Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 12:21 PM EDT

PDB ID	:	8CSQ / pdb_00008csq
EMDB ID	:	EMD-26967
Title	:	Human mitochondrial small subunit assembly intermediate (State B)
Authors	:	Harper, N.J.; Burnside, C.; Klinge, S.
Deposited on	:	2022-05-13
Resolution	:	2.54 Å(reported)
Based on initial models	:	6AAX, 6RW4, 2C2N

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 (i) 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 (i)) were used in the production of this report:

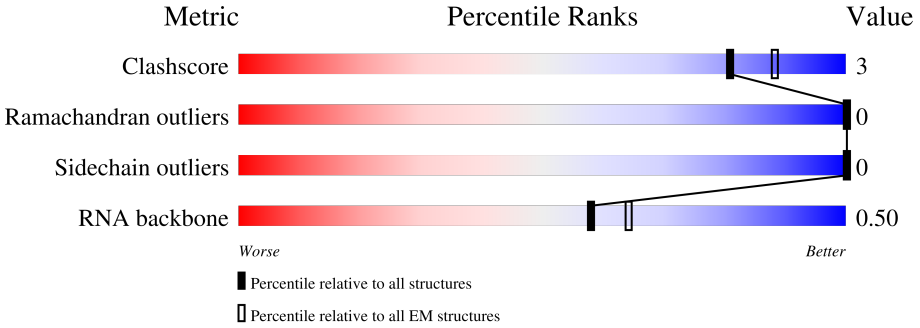
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

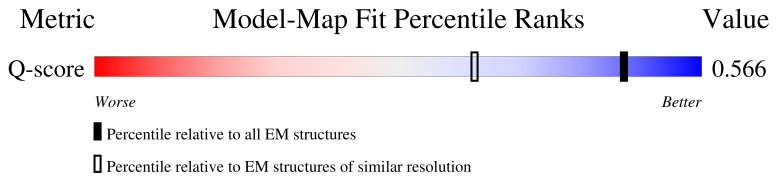
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.54 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	7403 (2.04 - 3.04)

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 <=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	0	218	20% 91% 6% •
2	1	323	15% 76% • 20%
3	3	199	14% 19% • 77%

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Mol	Chain	Length	Quality of chain
4	4	689	31% 73% 9% 18%
5	5	346	84% 8% 8%
6	7	456	5% 79% 9% 13%
7	8	390	5% 75% 8% 16%
8	A	955	15% 59% 21% 16%
9	B	296	70% 5% 26%
10	C	167	69% 7% 25%
11	D	430	8% 52% 46%
12	E	125	6% 74% 10% 16%
13	F	242	11% 76% 10% 14%
14	G	396	10% 68% 5% 27%
15	H	201	5% 58% 6% 35%
16	J	138	10% 76% 22%
17	K	128	9% 24% 73%
18	L	257	11% 57% 6% 37%
19	M	137	9% 80% 16%
20	N	130	9% 82% 16%
21	O	258	9% 74% 26%
22	P	142	12% 61% 35%
23	Q	87	5% 7% 93%
24	R	360	24% 76% 5% 19%
25	S	190	18% 69% 30%
26	T	173	18% 92% 5%
27	U	205	34% 81% 15%
28	V	414	5% 83% 13%

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Mol	Chain	Length	Quality of chain
29	W	187	7% 50% 48%
30	X	398	81% 8% 12%
31	Y	395	6% 27% 5% 69%
32	Z	106	12% 43% 9% 47%
33	a	437	44% 55% 5% 40%

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 67706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	211	1754	1108	333	308	5	0	0

- Molecule 2 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	259	2098	1333	353	402	10	0	0

- Molecule 3 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	45	395	254	81	60	0	0

- Molecule 4 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	566	4585	2940	774	843	28	0	0

- Molecule 5 is a protein called Dimethyladenosine transferase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	319	2568	1648	458	451	11	0	0

- Molecule 6 is a protein called Methyltransferase-like protein 17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	398	3145	2006	579	544	16	0	0

- Molecule 7 is a protein called Malonyl-CoA-acyl carrier protein transacylase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	8	326	2543	1617	463	446	17	0	0

- Molecule 8 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	A	802	17027	7635	3061	5529	802	0	0

- Molecule 9 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	220	1789	1142	324	313	10	0	0

- Molecule 10 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	126	1042	679	181	177	5	0	0

- Molecule 11 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D	232	1838	1155	345	329	9	0	0

- Molecule 12 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	105	839	526	154	155	4	0	0

- Molecule 13 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	208	1724	1104	312	297	11	0	0

- Molecule 14 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	G	291	2384	1516	414	440	14	0	0

- Molecule 15 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	H	130	1064	687	177	197	3	0	0

- Molecule 16 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 17 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	K	35	296	182	67	47	0	0

- Molecule 18 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	L	161	1363	869	253	234	7	0	0

- Molecule 19 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	M	115	913	578	181	148	6	0	0

- Molecule 20 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	N	109	859	557	155	144	3	0	0

- Molecule 21 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	O	190	1570	999	291	274	6	0	0

- Molecule 22 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	P	92	731	472	123	128	8	0	0

- Molecule 23 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Q	6	49	30	8	10	1	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 24 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	R	291	2382	1518	409	447	8	0	0

- Molecule 25 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	S	133	1100	709	196	194	1	0	0

- Molecule 26 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	T	164	1344	859	234	240	11	0	0

- Molecule 27 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	U	174	1468	905	295	264	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	V	359	2946	1891	491	552	12	0	0

- Molecule 29 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	W	98	775	491	138	142	4	0	0

- Molecule 30 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 31 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Y	123	1043	676	175	189	3	0	0

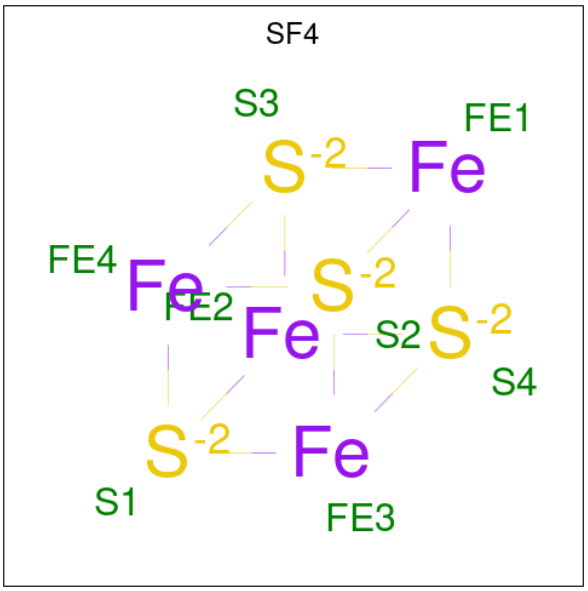
- Molecule 32 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Z	56	465	298	84	80	3	0	0

- Molecule 33 is a protein called GTPase Era, mitochondrial.

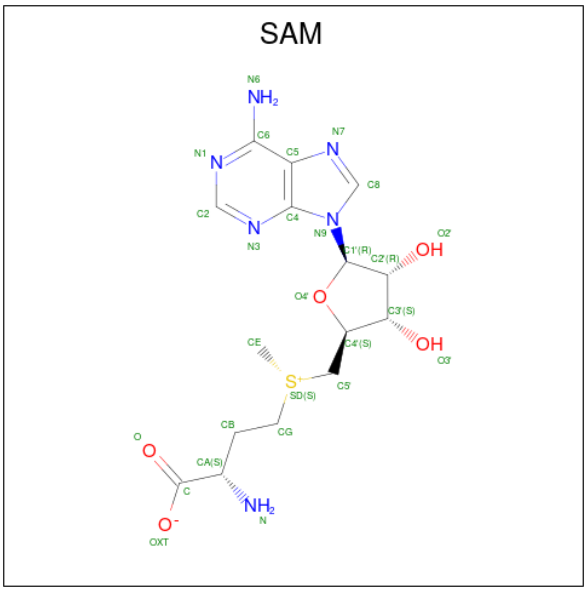
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	a	263	1785	1121	323	335	6	0	0

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
34	7	1	8	4	4	0

- Molecule 35 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
35	7	1	27	15	6	5	1	0

- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms			AltConf
			Total	K		
36	A	4	4	4		0

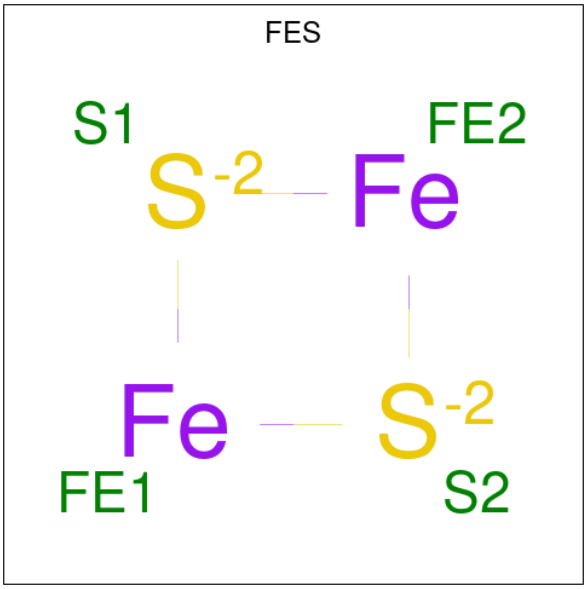
- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
37	A	25	25	25	0
37	B	1	1	1	0
37	X	1	1	1	0

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

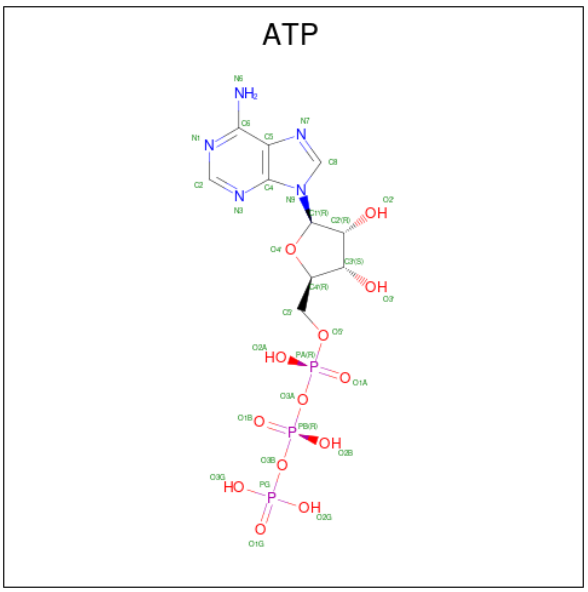
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
38	O	1	1	1	0

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



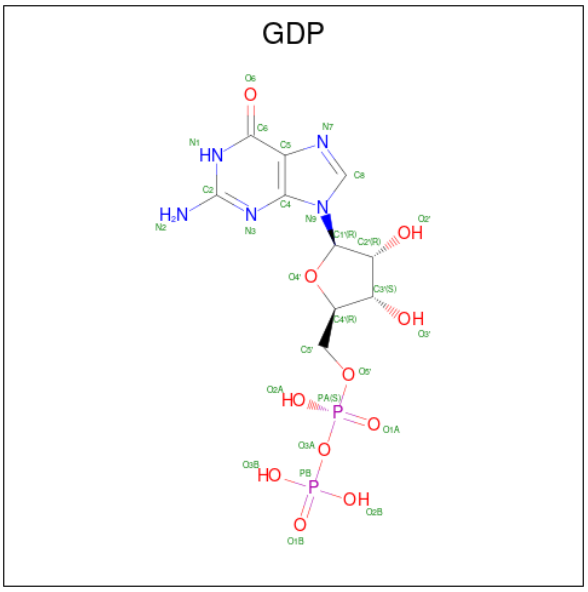
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
39	P	1	4	2	2	0
39	T	1	4	2	2	0

- 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	
40	X	1	31	10	5	13	3	0

- Molecule 41 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



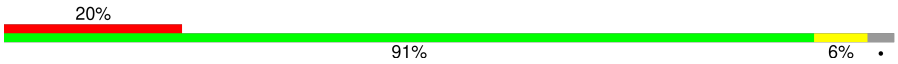
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	X	1	28	10	5	11	2	0

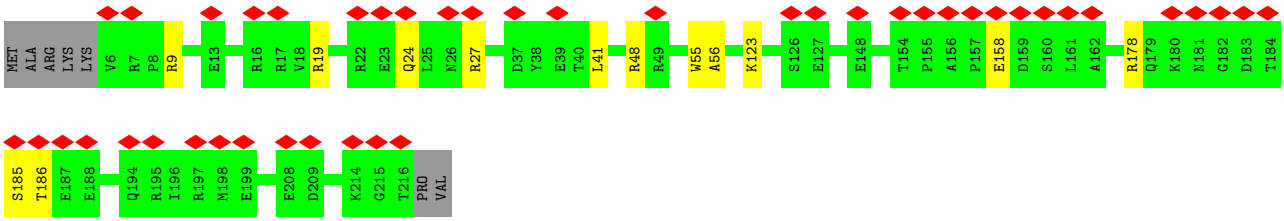
3 Residue-property plots (i)

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: 28S ribosomal protein S34, mitochondrial

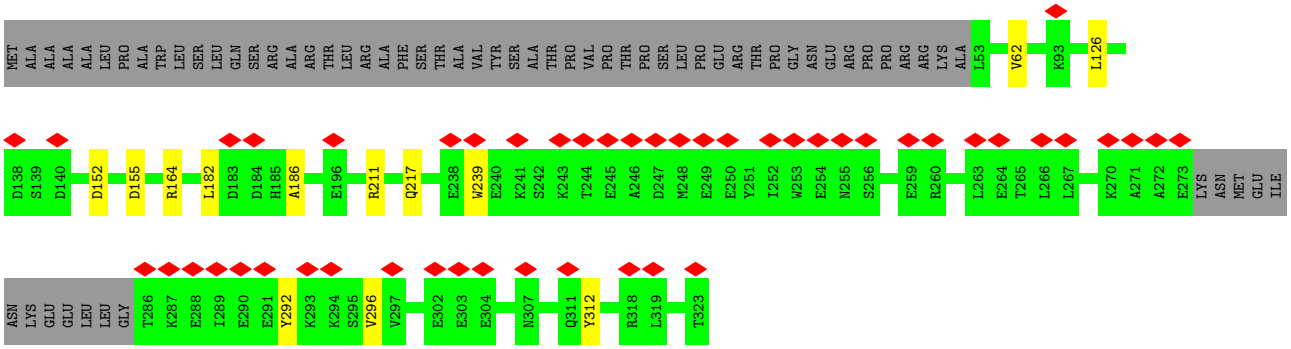
Chain 0:





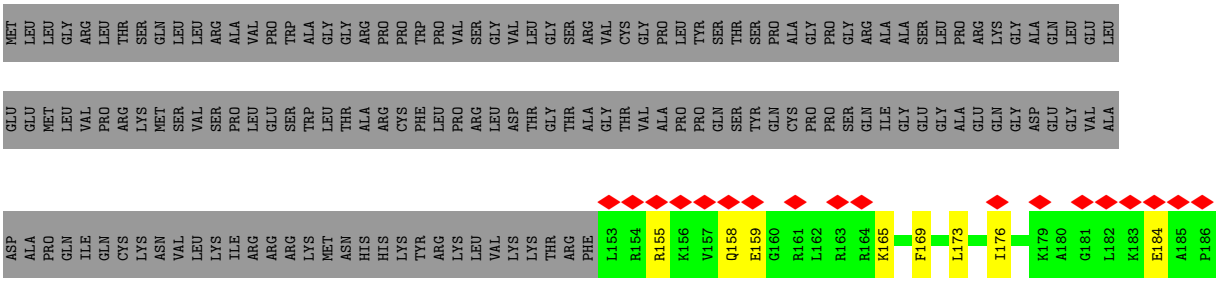
- Molecule 2: 28S ribosomal protein S35, mitochondrial

