	NAD	A	1701	36	45,48,48	0.94	2 (4%)	63,73,73	1.62	9 (14%)
40	ATP	X	402	36	29,33,33	1.28	4 (13%)	44,52,52	1.91	11 (25%)

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	FES	T	201	13,20	-	-	0/1/1/1
35	SRY	A	1703	-	-	1/20/87/87	0/3/3/3
41	GNP	X	403	-	-	5/18/38/38	0/3/3/3
34	SPM	A	1702	-	-	0/11/11/11	-
39	FES	P	201	16,5	-	-	0/1/1/1
33	NAD	A	1701	36	-	1/30/62/62	0/5/5/5
40	ATP	X	402	36	-	0/22/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	403	GNP	PB-O3A	4.26	1.64	1.59
40	X	402	ATP	C5-C4	4.13	1.46	1.39
41	X	403	GNP	PB-O1B	3.04	1.51	1.46
35	A	1703	SRY	CD1-N31	2.93	1.38	1.33
41	X	403	GNP	PG-N3B	2.92	1.71	1.63

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	X	402	ATP	C5-C4-N3	-5.99	118.94	126.75
33	A	1701	NAD	C5A-C4A-N3A	-5.84	119.13	126.75
40	X	402	ATP	N3-C4-N9	4.72	134.86	127.08
35	A	1703	SRY	C12-O42-C42	-4.58	101.17	108.38
33	A	1701	NAD	N3A-C4A-N9A	4.30	134.18	127.08

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

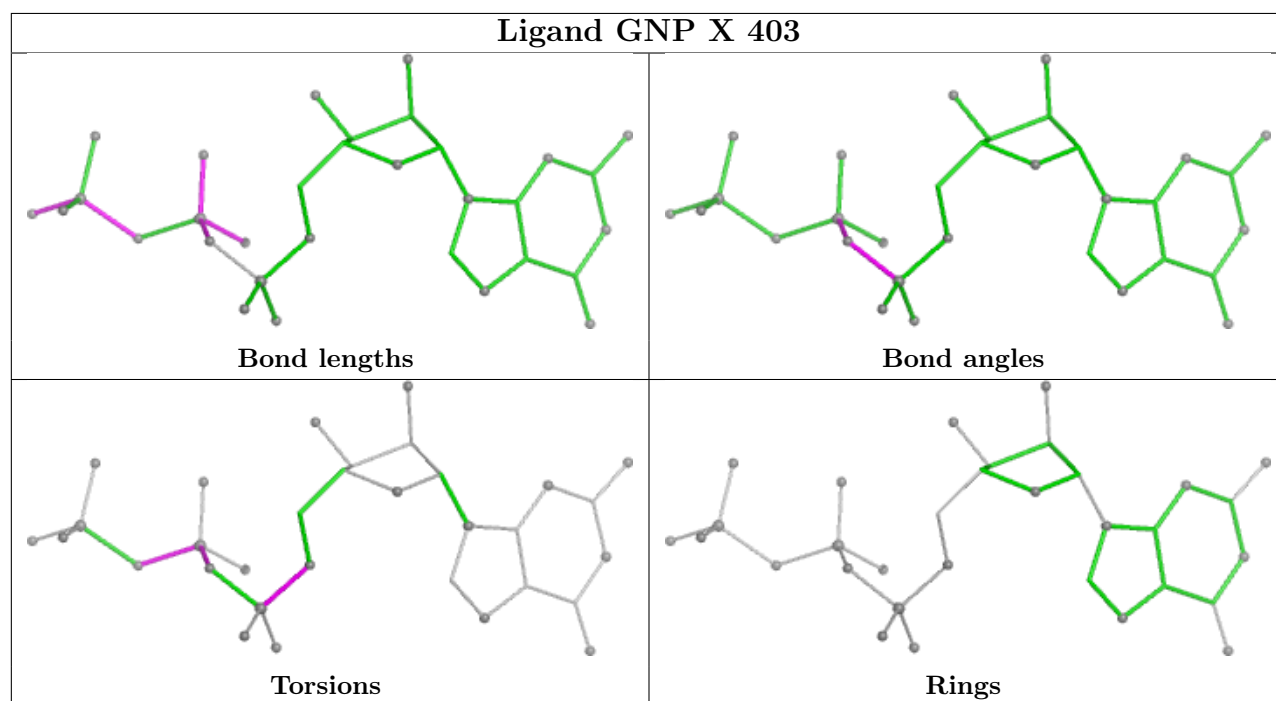
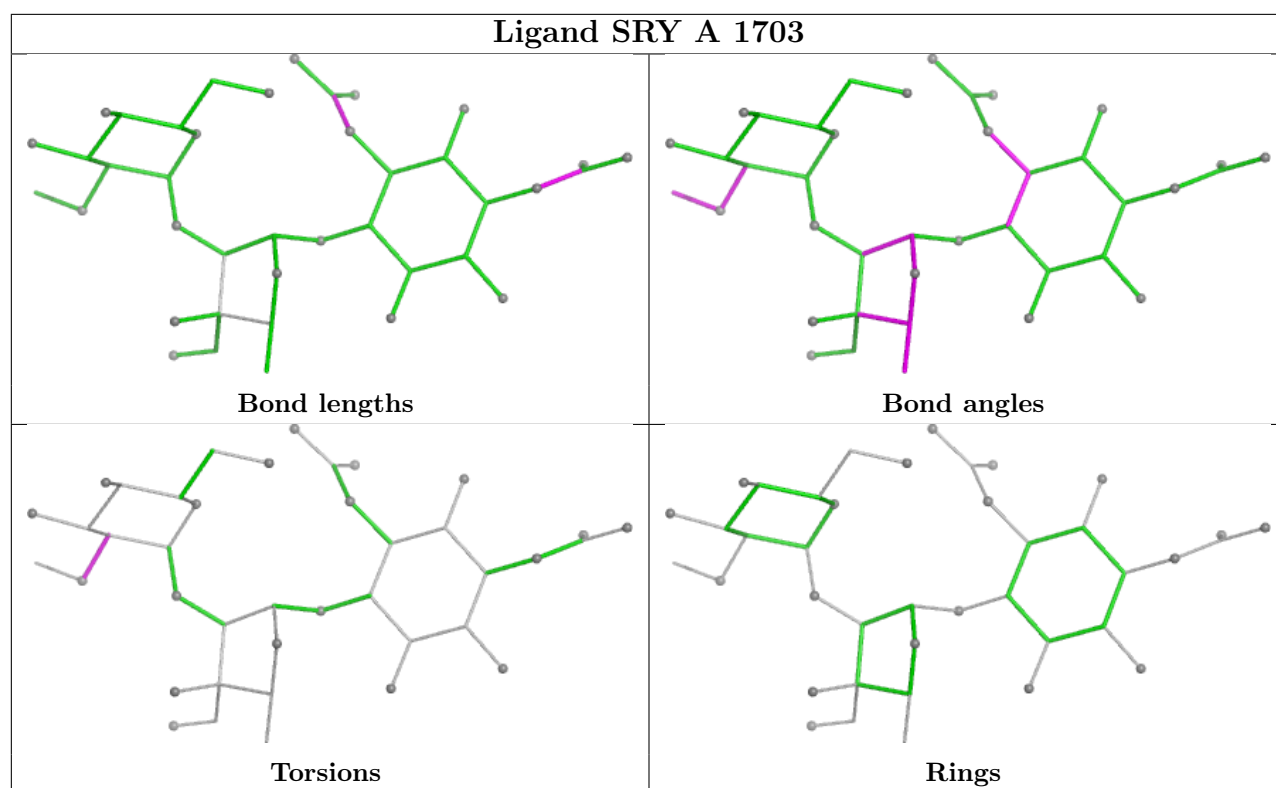
Mol	Chain	Res	Type	Atoms
41	X	403	GNP	PG-N3B-PB-O3A
41	X	403	GNP	PA-O3A-PB-O1B
41	X	403	GNP	PA-O3A-PB-O2B
41	X	403	GNP	PG-N3B-PB-O1B
35	A	1703	SRY	C13-C23-N23-CI3