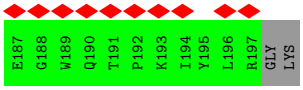
Chain 1:



- Molecule 3: Aurora kinase A-interacting protein

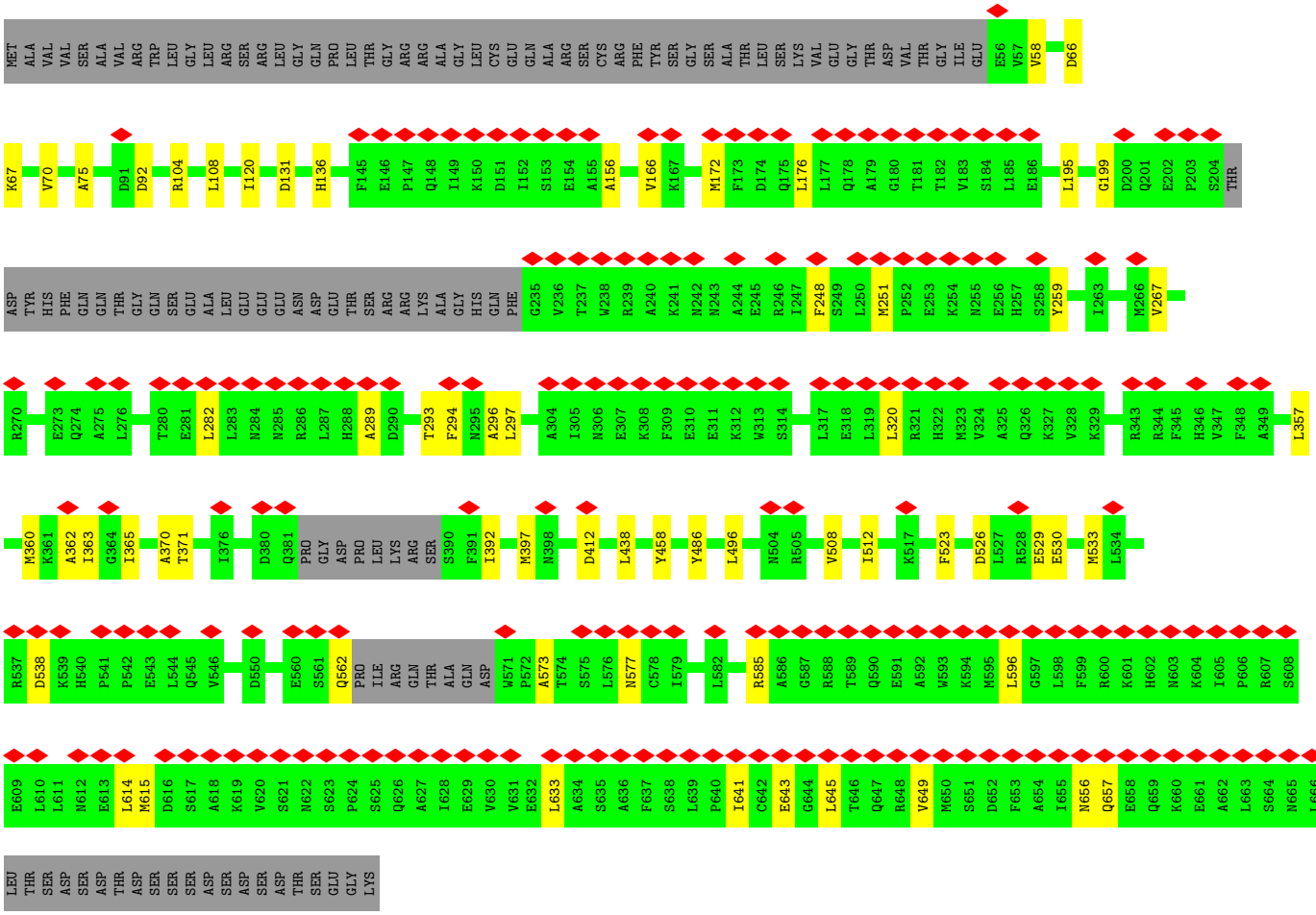
Chain 3:





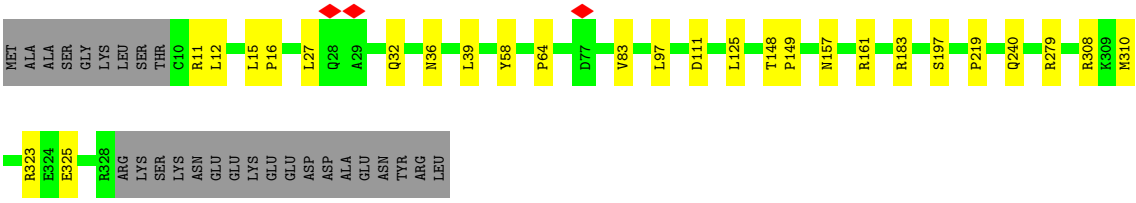
• Molecule 4: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain 4:



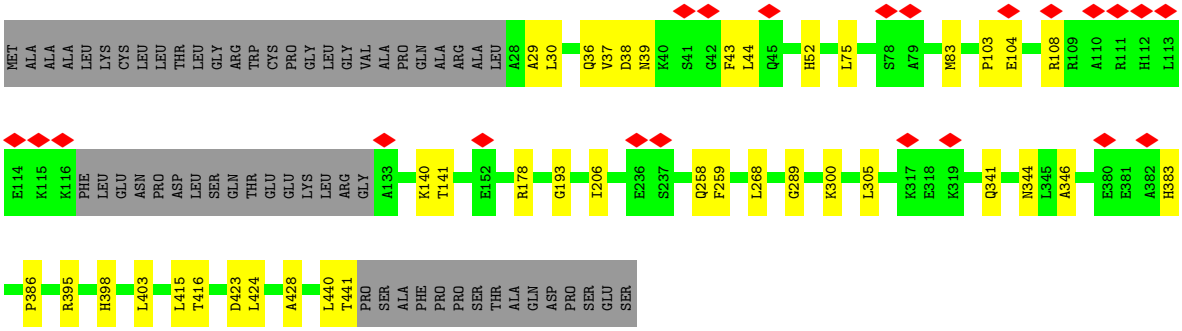
• Molecule 5: Dimethyladenosine transferase 1, mitochondrial

Chain 5:



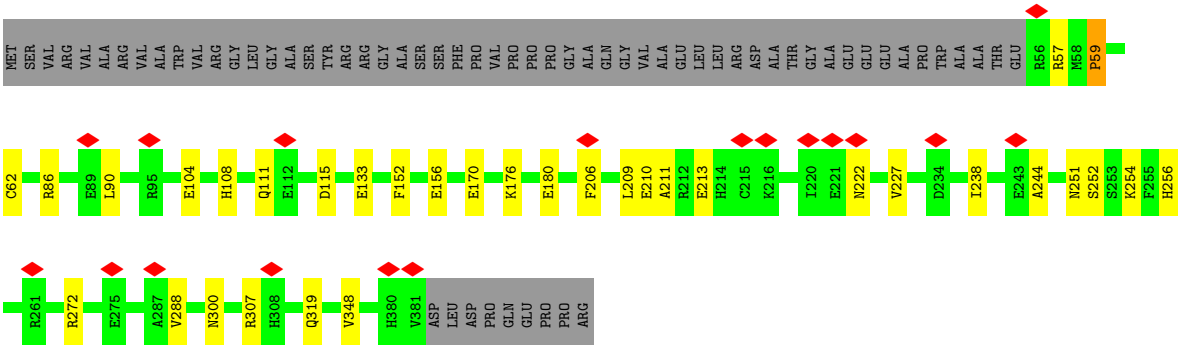
• Molecule 6: Methyltransferase-like protein 17, mitochondrial

Chain 7:



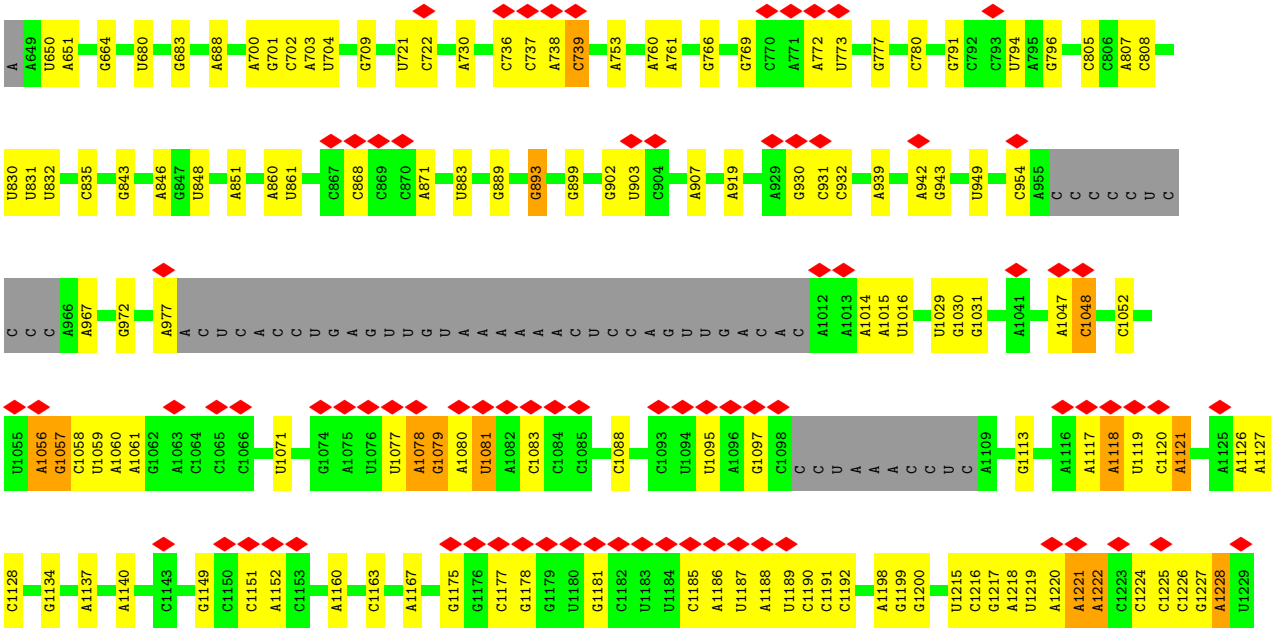
• Molecule 7: Malonyl-CoA-acyl carrier protein transacylase, mitochondrial

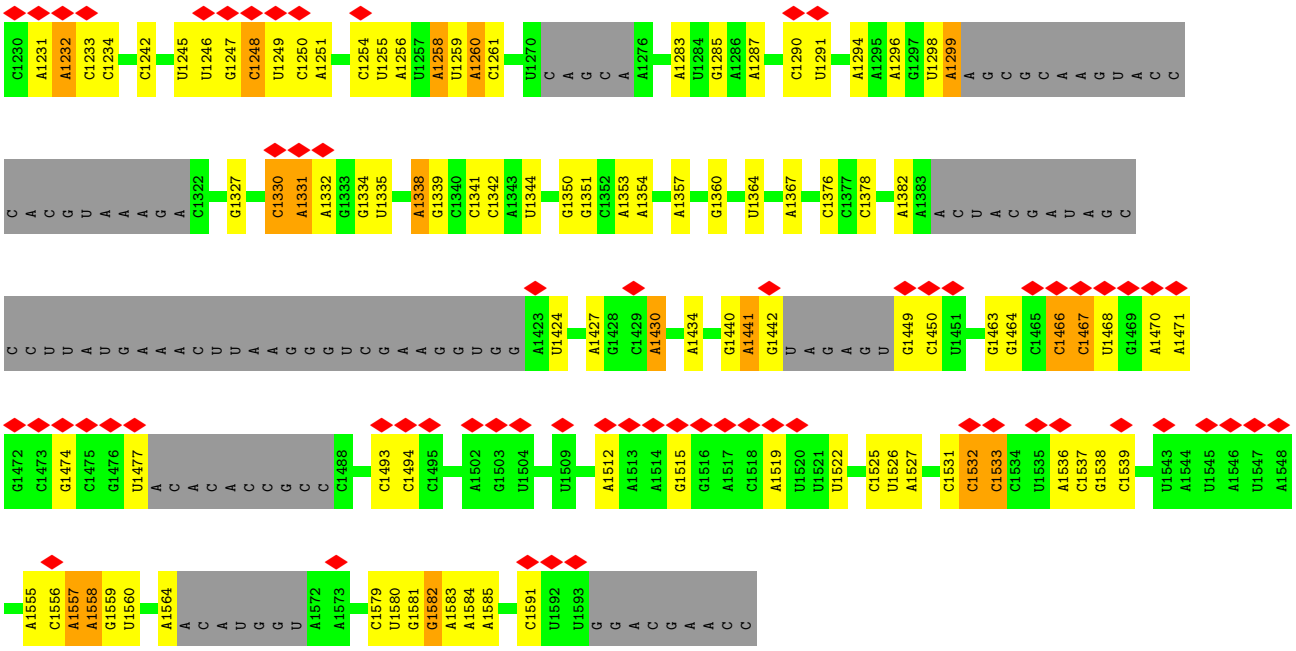
Chain 8:



• Molecule 8: 12S mitochondrial rRNA

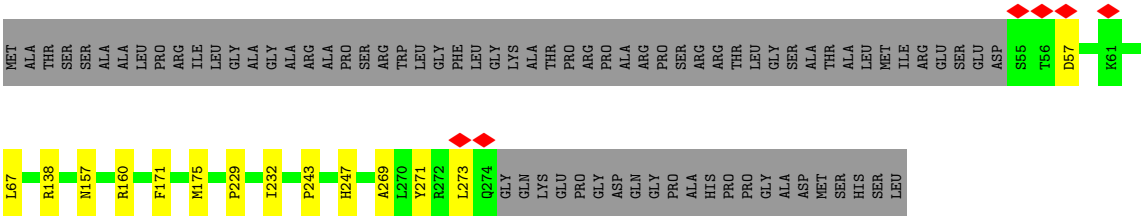
Chain A:





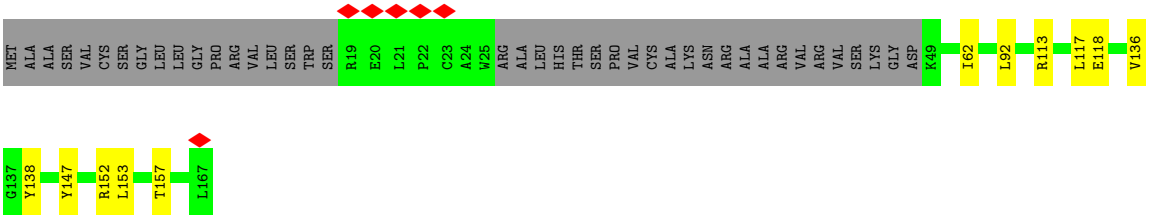
- Molecule 9: 28S ribosomal protein S2, mitochondrial

Chain B:



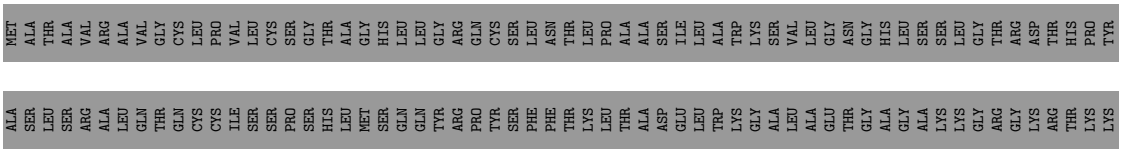
- Molecule 10: 28S ribosomal protein S24, mitochondrial

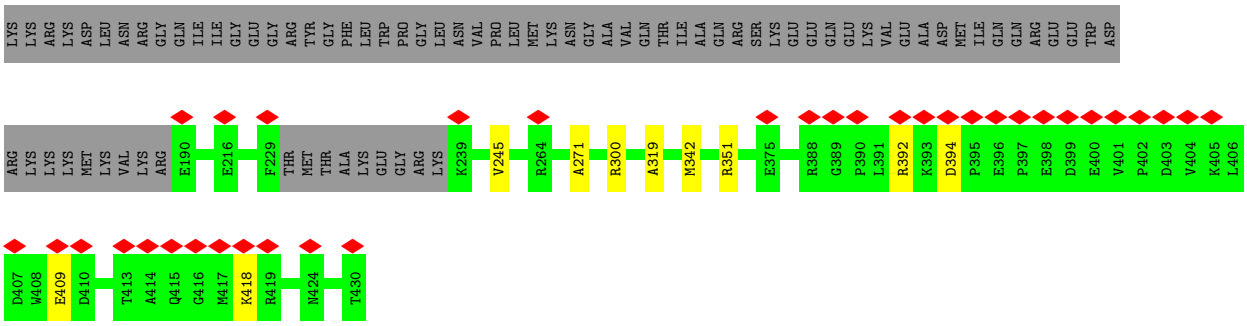
Chain C:



- Molecule 11: 28S ribosomal protein S5, mitochondrial

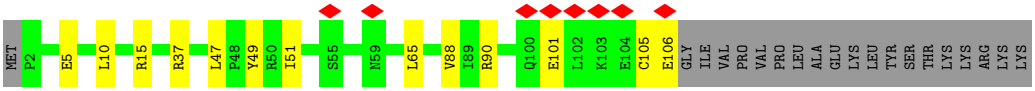
Chain D:





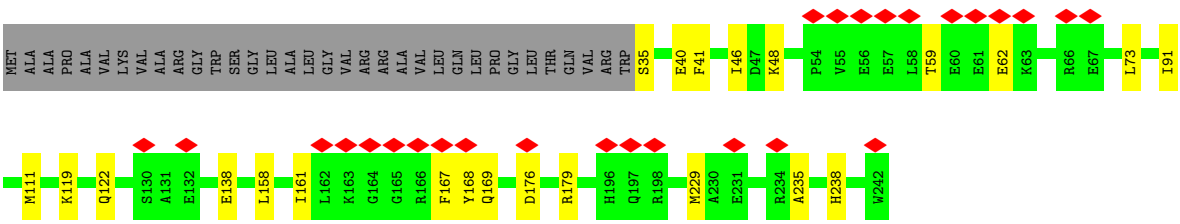
- Molecule 12: 28S ribosomal protein S6, mitochondrial

Chain E:



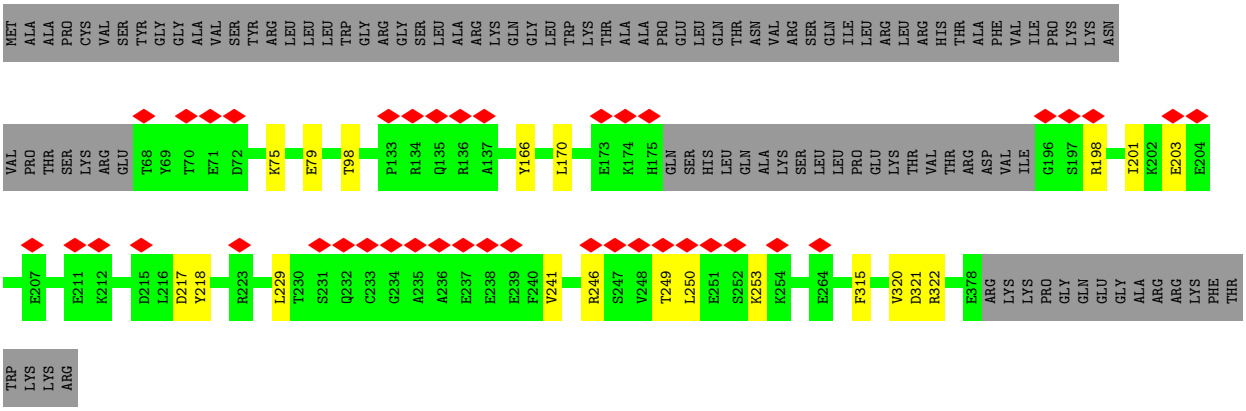
- Molecule 13: 28S ribosomal protein S7, mitochondrial

Chain F:



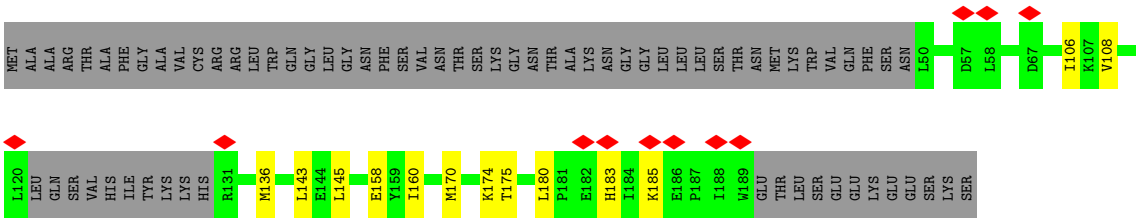
- Molecule 14: 28S ribosomal protein S9, mitochondrial

Chain G:



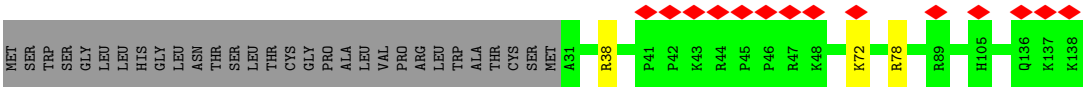
- Molecule 15: 28S ribosomal protein S10, mitochondrial

Chain H:



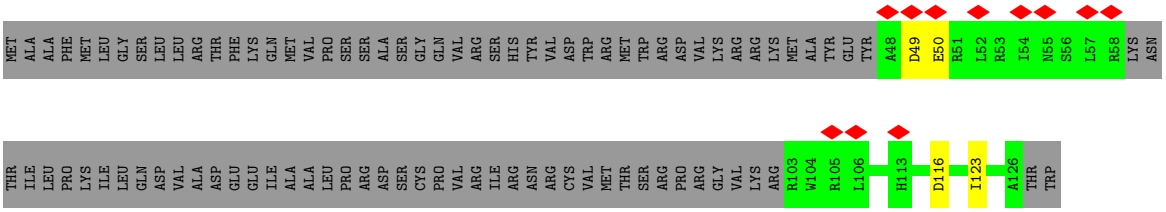
• Molecule 16: 28S ribosomal protein S12, mitochondrial

Chain J:



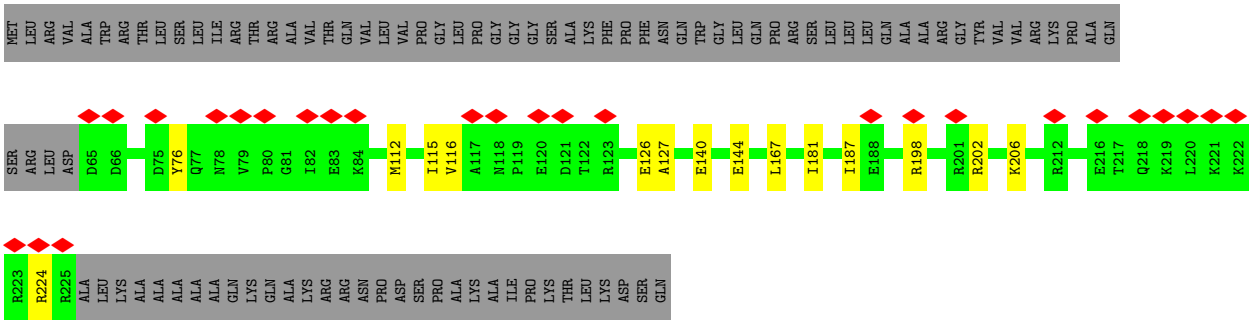
• Molecule 17: 28S ribosomal protein S14, mitochondrial

Chain K:



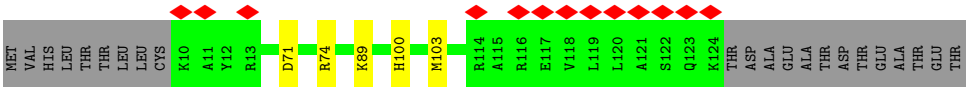
• Molecule 18: 28S ribosomal protein S15, mitochondrial

Chain L:



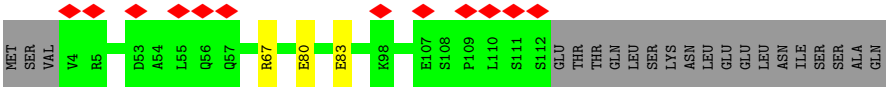
• Molecule 19: 28S ribosomal protein S16, mitochondrial

Chain M:



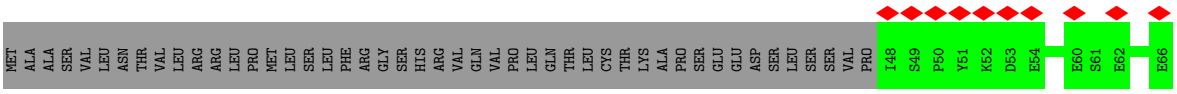
• Molecule 20: 28S ribosomal protein S17, mitochondrial

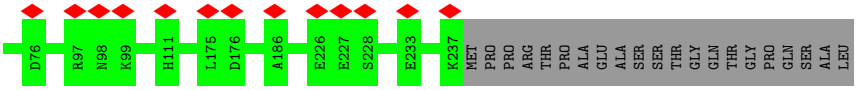
Chain N:



• Molecule 21: 28S ribosomal protein S18b, mitochondrial

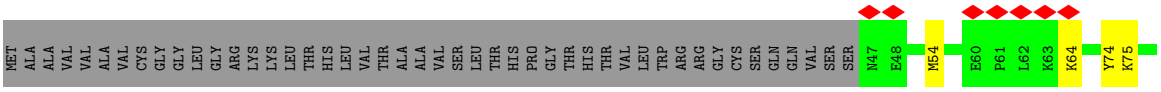
Chain O:

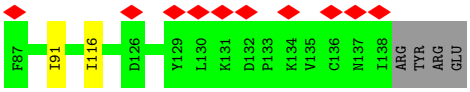




• Molecule 22: 28S ribosomal protein S18c, mitochondrial

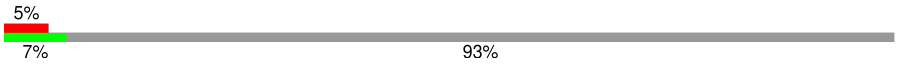
Chain P:

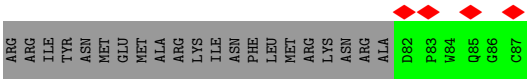




• Molecule 23: 28S ribosomal protein S21, mitochondrial

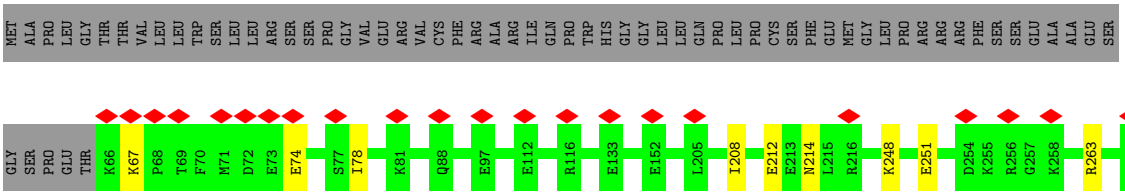
Chain Q:

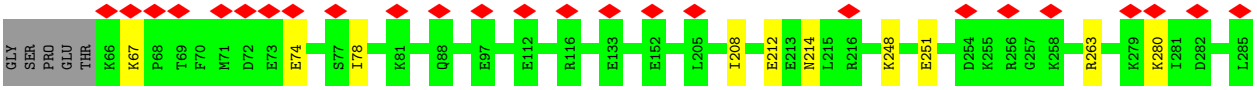


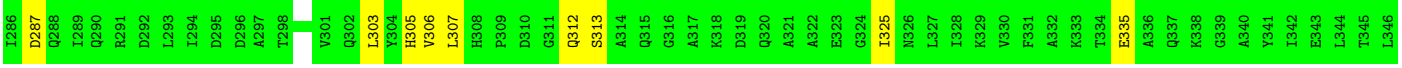


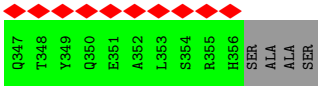
• Molecule 24: 28S ribosomal protein S22, mitochondrial

Chain R:



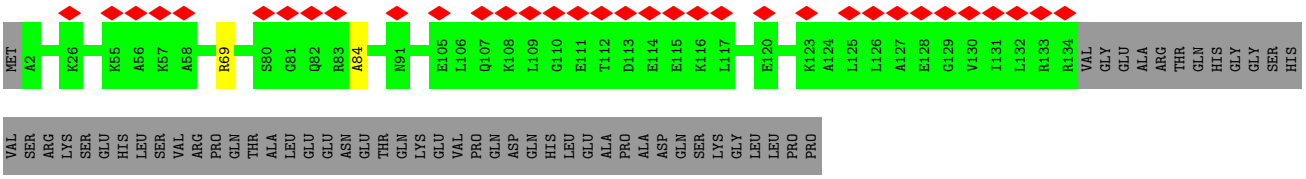






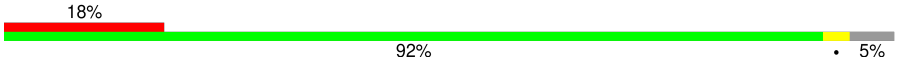
• Molecule 25: 28S ribosomal protein S23, mitochondrial

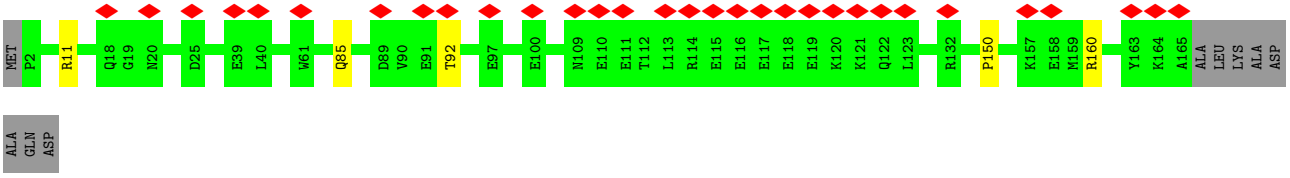
Chain S:



• Molecule 26: 28S ribosomal protein S25, mitochondrial

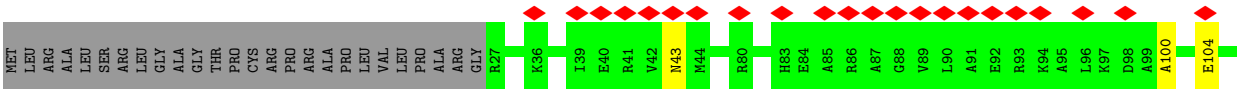
Chain T:

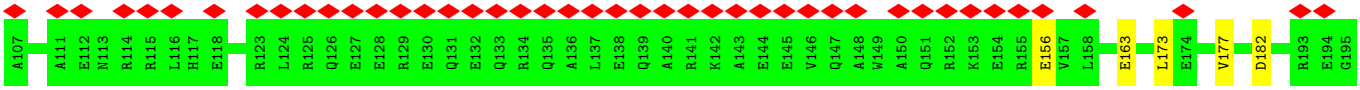


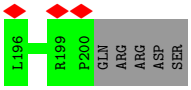


• Molecule 27: 28S ribosomal protein S26, mitochondrial

Chain U:

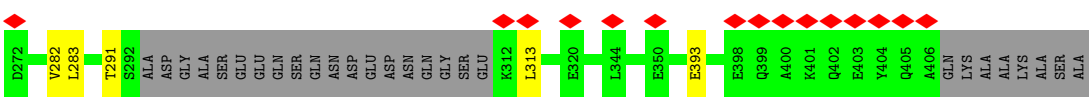






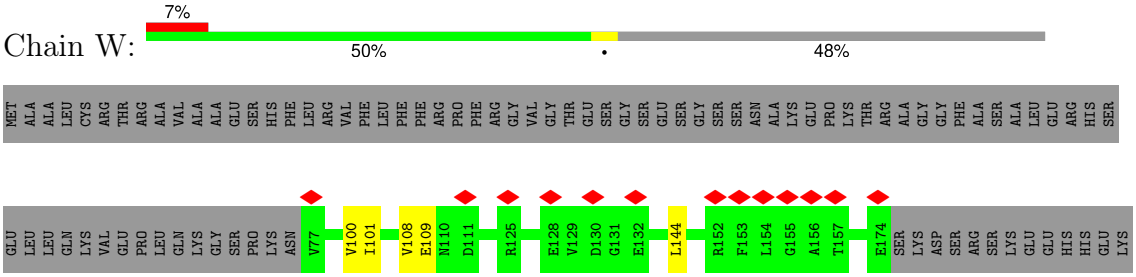
• Molecule 28: 28S ribosomal protein S27, mitochondrial

Chain V:



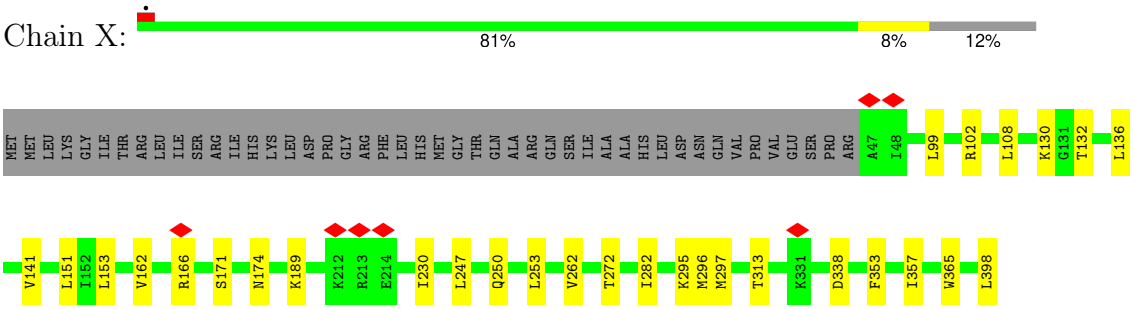
- Molecule 29: 28S ribosomal protein S28, mitochondrial

Chain W:



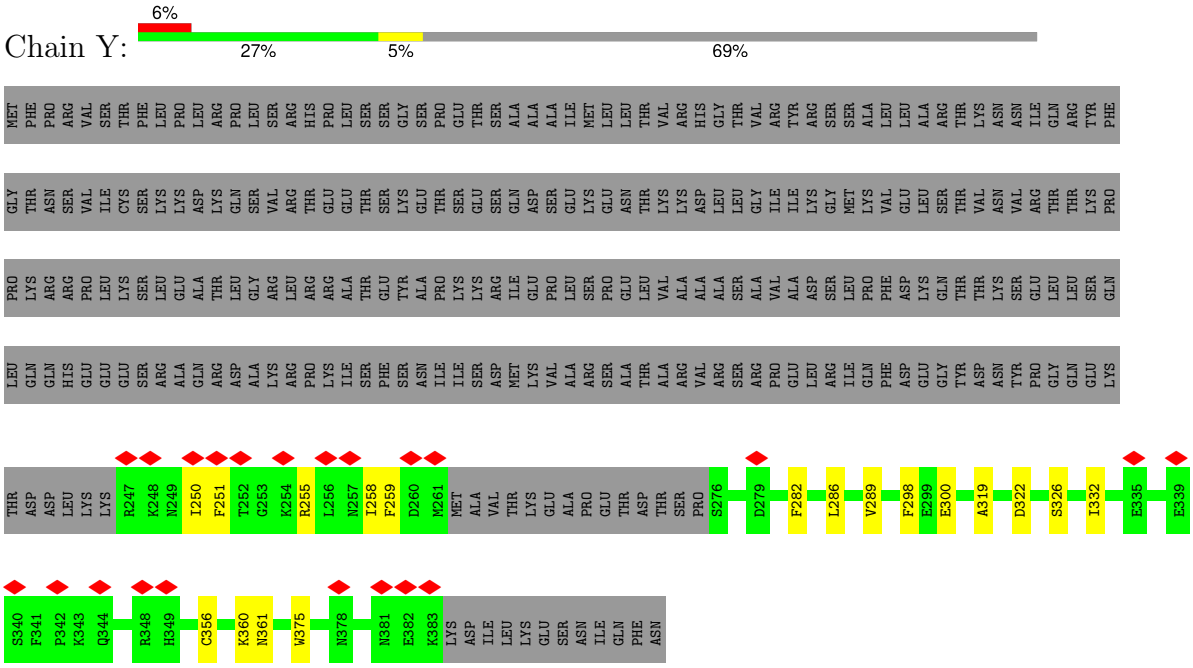
- Molecule 30: 28S ribosomal protein S29, mitochondrial

Chain X:



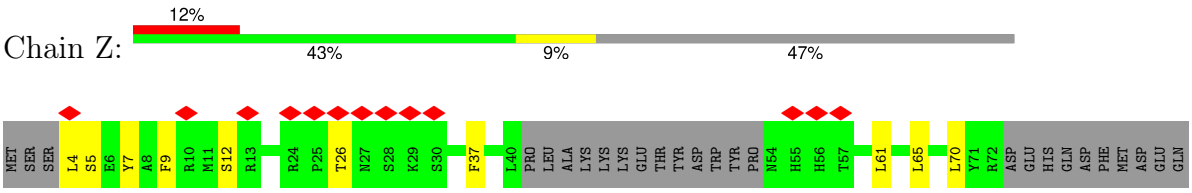
- Molecule 31: 28S ribosomal protein S31, mitochondrial

Chain Y:



- Molecule 32: 28S ribosomal protein S33, mitochondrial

Chain Z:



LYS ARG LEU LYS LYS LEU ARG GLY LYS GLU LYS PRO LYS LYS GLY GLU GLY LYS ARG ALA ALA LYS ARG LYS

• Molecule 33: GTPase Era, mitochondrial

Chain a:

MET ALA ALA PRO SER TRP ARG GLY ALA ARG LEU LEU VAL GLN SER VAL LEU ARG VAL TRP GLN VAL GLY PRO HIS VAL ALA ARG GLU ARG VAL ILE PRO PHE SER SER LEU LEU GLY PHE GLN ARG ARG CYS VAL SER CYS VAL ALA GLY SER ALA PHE SER GLY PRO ARG LEU ALA SER ALA

SER ARG SER ASN GLY GLN GLY SER ALA LEU ASP HIS PHE LEU GLY PHE SER GLN PRO ASP SER SER VAL THR PRO CYS VAL PRO ALA VAL SER MET ASN ARG ASP GLU GLN ASP VAL LEU LEU VAL HIS HIS PRO ASP MET PRO GLU ASN S111 R112 V113 L114 R115 V116 V117 L118 L119 G120

G125 L129 Q132 L133 L134 G135 R136 K137 V138 PHE PRO VAL SER ARG LYS VAL HIS THR THR ARG CYS GLN ALA L153 G154 V155 E158 K159 Q162 V163 I164 L165 L166 D167 T168 P169 G170 I171 ILE SER PRO GLY LYS GLN LYS ARG HIS HIS LEU GLU LEU SER LEU LEU E188

D189 P190 W191 K192 S193 M194 E195 S196 A197 D198 L199 L203 V204 D205 V206 S207 D208 K209 W210 T211 R212 L215 S216 P217 Q218 L219 L220 R221 C222 L223 T224 K225 Y226 S227 Q228 I229 C240 L241 K242 Q243 K244 L247 L250 E256 V259 K262 K263 L264 K265 M266 R267 Q268

A269 F270 H271 SER HIS PRO GLY THR HIS CYS PRO SER PRO ALA VAL LYS ASP PRO ASN THR GLN SER VAL GLY ASN P294 Q295 R296 I297 H301 E304 A310 L311 S312 Q313 E314 D315 V316 K317 T318 L319 K320 Q321 Y322 L323 L324 T325 Q326 A327 Q328 P329 G330 PRO TRP GLU TYR HIS

SER ALA VAL LEU THR SER GLN T343 P344 E345 E346 I347 C348 A349 N350 I351 I352 R353 E354 K355 L356 L357 E358 H359 L360 P361 Q362 E363 V364 P365 Y366 N367 V368 Q369 Q370 K371 T372 A373 V374 W375 E376 E377 G378 P379 G380 G381 E382 L383 V384 I385 Q386 Q387 K388 L389 L390 V391 P392 K393 E394 S395

Y396 V397 K398 L399 L400 I401 G402 P403 K404 G405 H406 V407 I408 S409 Q410 I411 A412 Q413 E414 A415 G416 H417 D418 L419 M420 D421 I422 F423 L424 C425 D426 V427 D428 I429 R430 L431 S432 V433 K434 L435 L436 K437

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	203950	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	56.870	Depositor
Minimum map value	-28.093	Depositor
Average map value	0.039	Depositor
Map value standard deviation	1.386	Depositor
Recommended contour level	8.5	Depositor
Map size (Å)	424.80002, 424.80002, 424.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.062, 1.062, 1.062	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: K, ATP, SAM, FES, ZN, MG, SF4, GDP

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	0	0.15	0/1800	0.32	0/2440
2	1	0.19	0/2143	0.35	0/2902
3	3	0.16	0/402	0.34	0/533
4	4	0.18	0/4686	0.39	0/6335
5	5	0.21	0/2624	0.40	0/3552
6	7	0.21	0/3234	0.39	1/4390 (0.0%)
7	8	0.19	0/2603	0.44	1/3520 (0.0%)
8	A	0.16	0/19038	0.31	0/29619
9	B	0.17	0/1832	0.34	0/2480
10	C	0.21	0/1074	0.42	0/1456
11	D	0.16	0/1877	0.35	0/2523
12	E	0.16	0/853	0.36	0/1151
13	F	0.18	0/1766	0.39	0/2373
14	G	0.19	0/2435	0.37	0/3269
15	H	0.21	0/1086	0.36	0/1473
16	J	0.15	0/855	0.33	0/1148
17	K	0.16	0/299	0.31	0/397
18	L	0.15	0/1387	0.30	0/1853
19	M	0.15	0/934	0.33	0/1255
20	N	0.14	0/877	0.30	0/1187
21	O	0.14	0/1624	0.29	0/2210
22	P	0.16	0/747	0.33	0/1004
23	Q	0.13	0/51	0.35	0/68
24	R	0.14	0/2429	0.32	0/3280
25	S	0.16	0/1127	0.31	0/1518
26	T	0.17	0/1375	0.34	0/1847
27	U	0.16	0/1490	0.34	0/1999
28	V	0.17	0/3007	0.33	0/4062
29	W	0.16	0/787	0.31	0/1060
30	X	0.19	0/2921	0.38	0/3954
31	Y	0.17	0/1073	0.36	0/1444
32	Z	0.18	0/473	0.45	0/631