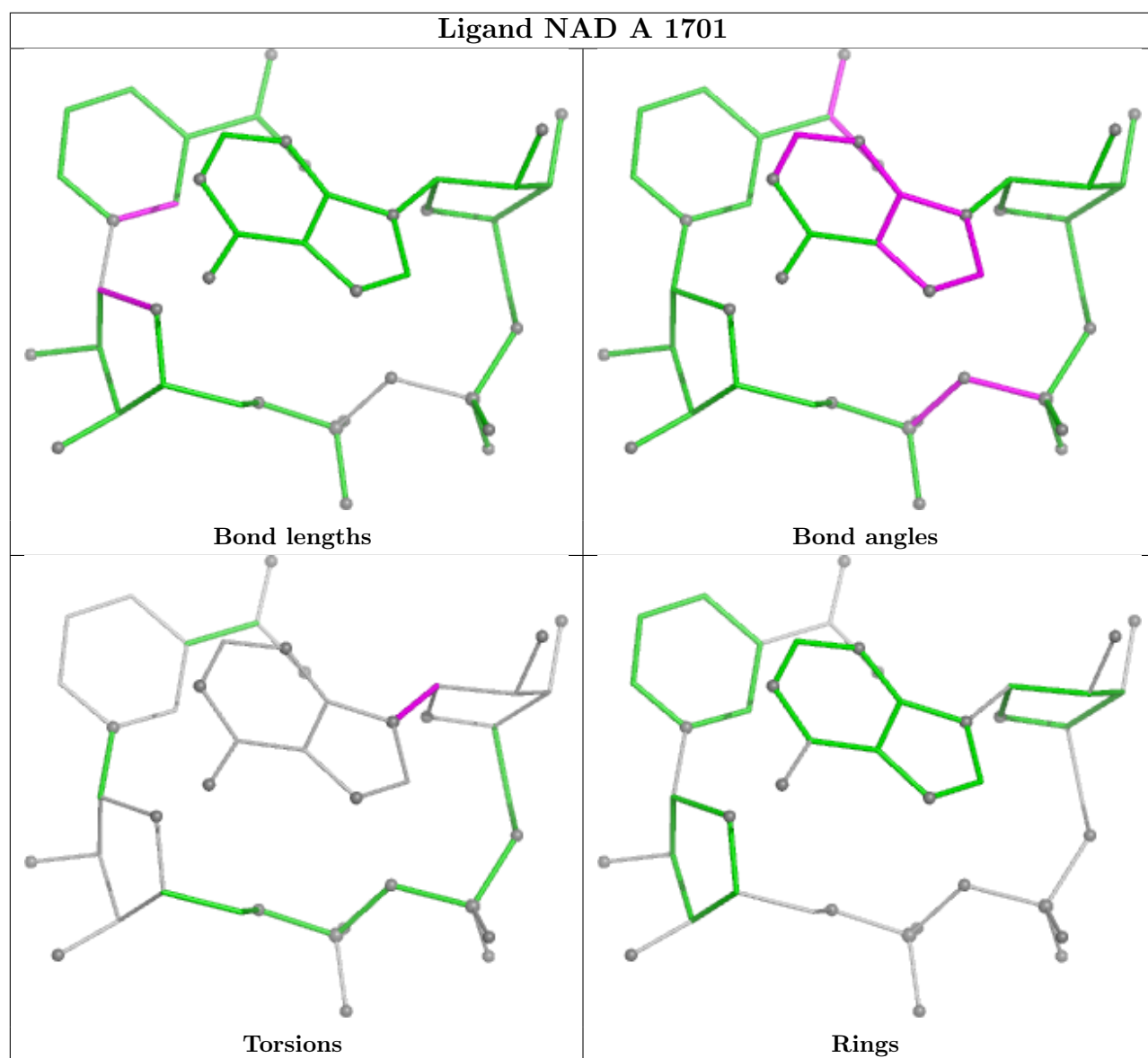
There are no ring outliers.

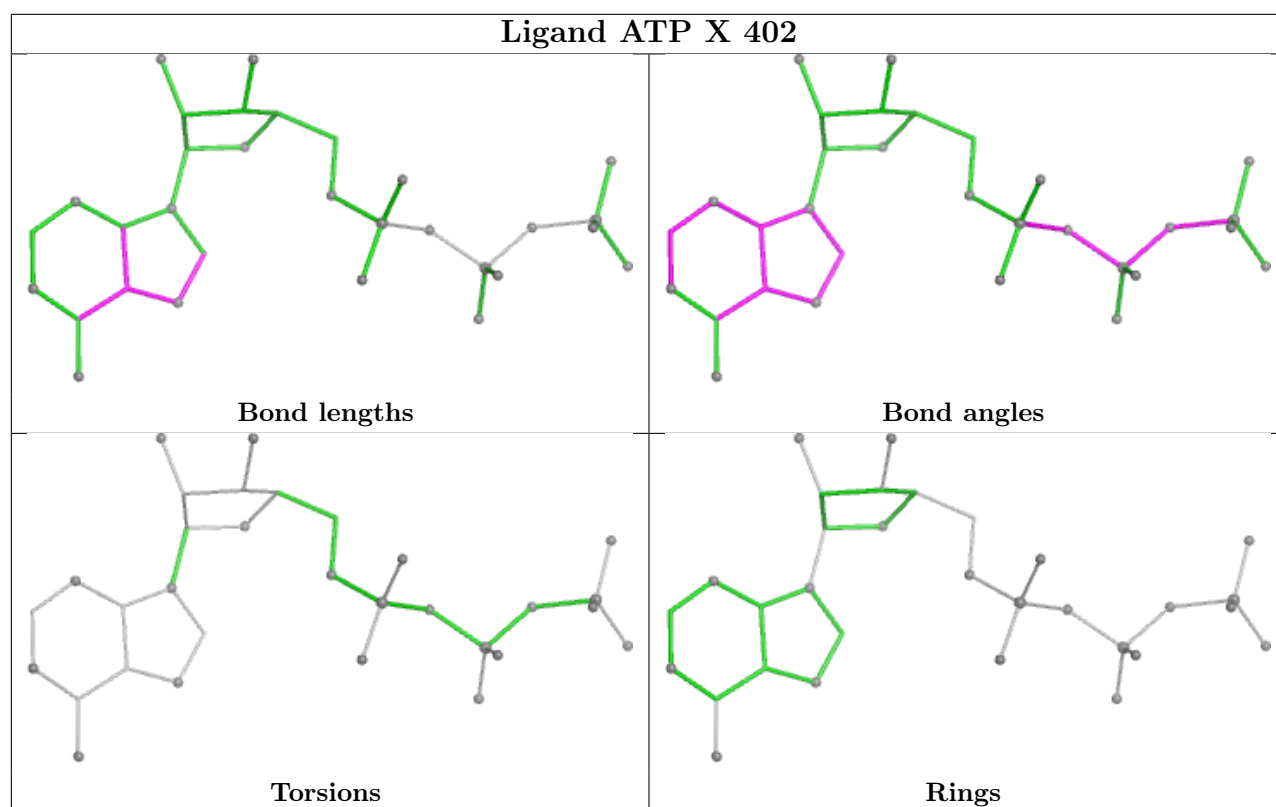
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	1701	NAD	1	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