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	a	0.15	0/1801	0.35	0/2447
All	All	0.17	0/70710	0.35	2/99380 (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
16	J	0	1
26	T	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	8	59	PRO	CA-N-CD	-6.22	103.30	112.00
6	7	103	PRO	CA-N-CD	-5.44	104.39	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	J	72	LYS	Peptide
26	T	160	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	0	1754	0	1754	9	0
2	1	2098	0	2115	11	0
3	3	395	0	432	6	0
4	4	4585	0	4595	46	0
5	5	2568	0	2655	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	7	3145	0	3159	25	0
7	8	2543	0	2561	20	0
8	A	17027	0	8651	54	0
9	B	1789	0	1781	7	0
10	C	1042	0	1033	10	0
11	D	1838	0	1858	6	0
12	E	839	0	848	10	0
13	F	1724	0	1769	20	0
14	G	2384	0	2351	16	0
15	H	1064	0	1089	10	0
16	J	839	0	887	2	0
17	K	296	0	304	4	0
18	L	1363	0	1442	14	0
19	M	913	0	943	3	0
20	N	859	0	922	2	0
21	O	1570	0	1533	0	0
22	P	731	0	761	6	0
23	Q	49	0	36	0	0
24	R	2382	0	2405	10	0
25	S	1100	0	1103	2	0
26	T	1344	0	1359	4	0
27	U	1468	0	1478	6	0
28	V	2946	0	2942	12	0
29	W	775	0	791	3	0
30	X	2849	0	2843	20	0
31	Y	1043	0	996	16	0
32	Z	465	0	475	10	0
33	a	1785	0	1599	16	0
34	7	8	0	0	0	0
35	7	27	0	22	1	0
36	A	4	0	0	0	0
37	A	25	0	0	0	0
37	B	1	0	0	0	0
37	X	1	0	0	0	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	28	0	12	1	0
All	All	67706	0	59516	329	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 (329) 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)
33:a:119:LEU:HD22	33:a:219:LEU:HD13	1.54	0.88
4:4:267:VAL:HG11	4:4:296:ALA:HB1	1.58	0.86
14:G:249:THR:HG22	14:G:250:LEU:HD12	1.56	0.85
13:F:48:LYS:NZ	14:G:321:ASP:OD1	2.10	0.84
11:D:409:GLU:OE2	11:D:418:LYS:NZ	2.10	0.83
8:A:738:A:O2'	8:A:739:C:O2	1.96	0.82
8:A:1515:G:O3'	18:L:224:ARG:NH2	2.15	0.79
18:L:112:MET:HE3	18:L:116:VAL:HG21	1.66	0.78
8:A:1118:A:O2'	11:D:351:ARG:NH2	2.17	0.78
5:5:183:ARG:O	5:5:197:SER:OG	2.01	0.78
6:7:193:GLY:O	35:7:502:SAM:N	2.18	0.77
6:7:440:LEU:HD12	6:7:441:THR:HG22	1.66	0.77
7:8:104:GLU:OE1	7:8:108:HIS:NE2	2.17	0.77
13:F:119:LYS:NZ	30:X:398:LEU:OXT	2.15	0.76
5:5:11:ARG:NH1	6:7:258:GLN:O	2.19	0.76
7:8:152:PHE:O	7:8:300:ASN:ND2	2.18	0.76
1:0:24:GLN:O	1:0:27:ARG:NH1	2.19	0.75
30:X:99:LEU:HD21	30:X:136:LEU:HD22	1.68	0.75
2:1:155:ASP:OD2	15:H:174:LYS:NZ	2.19	0.74
7:8:156:GLU:OE1	7:8:319:GLN:NE2	2.20	0.74
8:A:1248:C:HO2'	8:A:1251:A:HO2'	1.30	0.74
14:G:229:LEU:HD21	14:G:241:VAL:HG11	1.68	0.74
4:4:92:ASP:OD2	10:C:157:THR:OG1	2.05	0.73
2:1:312:TYR:OH	30:X:338:ASP:OD2	2.05	0.72
33:a:129:LEU:HD12	33:a:203:LEU:HD21	1.71	0.72
5:5:111:ASP:OD1	8:A:1079:G:N2	2.22	0.72
24:R:251:GLU:OE2	24:R:280:LYS:NZ	2.24	0.71
3:3:165:LYS:NZ	8:A:1149:G:OP2	2.21	0.70
33:a:317:LYS:O	33:a:321:GLN:NE2	2.25	0.70
6:7:75:LEU:HD22	6:7:83:MET:HE2	1.74	0.70
28:V:226:TYR:HE1	28:V:282:VAL:HG21	1.56	0.70
14:G:201:ILE:HD12	14:G:203:GLU:OE2	1.92	0.69
12:E:37:ARG:NH2	27:U:163:GLU:OE2	2.25	0.69
6:7:341:GLN:NE2	6:7:346:ALA:O	2.26	0.69
1:0:9:ARG:NE	8:A:805:C:O2	2.27	0.68
8:A:1559:G:OP2	8:A:1559:G:N2	2.18	0.68
30:X:272:THR:OG1	30:X:282:ILE:O	2.09	0.68
11:D:392:ARG:NH2	11:D:394:ASP:OD2	2.27	0.68
8:A:1121:A:OP1	11:D:300:ARG:NH2	2.26	0.68
33:a:244:LYS:O	33:a:247:LEU:HD12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:760:A:N1	8:A:780:C:O2'	2.27	0.67
10:C:152:ARG:NH1	31:Y:300:GLU:OE1	2.26	0.67
8:A:1016:U:O2'	22:P:91:ILE:O	2.13	0.67
18:L:115:ILE:HG21	18:L:181:ILE:HD13	1.74	0.67
13:F:167:PHE:O	13:F:169:GLN:NE2	2.27	0.66
24:R:67:LYS:NZ	24:R:307:LEU:O	2.29	0.66
1:0:19:ARG:NH1	8:A:808:C:OP1	2.29	0.66
22:P:54:MET:HE2	25:S:69:ARG:CZ	2.27	0.65
30:X:171:SER:OG	30:X:174:ASN:O	2.14	0.65
9:B:57:ASP:OD2	9:B:271:TYR:OH	2.09	0.63
19:M:71:ASP:OD1	19:M:74:ARG:NH2	2.32	0.63
8:A:1466:C:O2'	8:A:1467:C:OP1	2.13	0.63
8:A:1081:U:O2'	8:A:1083:C:OP2	2.06	0.62
32:Z:9:PHE:O	32:Z:12:SER:OG	2.14	0.62
24:R:312:GLN:N	24:R:335:GLU:OE2	2.32	0.62
8:A:1251:A:N6	8:A:1341:C:O2'	2.33	0.61
29:W:108:VAL:HG12	29:W:109:GLU:OE1	1.99	0.61
31:Y:356:CYS:SG	31:Y:360:LYS:NZ	2.73	0.61
18:L:112:MET:O	18:L:116:VAL:HG22	2.00	0.61
8:A:1248:C:O2'	8:A:1251:A:O2'	2.05	0.60
4:4:267:VAL:HG11	4:4:296:ALA:CB	2.31	0.59
8:A:1382:A:OP1	30:X:166:ARG:NH2	2.35	0.59
28:V:156:ASN:ND2	28:V:159:ASP:OD2	2.36	0.59
31:Y:286:LEU:O	31:Y:289:VAL:HG12	2.03	0.58
8:A:1224:C:O2'	8:A:1228:A:N6	2.36	0.58
5:5:279:ARG:HE	5:5:310:MET:HE2	1.68	0.58
8:A:1056:A:O2'	8:A:1057:G:O4'	2.21	0.58
33:a:119:LEU:HD23	33:a:120:GLY:N	2.19	0.57
15:H:183:HIS:O	15:H:183:HIS:ND1	2.35	0.57
5:5:27:LEU:HD11	5:5:32:GLN:HB2	1.85	0.57
7:8:57:ARG:NE	7:8:62:CYS:SG	2.78	0.57
6:7:415:LEU:HD22	6:7:428:ALA:HB2	1.87	0.57
4:4:131:ASP:OD2	4:4:136:HIS:ND1	2.30	0.57
14:G:198:ARG:N	14:G:246:ARG:O	2.34	0.57
14:G:217:ASP:OD1	14:G:218:TYR:N	2.38	0.57
28:V:226:TYR:CE1	28:V:282:VAL:HG21	2.36	0.57
6:7:39:ASN:OD1	6:7:43:PHE:N	2.37	0.56
4:4:538:ASP:O	4:4:585:ARG:NH1	2.39	0.56
6:7:37:VAL:HG11	6:7:44:LEU:HD11	1.88	0.56
6:7:398:HIS:HB3	6:7:416:THR:HG22	1.87	0.56
4:4:195:LEU:O	4:4:199:GLY:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:59:THR:OG1	13:F:62:GLU:OE1	2.23	0.56
6:7:178:ARG:HD3	6:7:206:ILE:HG23	1.88	0.56
6:7:268:LEU:HB2	6:7:305:LEU:HD21	1.88	0.56
8:A:1221:A:O2'	8:A:1222:A:OP2	2.24	0.56
28:V:291:THR:O	28:V:291:THR:HG22	2.06	0.56
24:R:74:GLU:OE2	24:R:78:ILE:HD11	2.05	0.56
6:7:300:LYS:NZ	6:7:344:ASN:O	2.35	0.55
8:A:1078:A:OP2	33:a:295:GLN:NE2	2.38	0.55
18:L:126:GLU:HB2	18:L:181:ILE:HD11	1.87	0.55
7:8:86:ARG:NH1	7:8:133:GLU:OE2	2.39	0.55
30:X:130:LYS:NZ	30:X:313:THR:OG1	2.37	0.55
4:4:615:MET:HE1	4:4:649:VAL:HG22	1.89	0.55
15:H:106:ILE:HD12	15:H:145:LEU:HD21	1.88	0.55
32:Z:26:THR:O	32:Z:26:THR:HG22	2.07	0.55
8:A:843:G:N2	8:A:846:A:OP2	2.38	0.55
18:L:76:TYR:OH	27:U:156:GLU:OE1	2.25	0.54
12:E:65:LEU:HD11	22:P:75:LYS:CD	2.36	0.54
4:4:360:MET:HE1	4:4:371:THR:HG21	1.90	0.54
33:a:119:LEU:CD2	33:a:219:LEU:HD13	2.32	0.54
10:C:136:VAL:HG22	10:C:153:LEU:HD23	1.89	0.53
15:H:180:LEU:O	15:H:185:LYS:NZ	2.41	0.53
8:A:702:C:OP1	8:A:848:U:O2'	2.25	0.53
4:4:523:PHE:HE2	4:4:562:GLN:HE21	1.50	0.53
6:7:29:ALA:C	6:7:30:LEU:HD12	2.33	0.53
6:7:423:ASP:OD2	6:7:424:LEU:N	2.42	0.53
5:5:64:PRO:HG3	5:5:83:VAL:HG13	1.91	0.53
18:L:116:VAL:HG12	18:L:126:GLU:HG3	1.89	0.53
31:Y:258:ILE:HG23	31:Y:259:PHE:CD1	2.44	0.53
8:A:899:G:O2'	8:A:907:A:N1	2.37	0.52
28:V:70:LEU:HD23	28:V:393:GLU:OE1	2.09	0.52
7:8:211:ALA:HB1	7:8:244:ALA:HB1	1.91	0.52
19:M:89:LYS:HA	19:M:103:MET:HE2	1.91	0.52
10:C:92:LEU:HD21	10:C:147:TYR:HE2	1.75	0.52
7:8:222:ASN:O	7:8:272:ARG:NH2	2.42	0.52
14:G:320:VAL:HG23	14:G:322:ARG:HG2	1.92	0.52
20:N:83:GLU:OE2	26:T:85:GLN:NE2	2.43	0.52
4:4:58:VAL:HG23	4:4:58:VAL:O	2.10	0.52
4:4:172:MET:O	4:4:176:LEU:HD23	2.10	0.52
4:4:370:ALA:N	4:4:412:ASP:OD1	2.41	0.52
24:R:305:HIS:NE2	24:R:313:SER:OG	2.35	0.51
1:0:48:ARG:NH2	8:A:701:G:O6	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1149:G:OP1	18:L:202:ARG:NH1	2.42	0.51
33:a:129:LEU:CD1	33:a:203:LEU:HD21	2.38	0.51
1:0:41:LEU:HD13	1:0:55:TRP:CG	2.46	0.51
19:M:100:HIS:H	19:M:103:MET:HE3	1.75	0.51
4:4:360:MET:HE1	4:4:371:THR:CG2	2.41	0.51
14:G:201:ILE:HD12	14:G:203:GLU:CD	2.36	0.51
4:4:645:LEU:O	4:4:649:VAL:HG23	2.11	0.51
6:7:140:LYS:O	6:7:141:THR:HG22	2.11	0.51
4:4:357:LEU:HD21	31:Y:251:PHE:HE1	1.76	0.51
8:A:1430:A:OP1	13:F:35:SER:N	2.44	0.51
8:A:1134:G:OP2	16:J:38:ARG:NH2	2.44	0.51
13:F:119:LYS:NZ	30:X:365:TRP:O	2.33	0.51
13:F:161:ILE:O	13:F:168:TYR:N	2.40	0.50
30:X:250:GLN:HA	30:X:253:LEU:HD12	1.94	0.50
24:R:212:GLU:OE1	24:R:248:LYS:NZ	2.37	0.50
24:R:208:ILE:O	24:R:214:ASN:ND2	2.42	0.50
4:4:656:ASN:OD1	4:4:657:GLN:N	2.41	0.50
5:5:15:LEU:HD21	5:5:39:LEU:HD22	1.94	0.50
5:5:325:GLU:N	5:5:325:GLU:OE1	2.44	0.50
4:4:596:LEU:HD22	4:4:633:LEU:HD13	1.94	0.50
30:X:189:LYS:CG	30:X:230:ILE:HD12	2.42	0.50
31:Y:361:ASN:ND2	32:Z:37:PHE:O	2.44	0.49
8:A:1441:A:H2	8:A:1449:G:H22	1.61	0.49
18:L:112:MET:HE1	18:L:127:ALA:HB2	1.95	0.49
13:F:238:HIS:NE2	33:a:315:ASP:OD1	2.46	0.49
17:K:49:ASP:OD1	17:K:50:GLU:N	2.45	0.49
3:3:176:ILE:HD11	18:L:206:LYS:HE3	1.94	0.49
13:F:73:LEU:HG	14:G:253:LYS:HE2	1.94	0.49
8:A:1260:A:H62	8:A:1330:C:H42	1.60	0.49
9:B:171:PHE:CE2	9:B:175:MET:HE3	2.48	0.49
12:E:105:CYS:SG	22:P:64:LYS:NZ	2.86	0.49
10:C:92:LEU:HD21	10:C:147:TYR:CE2	2.48	0.49
30:X:189:LYS:HG3	30:X:230:ILE:HD12	1.95	0.49
2:1:292:TYR:O	2:1:296:VAL:HG23	2.12	0.48
3:3:169:PHE:CZ	3:3:173:LEU:HD11	2.48	0.48
6:7:259:PHE:O	6:7:289:GLY:N	2.47	0.48
7:8:170:GLU:CD	7:8:288:VAL:HG13	2.39	0.48
7:8:227:VAL:HG22	7:8:238:ILE:CD1	2.43	0.48
8:A:700:A:N1	8:A:709:G:O2'	2.42	0.48
17:K:50:GLU:OE1	31:Y:375:TRP:NE1	2.47	0.48
4:4:529:GLU:CD	4:4:533:MET:HE2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:243:PRO:O	9:B:247:HIS:ND1	2.45	0.48
13:F:40:GLU:OE2	13:F:73:LEU:HD12	2.14	0.48
11:D:319:ALA:HB2	11:D:342:MET:HE1	1.96	0.48
28:V:57:MET:HE1	28:V:75:LEU:HD13	1.96	0.48
7:8:348:VAL:HG23	7:8:348:VAL:O	2.13	0.48
30:X:162:VAL:HB	30:X:272:THR:HG22	1.96	0.47
8:A:703:A:OP2	27:U:43:ASN:ND2	2.47	0.47
1:0:123:LYS:NZ	1:0:158:GLU:OE2	2.45	0.47
1:0:186:THR:O	1:0:186:THR:HG22	2.14	0.47
25:S:84:ALA:HB3	29:W:101:ILE:HD11	1.97	0.47
12:E:5:GLU:OE2	22:P:74:TYR:OH	2.23	0.47
14:G:166:TYR:CE2	14:G:170:LEU:HD11	2.50	0.47
2:1:62:VAL:HG12	2:1:62:VAL:O	2.15	0.47
3:3:155:ARG:O	3:3:158:GLN:N	2.47	0.47
4:4:66:ASP:OD1	4:4:67:LYS:N	2.44	0.47
4:4:259:TYR:HB3	4:4:282:LEU:HD13	1.97	0.47
28:V:190:LEU:HD22	28:V:226:TYR:OH	2.14	0.47
12:E:49:TYR:OH	12:E:90:ARG:NH1	2.48	0.47
12:E:15:ARG:NH1	27:U:182:ASP:OD1	2.47	0.47
9:B:67:LEU:HD11	9:B:138:ARG:NH2	2.29	0.47
4:4:70:VAL:HG21	15:H:158:GLU:OE1	2.14	0.46
13:F:46:ILE:O	13:F:46:ILE:HG22	2.15	0.46
8:A:1260:A:N6	8:A:1330:C:H42	2.14	0.46
5:5:148:THR:OG1	5:5:149:PRO:HD3	2.14	0.46
6:7:415:LEU:HD22	6:7:428:ALA:CB	2.44	0.46
20:N:67:ARG:NH1	20:N:80:GLU:OE2	2.49	0.46
31:Y:282:PHE:CE2	31:Y:286:LEU:HD11	2.51	0.46
33:a:133:LEU:HD23	33:a:165:LEU:HD11	1.97	0.46
4:4:397:MET:HE1	4:4:438:LEU:HD22	1.98	0.46
14:G:75:LYS:O	14:G:79:GLU:OE1	2.34	0.46
2:1:164:ARG:NH1	31:Y:319:ALA:O	2.44	0.46
3:3:184:GLU:OE2	3:3:184:GLU:N	2.47	0.46
24:R:325:ILE:HD12	24:R:325:ILE:H	1.80	0.46
26:T:92:THR:O	26:T:92:THR:HG22	2.16	0.46
8:A:1258:A:H61	8:A:1330:C:H5'	1.80	0.46
5:5:12:LEU:HD22	5:5:97:LEU:HD11	1.98	0.46
12:E:105:CYS:SG	12:E:106:GLU:N	2.89	0.46
14:G:98:THR:HG22	14:G:98:THR:O	2.15	0.46
5:5:58:TYR:CD2	5:5:125:LEU:HD11	2.50	0.46
14:G:198:ARG:NH1	14:G:201:ILE:HG23	2.31	0.46
5:5:64:PRO:CG	5:5:83:VAL:HG13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:122:GLN:NE2	13:F:138:GLU:O	2.44	0.45
15:H:108:VAL:HG22	15:H:143:LEU:CD2	2.46	0.45
7:8:170:GLU:OE1	7:8:288:VAL:HG13	2.17	0.45
8:A:1231:A:H2'	8:A:1232:A:H4'	1.97	0.45
30:X:295:LYS:NZ	41:X:503:GDP:O3A	2.50	0.45
10:C:62:ILE:HD11	17:K:116:ASP:O	2.17	0.45
11:D:245:VAL:HG22	11:D:271:ALA:HB1	1.99	0.45
4:4:392:ILE:HD12	31:Y:250:ILE:HG21	1.99	0.45
4:4:573:ALA:O	4:4:577:ASN:ND2	2.50	0.45
4:4:643:GLU:OE2	4:4:643:GLU:N	2.45	0.45
5:5:36:ASN:ND2	5:5:219:PRO:O	2.46	0.45
8:A:1059:U:N3	8:A:1060:A:N7	2.65	0.45
30:X:153:LEU:HD22	30:X:296:MET:HE2	1.99	0.45
4:4:120:ILE:HD13	32:Z:65:LEU:HD11	1.98	0.45
2:1:239:TRP:CZ2	32:Z:7:TYR:HA	2.52	0.44
4:4:523:PHE:CE2	4:4:562:GLN:NE2	2.80	0.44
10:C:138:TYR:OH	32:Z:65:LEU:HD12	2.17	0.44
1:0:178:ARG:NH2	1:0:185:SER:O	2.51	0.44
4:4:293:THR:O	4:4:297:LEU:HD23	2.17	0.44
13:F:46:ILE:HG23	14:G:315:PHE:CZ	2.52	0.44
8:A:1532:C:H3'	8:A:1533:C:C5'	2.47	0.44
12:E:10:LEU:CD2	12:E:88:VAL:HG22	2.48	0.44
28:V:225:LEU:HD11	28:V:283:LEU:HD22	1.99	0.44
8:A:1048:C:O2'	18:L:198:ARG:N	2.50	0.44
28:V:75:LEU:C	28:V:75:LEU:HD23	2.43	0.44
4:4:248:PHE:HA	4:4:251:MET:HE2	1.98	0.44
4:4:289:ALA:HB3	4:4:294:PHE:CE2	2.53	0.44
8:A:1580:U:O2'	8:A:1582:G:OP1	2.28	0.44
28:V:29:LEU:HD11	28:V:184:TYR:CD2	2.52	0.44
30:X:151:LEU:HD21	30:X:247:LEU:HD22	1.99	0.44
13:F:91:ILE:HG23	13:F:111:MET:HE2	2.00	0.44
27:U:100:ALA:O	27:U:104:GLU:OE1	2.35	0.44
2:1:152:ASP:OD1	15:H:175:THR:HG23	2.17	0.44
6:7:36:GLN:NE2	6:7:440:LEU:HD11	2.32	0.44
6:7:104:GLU:O	6:7:108:ARG:NE	2.48	0.44
7:8:209:LEU:O	7:8:213:GLU:OE1	2.36	0.44
8:A:1031:G:H21	22:P:116:ILE:CD1	2.30	0.44
6:7:43:PHE:CE1	6:7:52:HIS:HA	2.53	0.44
31:Y:322:ASP:OD1	31:Y:322:ASP:O	2.36	0.43
2:1:182:LEU:HD22	2:1:186:ALA:HB1	2.01	0.43
4:4:75:ALA:HB2	31:Y:298:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:395:ARG:NE	8:A:1256:A:OP1	2.41	0.43
32:Z:4:LEU:HD23	32:Z:5:SER:O	2.19	0.43
4:4:363:ILE:HD11	4:4:365:ILE:HD12	1.99	0.43
9:B:229:PRO:HA	9:B:232:ILE:HD13	2.01	0.43
18:L:116:VAL:HG12	18:L:126:GLU:CG	2.49	0.43
24:R:303:LEU:HA	24:R:306:VAL:HG12	2.00	0.43
7:8:86:ARG:O	7:8:90:LEU:HD13	2.19	0.43
8:A:683:G:O2'	26:T:150:PRO:O	2.34	0.43
13:F:235:ALA:HB2	33:a:259:VAL:HG11	2.01	0.43
5:5:240:GLN:OE1	5:5:308:ARG:HD2	2.19	0.43
4:4:104:ARG:O	4:4:108:LEU:HD13	2.18	0.43
4:4:120:ILE:HD13	32:Z:65:LEU:CD1	2.49	0.43
6:7:38:ASP:HA	6:7:440:LEU:HD23	2.00	0.43
12:E:101:GLU:OE2	12:E:101:GLU:N	2.50	0.43
4:4:641:ILE:O	4:4:641:ILE:HG22	2.19	0.43
8:A:1140:A:H2	8:A:1163:C:H42	1.66	0.42
4:4:529:GLU:OE1	4:4:533:MET:HE2	2.18	0.42
10:C:138:TYR:CE2	32:Z:70:LEU:HD13	2.54	0.42
33:a:132:GLN:OE1	33:a:313:GLN:NE2	2.53	0.42
4:4:156:ALA:HB3	4:4:172:MET:HE2	2.01	0.42
6:7:383:HIS:O	6:7:383:HIS:ND1	2.52	0.42
33:a:206:VAL:HG23	33:a:250:LEU:CD1	2.50	0.42
4:4:508:VAL:HG12	4:4:508:VAL:O	2.19	0.42
8:A:893:G:N7	16:J:78:ARG:NH1	2.67	0.42
8:A:1298:U:H2'	8:A:1299:A:O4'	2.20	0.42
9:B:269:ALA:O	9:B:273:LEU:HD13	2.20	0.42
10:C:113:ARG:NH2	10:C:118:GLU:OE2	2.51	0.42
30:X:262:VAL:HG21	30:X:297:MET:HE1	2.00	0.42
6:7:398:HIS:CB	6:7:416:THR:HG22	2.49	0.42
8:A:932:C:N3	26:T:11:ARG:NH2	2.68	0.42
4:4:526:ASP:O	4:4:530:GLU:OE1	2.36	0.42
7:8:251:ASN:OD1	7:8:254:LYS:HG2	2.19	0.42
24:R:263:ARG:NH2	24:R:287:ASP:OD2	2.44	0.42
6:7:386:PRO:HB2	6:7:403:LEU:HD22	2.02	0.42
9:B:157:ASN:OD1	9:B:160:ARG:NH1	2.48	0.42
5:5:323:ARG:NH1	8:A:1088:C:O2	2.50	0.42
8:A:1493:C:N4	8:A:1555:A:N1	2.67	0.42
14:G:198:ARG:HH11	14:G:201:ILE:HG23	1.85	0.42
30:X:108:LEU:HD23	30:X:141:VAL:HG21	2.02	0.42
2:1:217:GLN:NE2	31:Y:326:SER:O	2.52	0.41
32:Z:61:LEU:HD12	32:Z:65:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:206:PHE:O	7:8:210:GLU:OE1	2.37	0.41
8:A:1029:U:H2'	8:A:1030:G:H5'	2.01	0.41
7:8:176:LYS:O	7:8:180:GLU:OE1	2.38	0.41
4:4:458:TYR:HB3	4:4:486:TYR:CD1	2.56	0.41
8:A:1557:A:H2'	8:A:1558:A:N7	2.35	0.41
15:H:108:VAL:HG22	15:H:143:LEU:HD23	2.03	0.41
18:L:140:GLU:O	18:L:144:GLU:HG3	2.19	0.41
10:C:92:LEU:HD11	10:C:117:LEU:HD21	2.03	0.41
33:a:117:VAL:HG22	33:a:166:LEU:HD12	2.03	0.41
2:1:126:LEU:HD21	4:4:70:VAL:HG13	2.02	0.41
4:4:362:ALA:HB1	31:Y:255:ARG:NH1	2.36	0.41
4:4:496:LEU:HD21	4:4:512:ILE:HD12	2.03	0.41
1:0:56:ALA:HB1	28:V:313:LEU:HD11	2.03	0.41
13:F:46:ILE:HG23	14:G:315:PHE:HZ	1.86	0.41
15:H:136:MET:HG2	17:K:123:ILE:HD13	2.03	0.41
18:L:167:LEU:HD11	18:L:187:ILE:HG21	2.01	0.41
4:4:166:VAL:HG13	4:4:195:LEU:HD23	2.03	0.41
7:8:307:ARG:NH2	8:A:1231:A:N1	2.69	0.41
8:A:1071:U:OP1	8:A:1581:G:O2'	2.14	0.41
8:A:1330:C:H1'	8:A:1331:A:OP2	2.21	0.41
12:E:47:LEU:HD13	12:E:51:ILE:HD12	2.03	0.41
13:F:41:PHE:CZ	13:F:73:LEU:HD13	2.56	0.41
27:U:173:LEU:O	27:U:177:VAL:HG23	2.20	0.41
30:X:102:ARG:NH1	30:X:132:THR:O	2.50	0.41
4:4:320:LEU:HB3	31:Y:258:ILE:HD13	2.03	0.41
5:5:157:ASN:O	5:5:161:ARG:N	2.54	0.41
7:8:111:GLN:NE2	7:8:115:ASP:OD1	2.53	0.41
7:8:59:PRO:HD2	7:8:59:PRO:O	2.21	0.40
13:F:235:ALA:CB	33:a:259:VAL:HG11	2.51	0.40
33:a:219:LEU:O	33:a:223:LEU:HD12	2.22	0.40
3:3:155:ARG:O	3:3:159:GLU:OE1	2.39	0.40
4:4:596:LEU:HD11	4:4:614:LEU:HD13	2.04	0.40
30:X:151:LEU:CD2	30:X:247:LEU:HD22	2.50	0.40
5:5:15:LEU:HD23	5:5:16:PRO:O	2.21	0.40
8:A:1338:A:C2	8:A:1339:G:C8	3.09	0.40
13:F:158:LEU:HD11	13:F:229:MET:SD	2.62	0.40
2:1:211:ARG:HE	31:Y:332:ILE:HD12	1.87	0.40
13:F:176:ASP:HA	13:F:179:ARG:HE	1.87	0.40
28:V:35:VAL:O	28:V:35:VAL:HG12	2.22	0.40
7:8:252:SER:O	7:8:256:HIS:N	2.55	0.40
15:H:160:ILE:HD12	15:H:170:MET:HE1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:100:VAL:HG11	29:W:144:LEU:HD11	2.03	0.40
30:X:353:PHE:CZ	30:X:357:ILE:HD11	2.56	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	0	209/218 (96%)	208 (100%)	1 (0%)	0	100	100
2	1	255/323 (79%)	251 (98%)	4 (2%)	0	100	100
3	3	43/199 (22%)	42 (98%)	1 (2%)	0	100	100
4	4	558/689 (81%)	549 (98%)	9 (2%)	0	100	100
5	5	317/346 (92%)	311 (98%)	6 (2%)	0	100	100
6	7	394/456 (86%)	381 (97%)	13 (3%)	0	100	100
7	8	324/390 (83%)	316 (98%)	8 (2%)	0	100	100
9	B	218/296 (74%)	216 (99%)	2 (1%)	0	100	100
10	C	122/167 (73%)	120 (98%)	2 (2%)	0	100	100
11	D	228/430 (53%)	223 (98%)	5 (2%)	0	100	100
12	E	103/125 (82%)	103 (100%)	0	0	100	100
13	F	206/242 (85%)	203 (98%)	3 (2%)	0	100	100
14	G	287/396 (72%)	281 (98%)	6 (2%)	0	100	100
15	H	126/201 (63%)	124 (98%)	2 (2%)	0	100	100
16	J	106/138 (77%)	102 (96%)	4 (4%)	0	100	100
17	K	31/128 (24%)	30 (97%)	1 (3%)	0	100	100
18	L	159/257 (62%)	158 (99%)	1 (1%)	0	100	100
19	M	113/137 (82%)	113 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	N	107/130 (82%)	107 (100%)	0	0	100	100
21	O	188/258 (73%)	185 (98%)	3 (2%)	0	100	100
22	P	90/142 (63%)	89 (99%)	1 (1%)	0	100	100
23	Q	4/87 (5%)	4 (100%)	0	0	100	100
24	R	289/360 (80%)	284 (98%)	5 (2%)	0	100	100
25	S	131/190 (69%)	130 (99%)	1 (1%)	0	100	100
26	T	162/173 (94%)	160 (99%)	2 (1%)	0	100	100
27	U	172/205 (84%)	168 (98%)	4 (2%)	0	100	100
28	V	355/414 (86%)	349 (98%)	6 (2%)	0	100	100
29	W	96/187 (51%)	95 (99%)	1 (1%)	0	100	100
30	X	350/398 (88%)	346 (99%)	4 (1%)	0	100	100
31	Y	119/395 (30%)	118 (99%)	1 (1%)	0	100	100
32	Z	52/106 (49%)	47 (90%)	5 (10%)	0	100	100
33	a	253/437 (58%)	248 (98%)	5 (2%)	0	100	100
All	All	6167/8620 (72%)	6061 (98%)	106 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	0	184/190 (97%)	184 (100%)	0	100	100
2	1	239/291 (82%)	239 (100%)	0	100	100
3	3	40/166 (24%)	40 (100%)	0	100	100
4	4	506/609 (83%)	506 (100%)	0	100	100
5	5	286/309 (93%)	286 (100%)	0	100	100
6	7	339/385 (88%)	339 (100%)	0	100	100
7	8	270/317 (85%)	270 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	B	194/249 (78%)	194 (100%)	0	100	100
10	C	111/143 (78%)	111 (100%)	0	100	100
11	D	196/357 (55%)	196 (100%)	0	100	100
12	E	89/107 (83%)	89 (100%)	0	100	100
13	F	185/209 (88%)	185 (100%)	0	100	100
14	G	253/342 (74%)	253 (100%)	0	100	100
15	H	120/180 (67%)	120 (100%)	0	100	100
16	J	93/118 (79%)	93 (100%)	0	100	100
17	K	30/113 (26%)	30 (100%)	0	100	100
18	L	151/226 (67%)	151 (100%)	0	100	100
19	M	94/113 (83%)	94 (100%)	0	100	100
20	N	95/115 (83%)	95 (100%)	0	100	100
21	O	171/230 (74%)	171 (100%)	0	100	100
22	P	83/123 (68%)	83 (100%)	0	100	100
23	Q	5/79 (6%)	5 (100%)	0	100	100
24	R	261/318 (82%)	261 (100%)	0	100	100
25	S	115/164 (70%)	115 (100%)	0	100	100
26	T	151/157 (96%)	151 (100%)	0	100	100
27	U	150/174 (86%)	150 (100%)	0	100	100
28	V	323/364 (89%)	323 (100%)	0	100	100
29	W	85/158 (54%)	85 (100%)	0	100	100
30	X	311/351 (89%)	311 (100%)	0	100	100
31	Y	113/357 (32%)	113 (100%)	0	100	100
32	Z	51/95 (54%)	51 (100%)	0	100	100
33	a	151/386 (39%)	151 (100%)	0	100	100
All	All	5445/7495 (73%)	5445 (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 (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	111	HIS