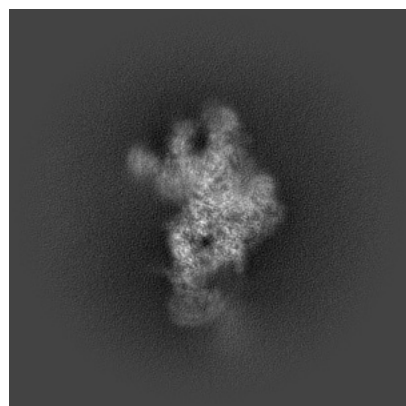
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18440. These allow visual inspection of the internal detail of the map and identification of artifacts.

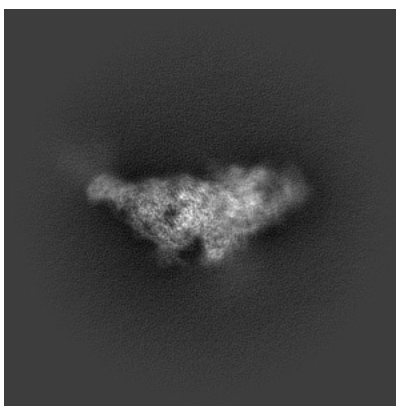
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

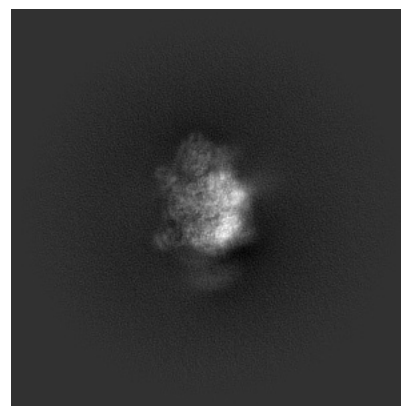
6.1.1 Primary map



X

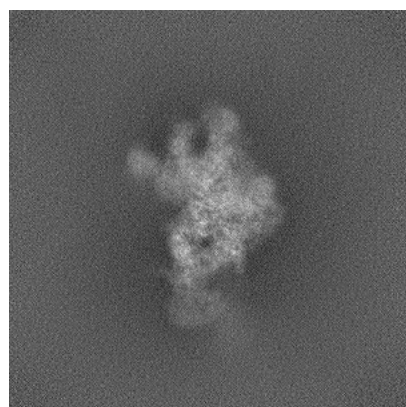


Y

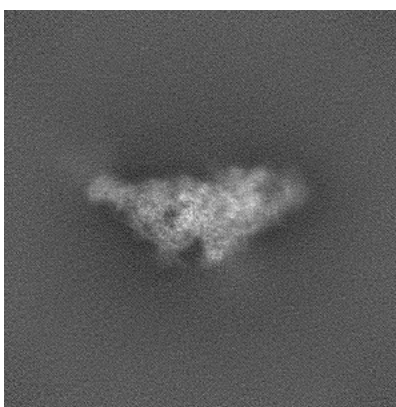


Z

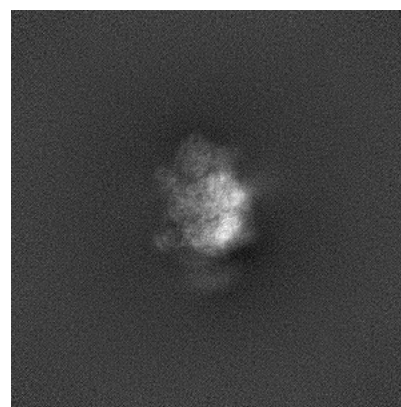
6.1.2 Raw map



X



Y

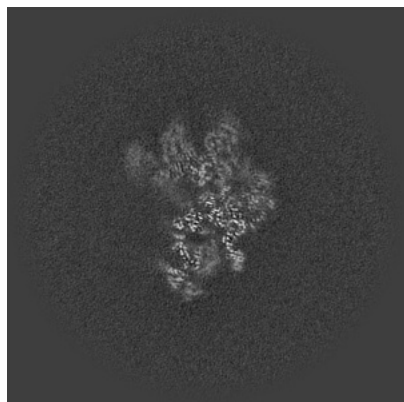


Z

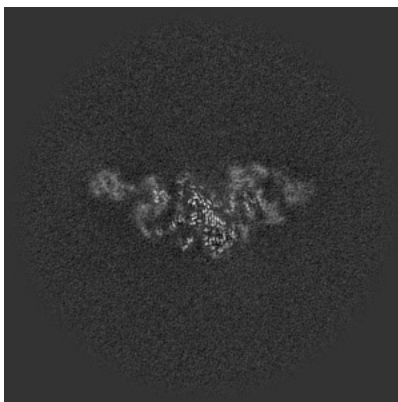
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