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Mol	Chain	Res	Type
2	1	231	HIS
4	4	373	HIS
4	4	577	ASN
4	4	602	HIS
5	5	95	GLN
5	5	137	HIS
5	5	171	GLN
5	5	229	HIS
5	5	254	GLN
5	5	272	GLN
5	5	316	GLN
6	7	51	GLN
6	7	86	GLN
6	7	98	HIS
6	7	187	GLN
6	7	398	HIS
6	7	400	HIS
7	8	136	HIS
7	8	300	ASN
7	8	344	GLN
9	B	74	ASN
9	B	167	HIS
10	C	57	HIS
10	C	156	GLN
11	D	361	GLN
12	E	54	HIS
14	G	255	GLN
16	J	134	HIS
17	K	113	HIS
19	M	75	HIS
21	O	169	GLN
21	O	223	HIS
22	P	71	HIS
24	R	221	GLN
24	R	278	ASN
24	R	308	HIS
25	S	82	GLN
26	T	18	GLN
27	U	65	GLN
27	U	79	GLN
28	V	87	HIS
28	V	380	GLN

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Mol	Chain	Res	Type
28	V	381	GLN
29	W	173	GLN
30	X	154	HIS
30	X	394	HIS
31	Y	257	ASN
31	Y	292	GLN
33	a	321	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	A	792/955 (82%)	187 (23%)	6 (0%)

All (187) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	650	U
8	A	651	A
8	A	664	G
8	A	680	U
8	A	688	A
8	A	704	U
8	A	721	U
8	A	722	C
8	A	730	A
8	A	736	C
8	A	737	C
8	A	739	C
8	A	753	A
8	A	761	A
8	A	766	G
8	A	769	G
8	A	772	A
8	A	773	U
8	A	777	G
8	A	791	G
8	A	794	U
8	A	796	G
8	A	807	A
8	A	830	U
8	A	831	U

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Mol	Chain	Res	Type
8	A	832	U
8	A	835	C
8	A	851	A
8	A	860	A
8	A	861	U
8	A	868	C
8	A	871	A
8	A	883	U
8	A	889	G
8	A	893	G
8	A	902	G
8	A	903	U
8	A	919	A
8	A	930	G
8	A	931	C
8	A	939	A
8	A	942	A
8	A	943	G
8	A	949	U
8	A	954	C
8	A	967	A
8	A	972	G
8	A	977	A
8	A	1014	A
8	A	1015	A
8	A	1047	A
8	A	1048	C
8	A	1052	C
8	A	1056	A
8	A	1057	G
8	A	1058	C
8	A	1061	A
8	A	1077	U
8	A	1078	A
8	A	1079	G
8	A	1080	A
8	A	1081	U
8	A	1095	U
8	A	1097	G
8	A	1113	G
8	A	1117	A
8	A	1118	A

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Mol	Chain	Res	Type
8	A	1119	U
8	A	1120	C
8	A	1121	A
8	A	1126	A
8	A	1127	A
8	A	1128	C
8	A	1137	A
8	A	1151	C
8	A	1152	A
8	A	1160	A
8	A	1167	A
8	A	1175	G
8	A	1177	C
8	A	1178	G
8	A	1181	G
8	A	1185	C
8	A	1186	A
8	A	1187	U
8	A	1188	A
8	A	1189	U
8	A	1190	C
8	A	1191	C
8	A	1192	C
8	A	1198	A
8	A	1199	G
8	A	1200	G
8	A	1215	U
8	A	1216	C
8	A	1217	G
8	A	1218	A
8	A	1219	U
8	A	1220	A
8	A	1221	A
8	A	1222	A
8	A	1225	C
8	A	1226	C
8	A	1227	G
8	A	1228	A
8	A	1232	A
8	A	1233	C
8	A	1234	C
8	A	1242	C

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Mol	Chain	Res	Type
8	A	1245	U
8	A	1246	U
8	A	1247	G
8	A	1248	C
8	A	1249	U
8	A	1250	C
8	A	1254	C
8	A	1255	U
8	A	1258	A
8	A	1259	U
8	A	1260	A
8	A	1261	C
8	A	1283	A
8	A	1285	G
8	A	1287	A
8	A	1290	C
8	A	1291	U
8	A	1294	A
8	A	1296	A
8	A	1299	A
8	A	1327	G
8	A	1330	C
8	A	1331	A
8	A	1332	A
8	A	1334	G
8	A	1335	U
8	A	1338	A
8	A	1342	C
8	A	1344	U
8	A	1350	G
8	A	1351	G
8	A	1353	A
8	A	1354	A
8	A	1357	A
8	A	1360	G
8	A	1364	U
8	A	1367	A
8	A	1376	C
8	A	1378	C
8	A	1424	U
8	A	1427	A
8	A	1430	A

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Mol	Chain	Res	Type
8	A	1434	A
8	A	1440	G
8	A	1441	A
8	A	1442	G
8	A	1450	C
8	A	1463	G
8	A	1464	G
8	A	1467	C
8	A	1468	U
8	A	1470	A
8	A	1471	A
8	A	1474	G
8	A	1477	U
8	A	1494	C
8	A	1512	A
8	A	1519	A
8	A	1522	U
8	A	1525	C
8	A	1526	U
8	A	1527	A
8	A	1532	C
8	A	1533	C
8	A	1537	C
8	A	1538	G
8	A	1539	C
8	A	1556	C
8	A	1557	A
8	A	1558	A
8	A	1560	U
8	A	1564	A
8	A	1579	C
8	A	1582	G
8	A	1583	A
8	A	1584	A
8	A	1585	A
8	A	1591	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1077	U
8	A	1225	C

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Mol	Chain	Res	Type
8	A	1330	C
8	A	1466	C
8	A	1531	C
8	A	1536	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 32 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
35	SAM	7	502	-	27,29,29	1.11	5 (18%)	34,42,42	1.99	8 (23%)
34	SF4	7	501	6	0,12,12	-	-	-		
39	FES	P	201	12,22	0,4,4	-	-	-		
39	FES	T	201	19,26	0,4,4	-	-	-		
40	ATP	X	501	37	32,33,33	0.51	0	48,52,52	0.68	1 (2%)
41	GDP	X	503	-	29,30,30	3.28	10 (34%)	45,47,47	2.29	15 (33%)

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
35	SAM	7	502	-	-	2/17/33/33	0/3/3/3
34	SF4	7	501	6	-	-	0/6/5/5
39	FES	P	201	12,22	-	-	0/1/1/1
39	FES	T	201	19,26	-	-	0/1/1/1
40	ATP	X	501	37	-	0/22/38/38	0/3/3/3
41	GDP	X	503	-	-	3/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	503	GDP	O6-C6	9.76	1.42	1.23
41	X	503	GDP	C2-N1	7.67	1.56	1.37
41	X	503	GDP	PA-O3A	7.35	1.67	1.59
41	X	503	GDP	C2-N2	5.23	1.46	1.34
41	X	503	GDP	C2-N3	5.21	1.45	1.33
41	X	503	GDP	C2'-C3'	-2.93	1.45	1.53
35	7	502	SAM	C2-N3	2.60	1.38	1.33
41	X	503	GDP	C6-N1	2.55	1.43	1.38
35	7	502	SAM	C2-N1	2.47	1.38	1.33
41	X	503	GDP	PB-O3B	-2.35	1.46	1.54
41	X	503	GDP	PA-O5'	2.30	1.68	1.59
35	7	502	SAM	OXT-C	-2.25	1.23	1.30
41	X	503	GDP	PB-O2B	-2.19	1.46	1.54
35	7	502	SAM	C8-N7	2.07	1.35	1.31
35	7	502	SAM	C5-N7	-2.06	1.35	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	X	503	GDP	C8-N7-C5	6.81	116.39	104.26
41	X	503	GDP	N9-C8-N7	-6.74	100.90	113.40
35	7	502	SAM	N3-C2-N1	-5.57	120.15	128.58
41	X	503	GDP	C2-N1-C6	-4.84	116.33	125.11
35	7	502	SAM	C5-C4-N3	-4.68	120.27	126.72
41	X	503	GDP	C8-N9-C4	3.96	113.44	106.03
35	7	502	SAM	N9-C8-N7	-3.83	108.51	113.94
41	X	503	GDP	C6-C5-C4	3.54	124.16	118.83
35	7	502	SAM	C2-N3-C4	3.50	120.38	111.83
35	7	502	SAM	C5-N7-C8	3.39	108.78	103.45
41	X	503	GDP	C4-C5-N7	-3.22	105.57	110.67
35	7	502	SAM	N3-C4-N9	3.01	132.29	127.17
41	X	503	GDP	C2-N3-C4	2.94	117.37	112.30
41	X	503	GDP	O2B-PB-O3A	2.78	113.95	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	X	503	GDP	N9-C4-N3	2.71	131.38	125.95
41	X	503	GDP	O3B-PB-O3A	2.69	113.65	104.64
35	7	502	SAM	OXT-C-O	-2.62	118.15	124.08
41	X	503	GDP	O2A-PA-O1A	-2.34	101.55	112.44
35	7	502	SAM	C4-C5-N7	-2.34	107.91	110.58
41	X	503	GDP	C3'-C2'-C1'	2.20	105.63	101.46
41	X	503	GDP	C5-C4-N3	-2.18	124.92	128.39
41	X	503	GDP	O6-C6-C5	-2.09	121.01	126.53
40	X	501	ATP	O3'-C3'-C4'	-2.08	105.11	111.08
41	X	503	GDP	N1-C2-N3	-2.02	119.62	123.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	7	502	SAM	CB-CG-SD-CE
35	7	502	SAM	CB-CG-SD-C5'
41	X	503	GDP	C5'-O5'-PA-O1A
41	X	503	GDP	PB-O3A-PA-O1A
41	X	503	GDP	O4'-C4'-C5'-O5'

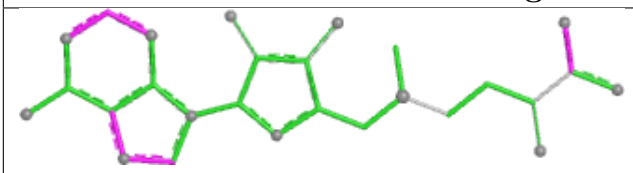
There are no ring outliers.

2 monomers are involved in 2 short contacts:

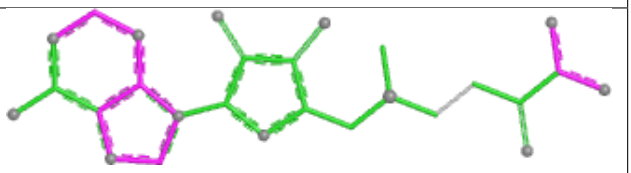
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	7	502	SAM	1	0
41	X	503	GDP	1	0

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 then 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.