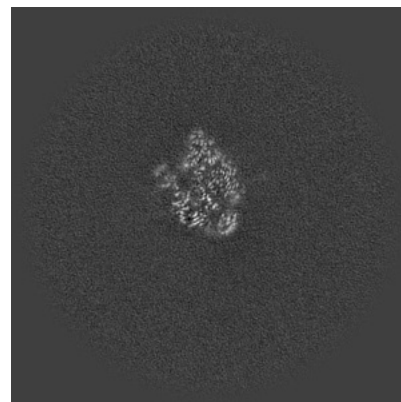
6.2.1 Primary map



X Index: 256

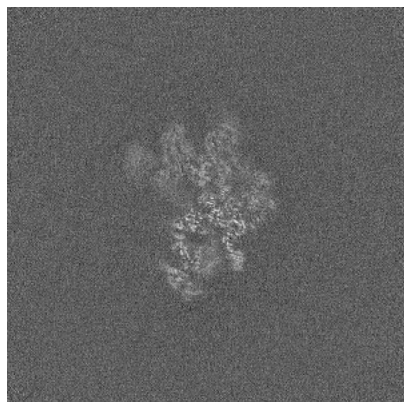


Y Index: 256

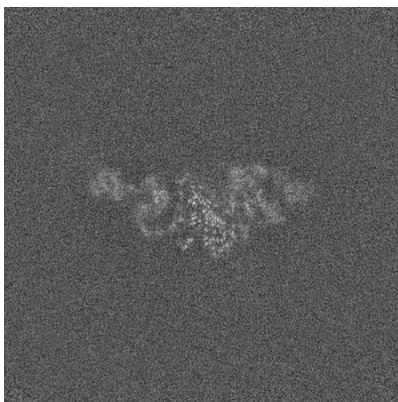


Z Index: 256

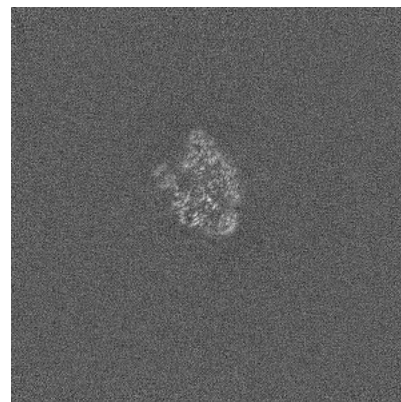
6.2.2 Raw map



X Index: 256



Y Index: 256

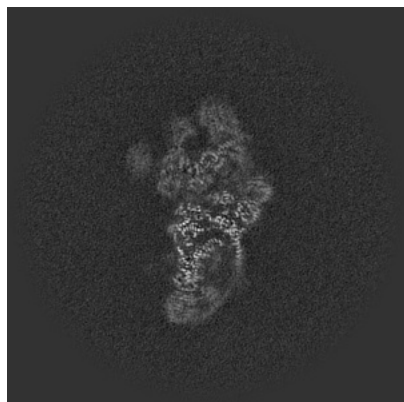


Z Index: 256

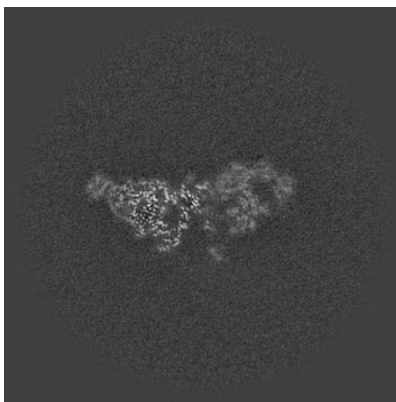
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

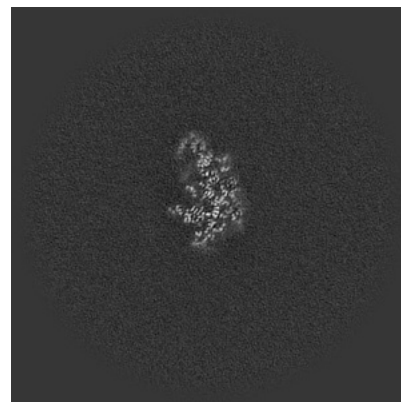
6.3.1 Primary map



X Index: 271

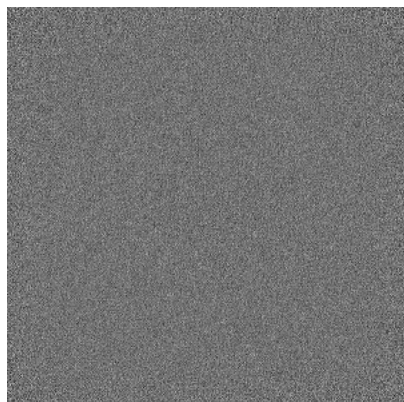


Y Index: 230

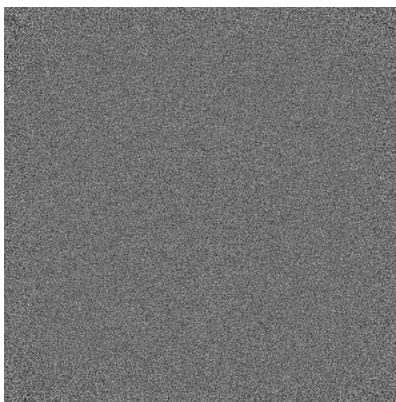


Z Index: 239

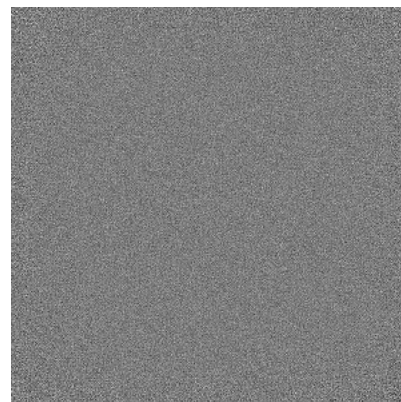
6.3.2 Raw map



X Index: 0



Y Index: 0

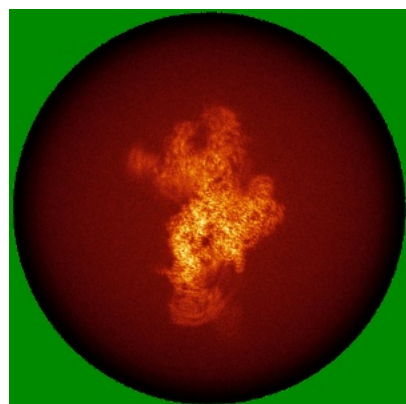


Z Index: 0

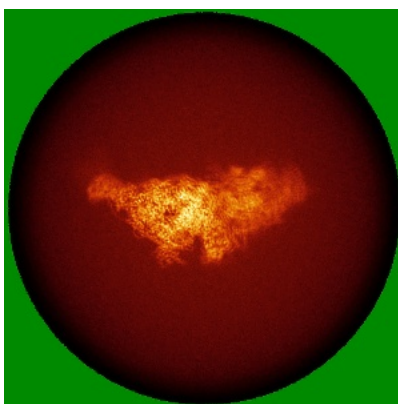
The images above show the largest variance slices of the map in three orthogonal directions.

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

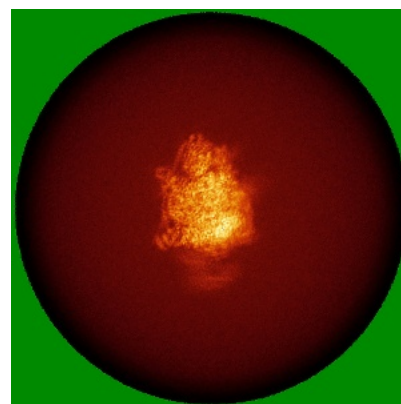
6.4.1 Primary map



X

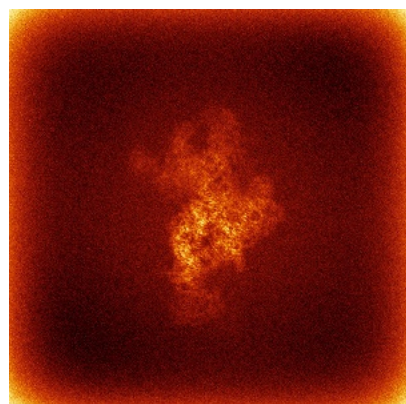


Y

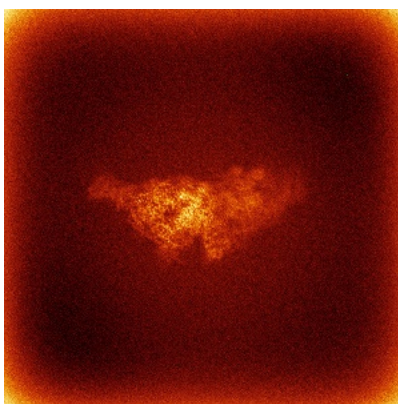


Z

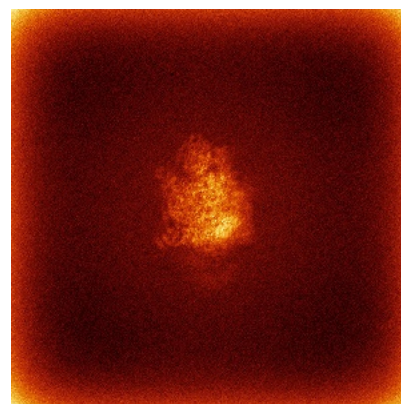
6.4.2 Raw map



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](#)

6.5.1 Primary map



X



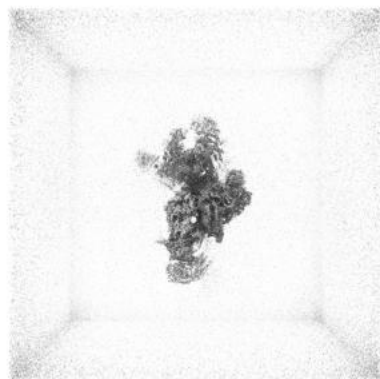
Y



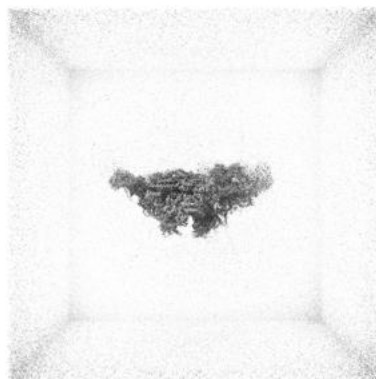
Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

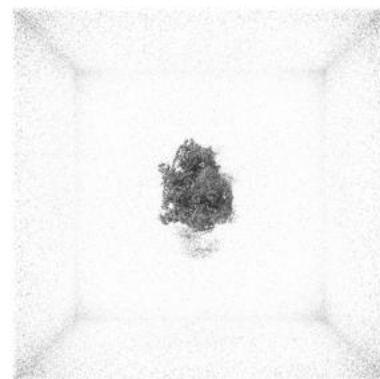
6.5.2 Raw map



X



Y



Z

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

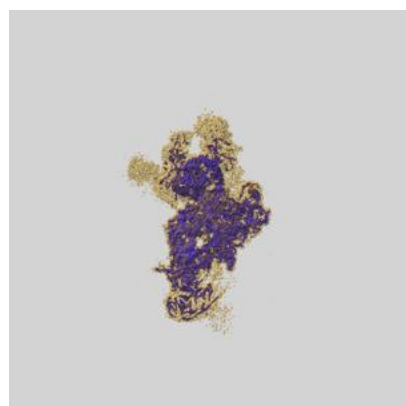
6.6 Mask visualisation [i](#)

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

A mask typically either:

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

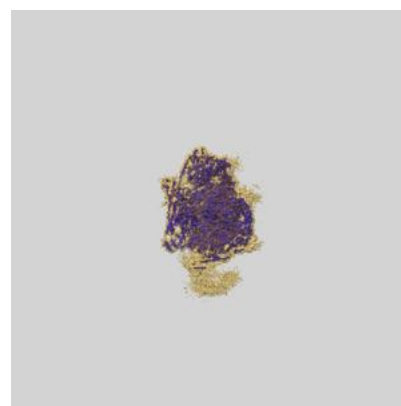
6.6.1 emd_18440_msk_1.map [i](#)



X



Y

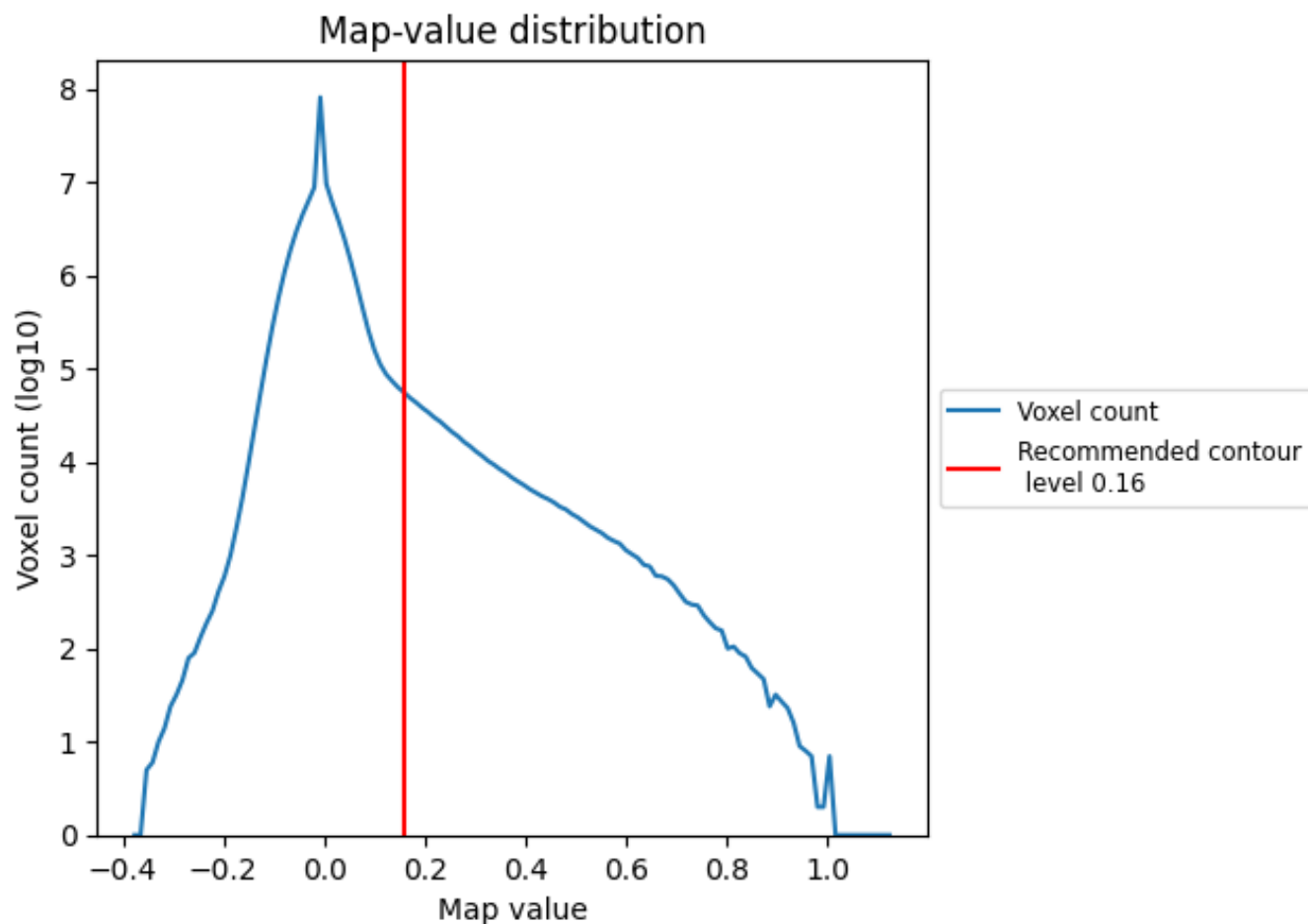


Z

7 Map analysis [i](#)

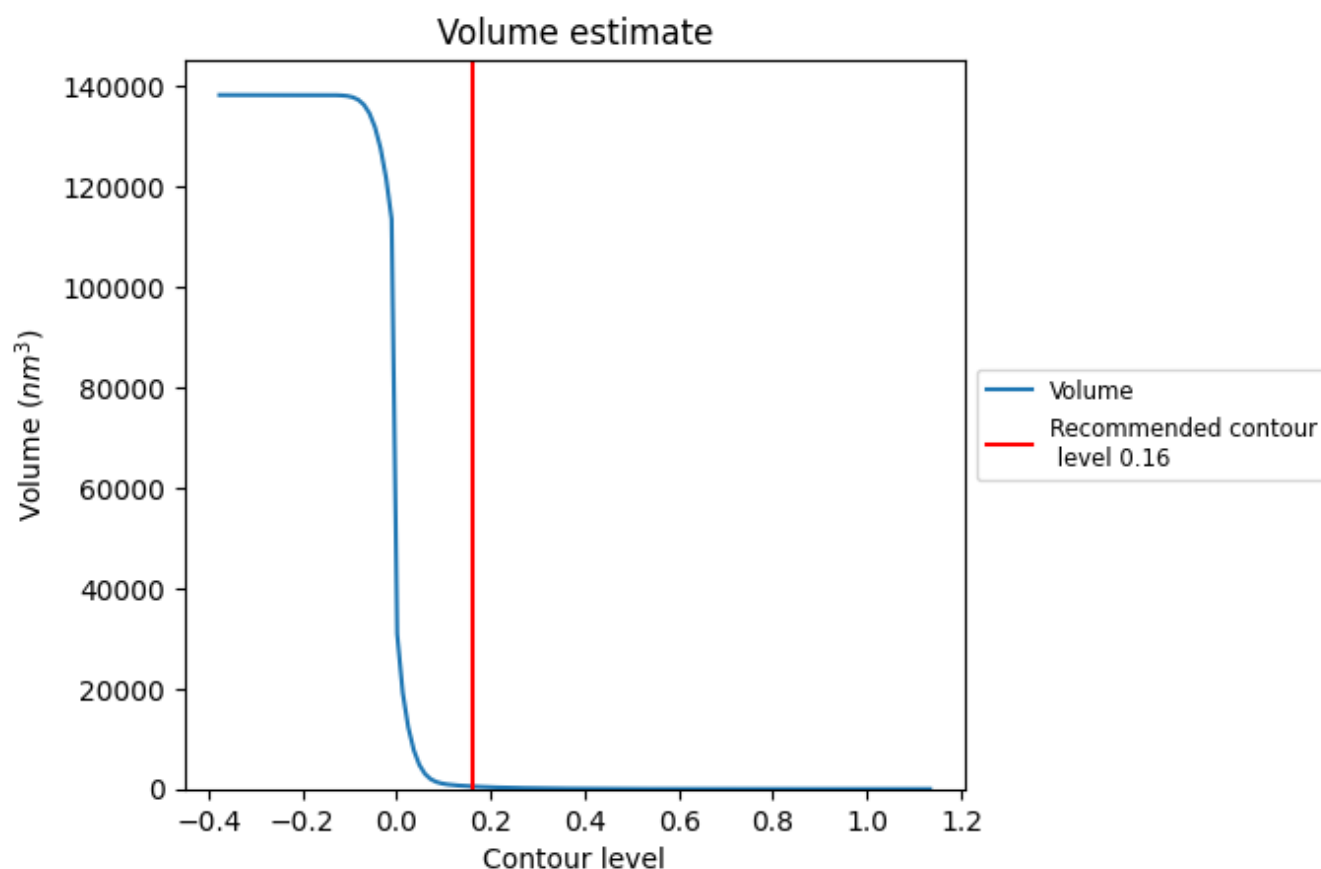
This section contains the results of statistical analysis of the map.

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.

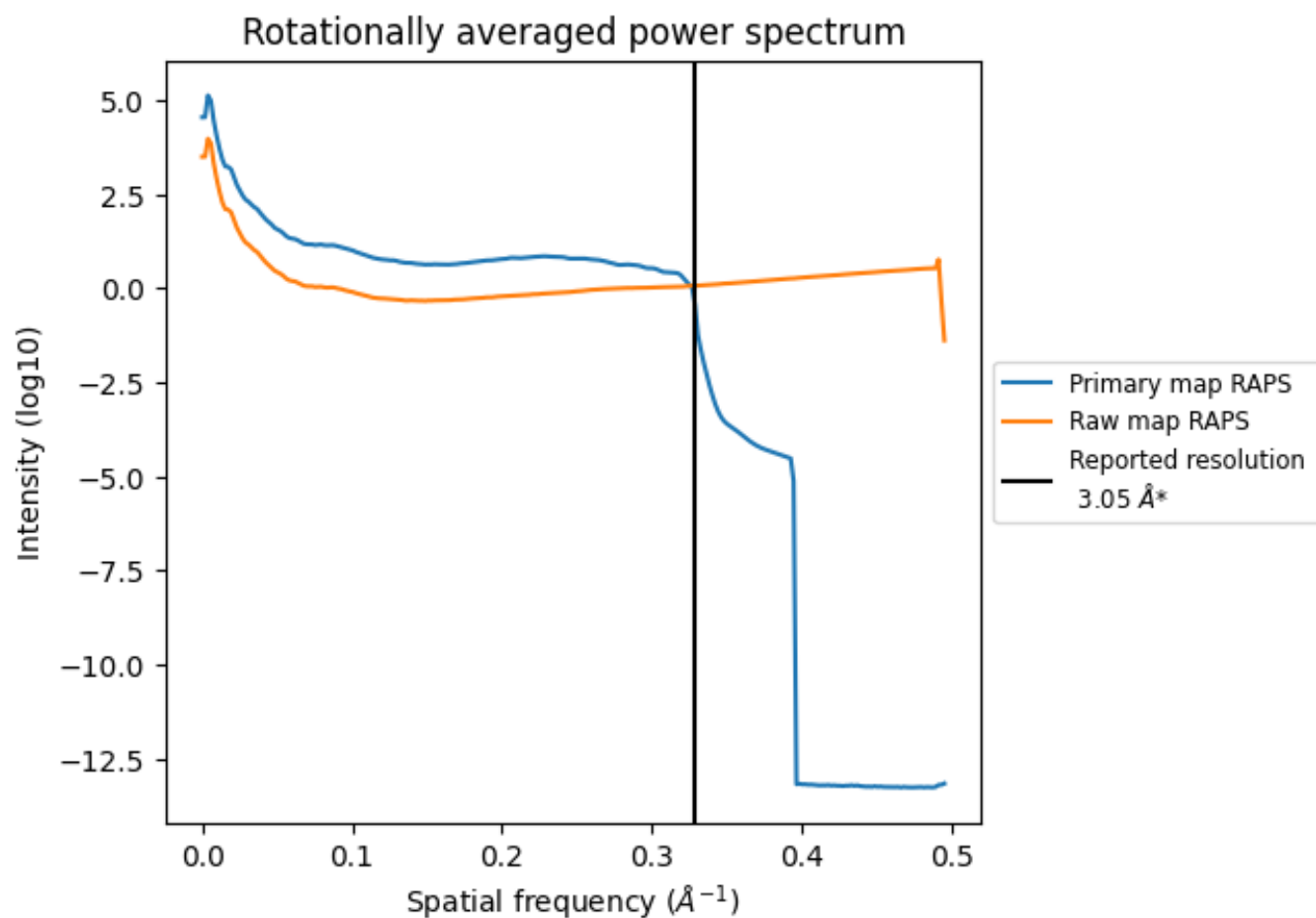
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 516 nm^3 ; this corresponds to an approximate mass of 466 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 ⓘ

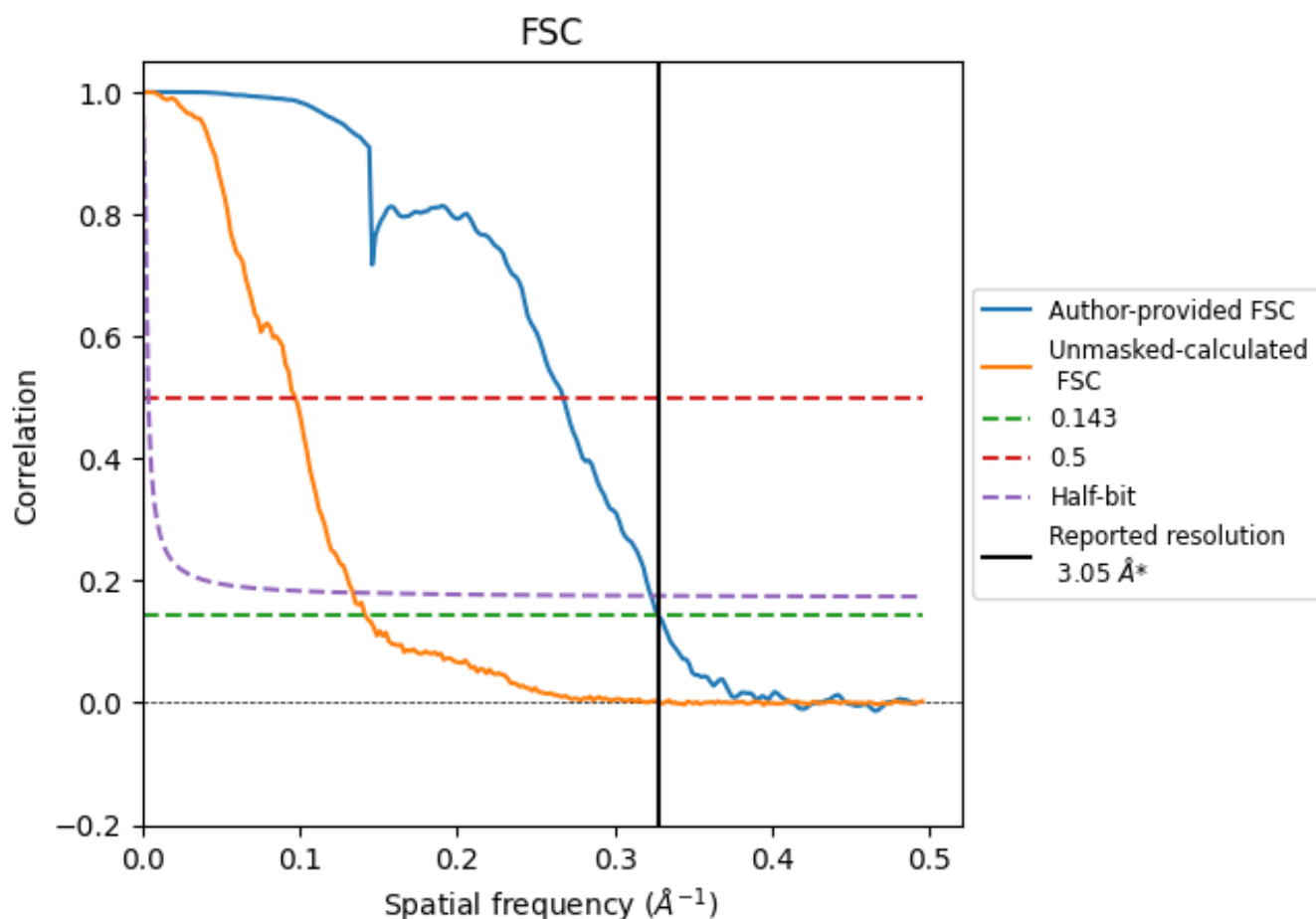


*Reported resolution corresponds to spatial frequency of 0.328 Å⁻¹

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 0.328 Å⁻¹

8.2 Resolution estimates [i](#)

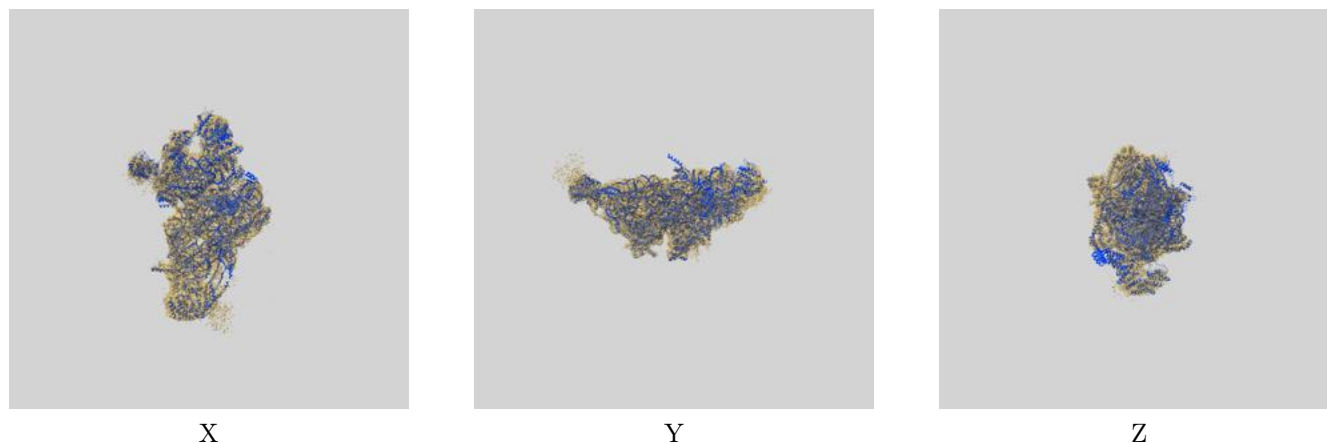
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.05	3.74	3.10
Unmasked-calculated*	7.06	10.31	7.47

*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 7.06 differs from the reported value 3.05 by more than 10 %

9 Map-model fit [i](#)

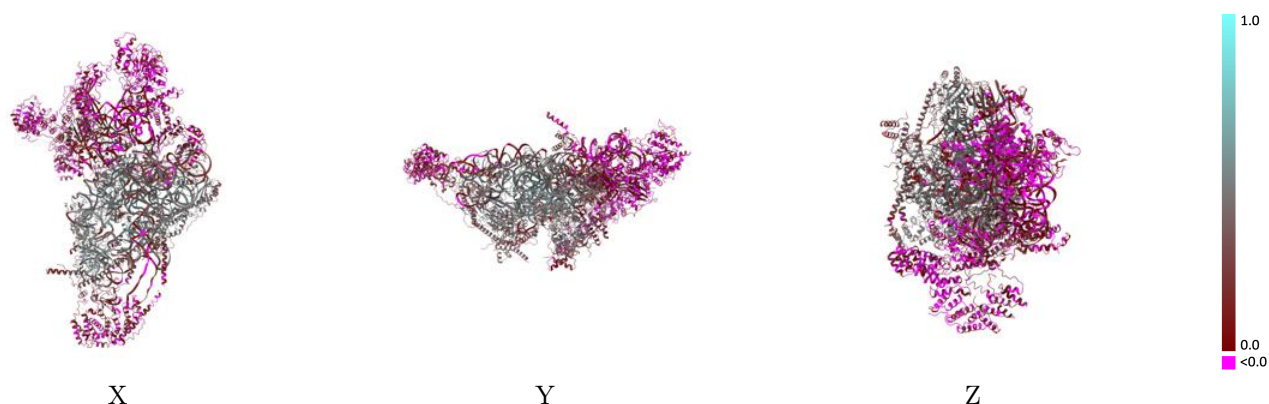
This section contains information regarding the fit between EMDB map EMD-18440 and PDB model 8QRM. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



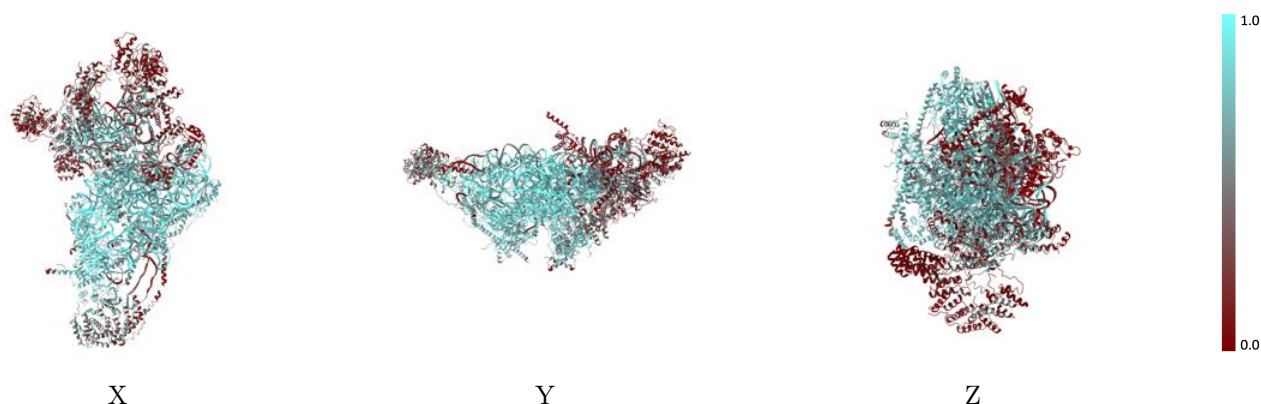
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



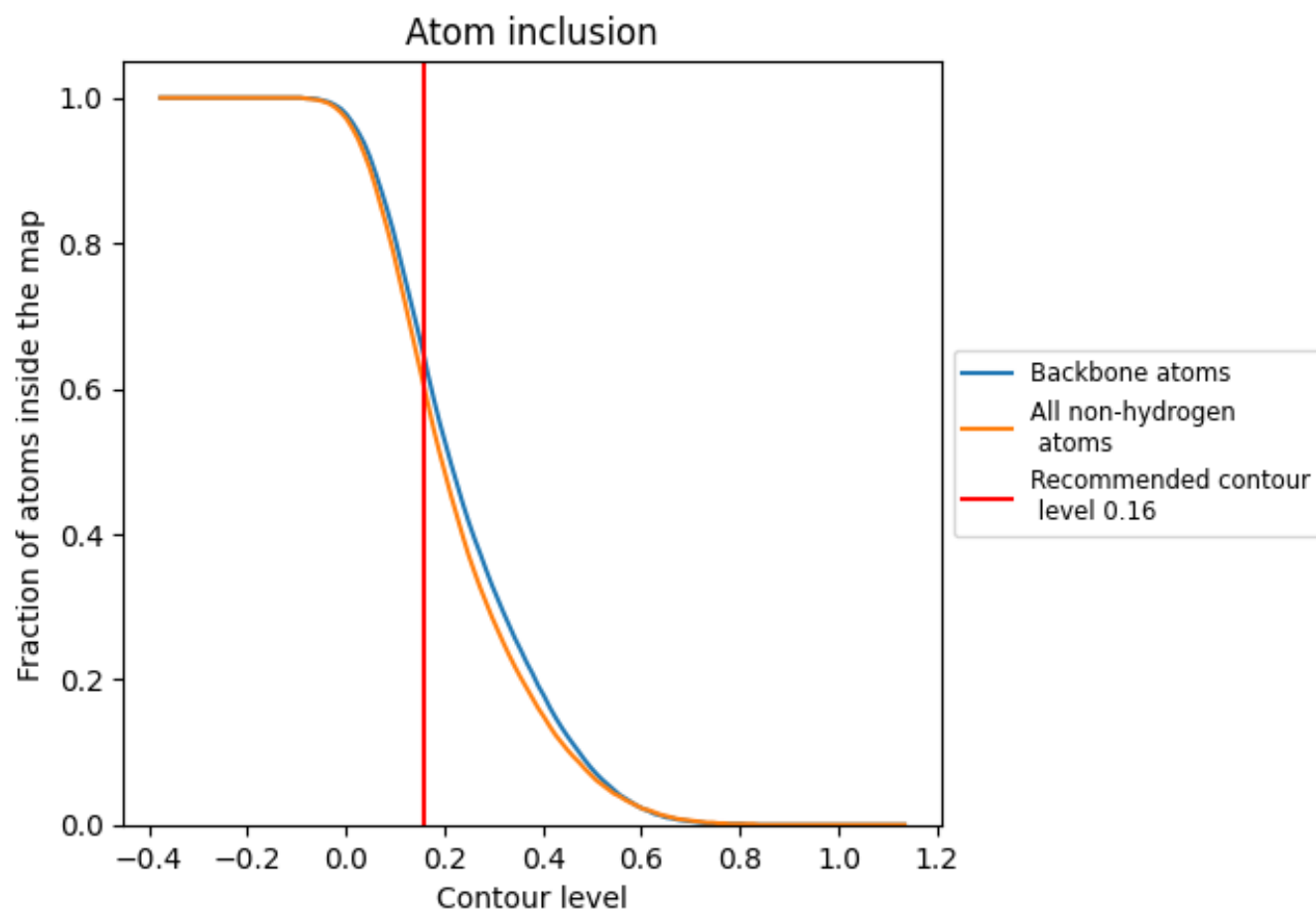
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 60% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5980	 0.2550
0	 0.6400	 0.2420
1	 0.2980	 0.0370
2	 0.1590	 0.1170
3	 0.7650	 0.4080
4	 0.1590	 0.0330
8	 0.0910	 0.1130
A	 0.7900	 0.3350
B	 0.8020	 0.4190
C	 0.6090	 0.2640
D	 0.6620	 0.3710
E	 0.7060	 0.4030
F	 0.2260	 0.0170
G	 0.4190	 0.1170
H	 0.4210	 0.1020
I	 0.6630	 0.3230
J	 0.7710	 0.4120
K	 0.5230	 0.1800
L	 0.7480	 0.3850
M	 0.8300	 0.4260
N	 0.8040	 0.4150
O	 0.8290	 0.4150
P	 0.8090	 0.4160
Q	 0.7260	 0.4030
R	 0.8200	 0.4180
S	 0.7180	 0.3320
T	 0.7510	 0.4130
U	 0.7490	 0.3440
V	 0.4510	 0.0760
W	 0.7210	 0.3620
X	 0.2060	 -0.0040
Y	 0.2840	 0.0600
Z	 0.4040	 0.1140