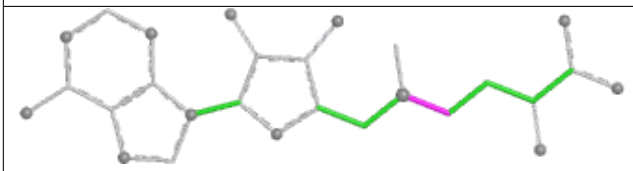
Ligand SAM 7 502



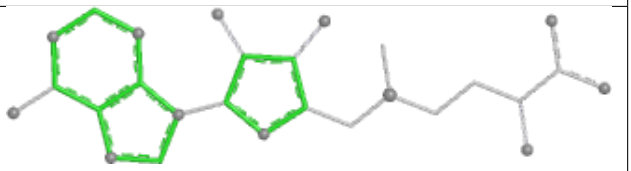
Bond lengths



Bond angles

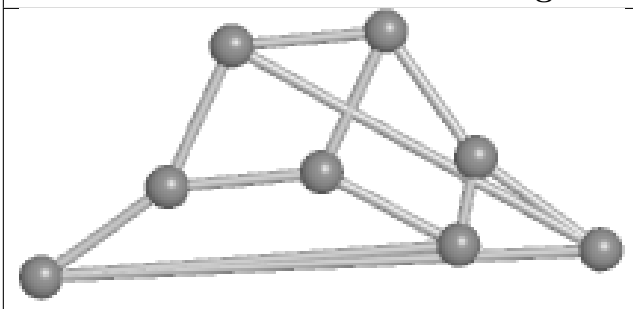


Torsions

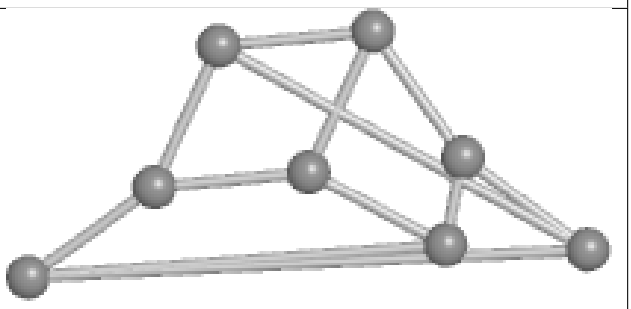


Rings

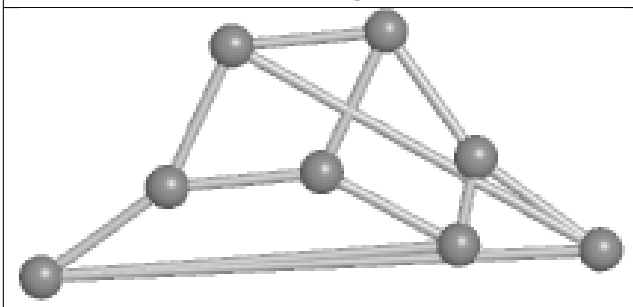
Ligand SF4 7 501



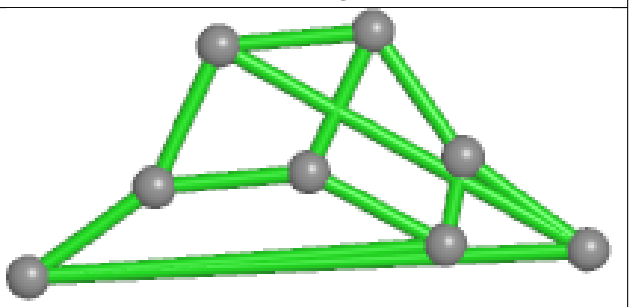
Bond lengths



Bond angles

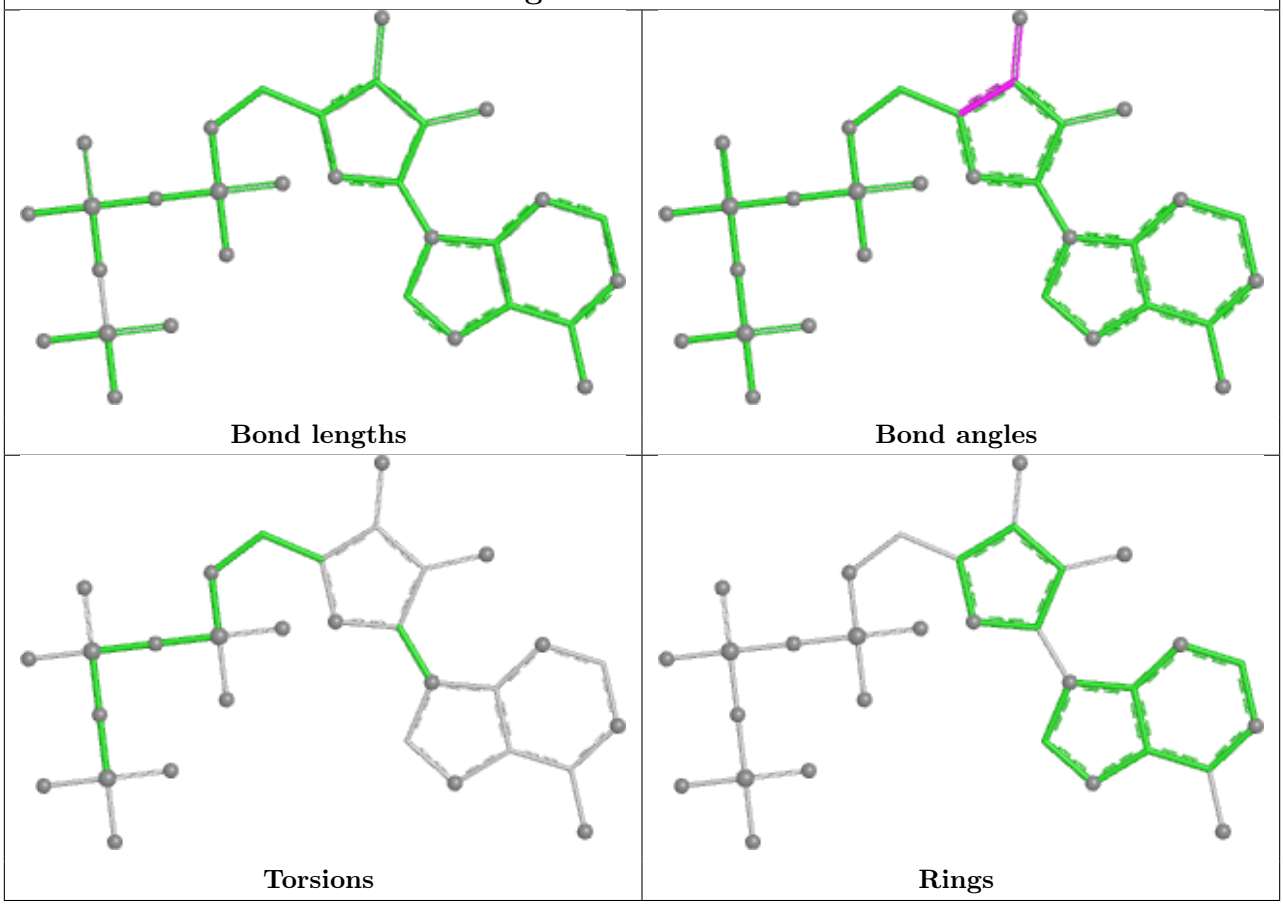


Torsions

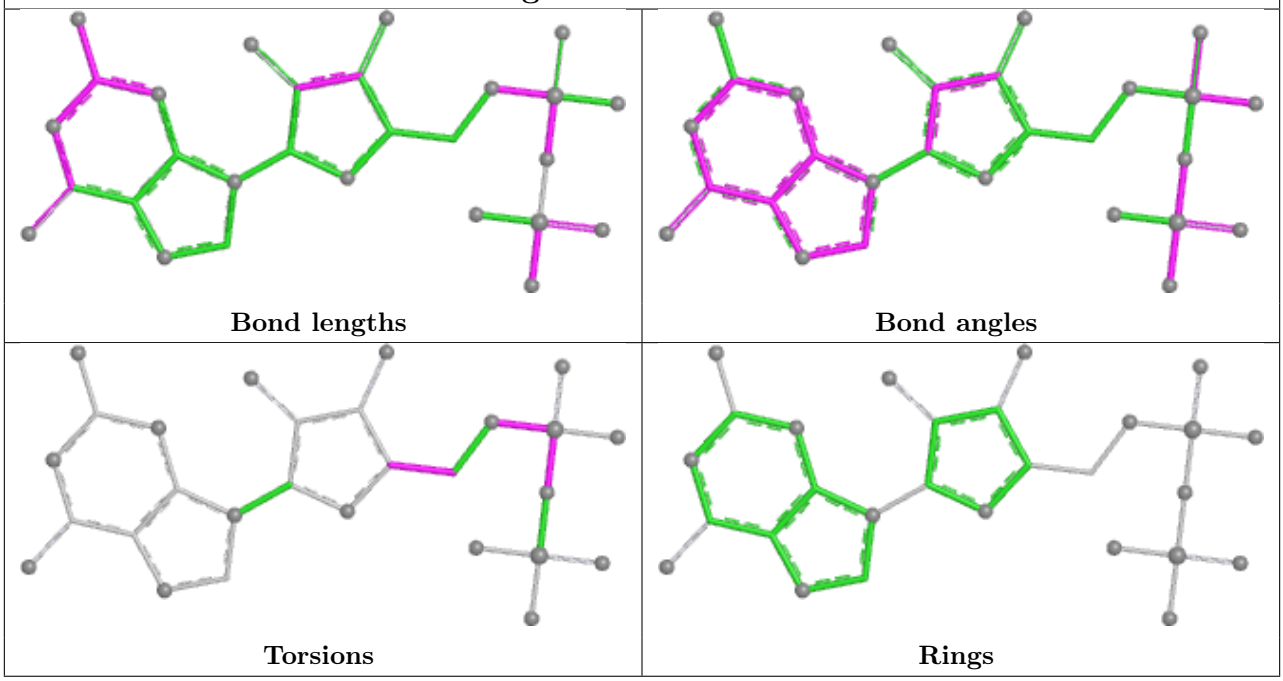


Rings

Ligand ATP X 501



Ligand GDP X 503



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.

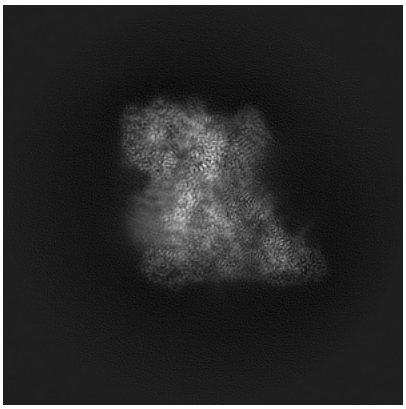
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26967. These allow visual inspection of the internal detail of the map and identification of artifacts.

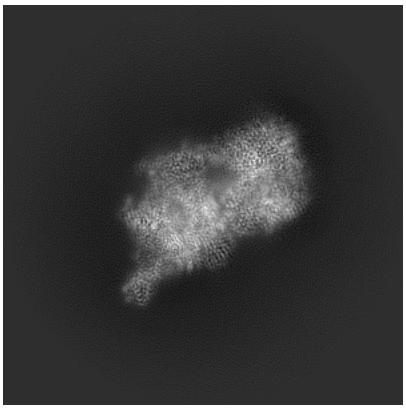
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

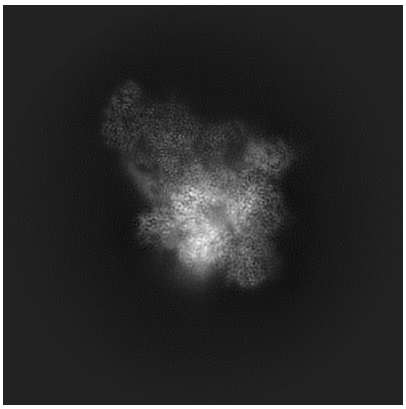
6.1.1 Primary map



X

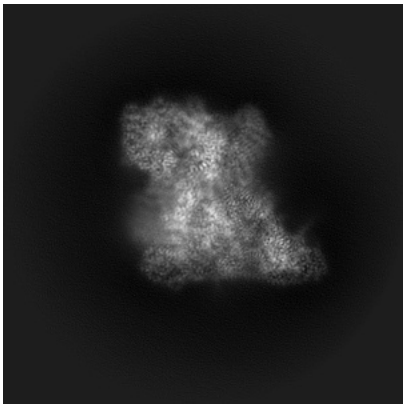


Y

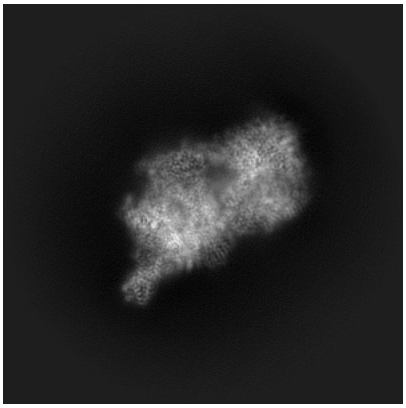


Z

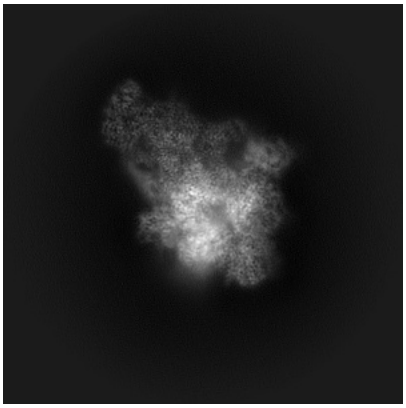
6.1.2 Raw map



X



Y

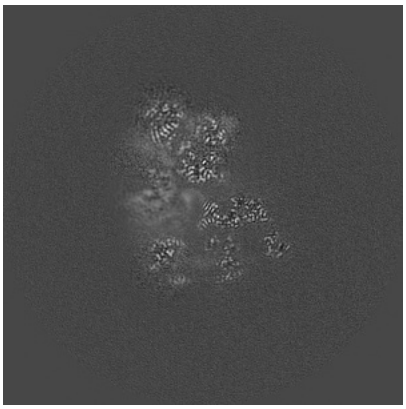


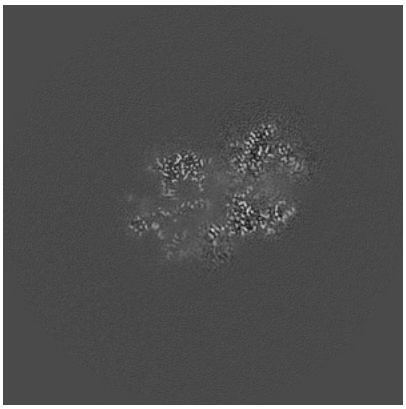
Z

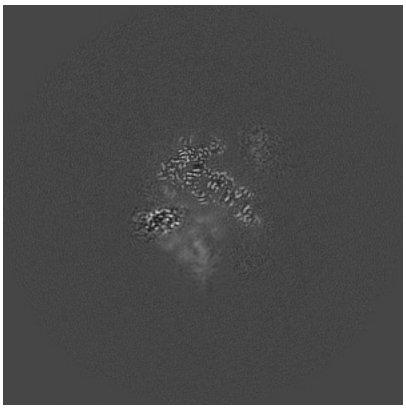
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

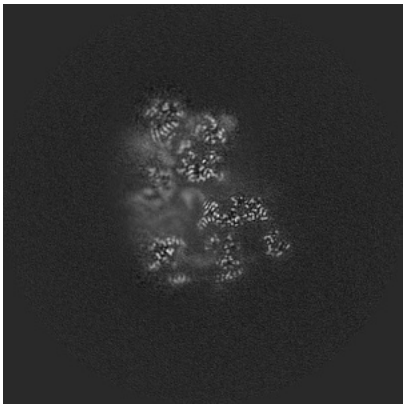
6.2.1 Primary map

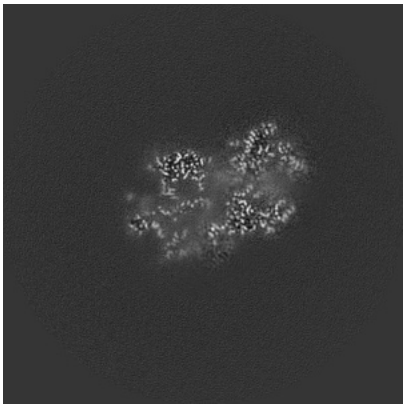

X Index: 200

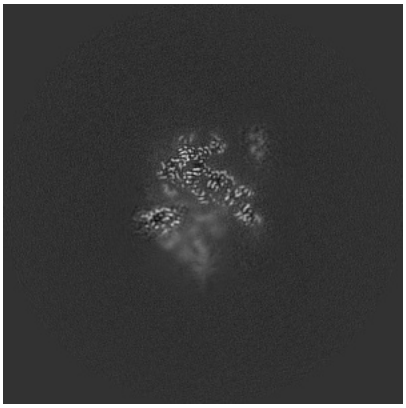

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

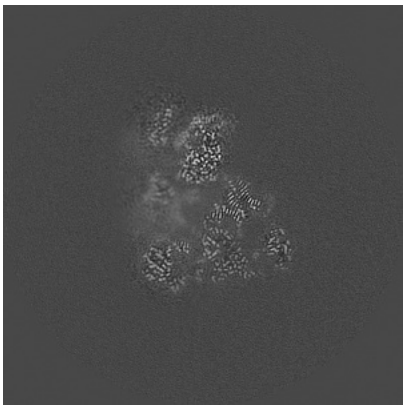

Y Index: 200


Z Index: 200

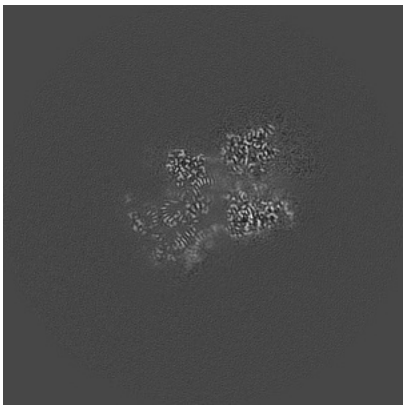
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

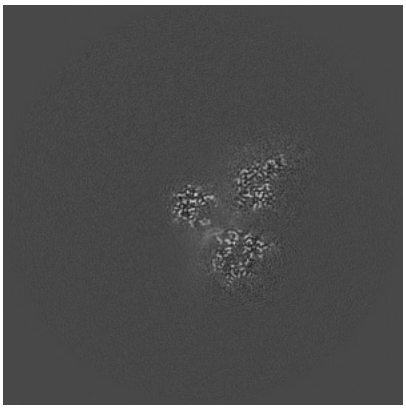
6.3.1 Primary map



X Index: 190

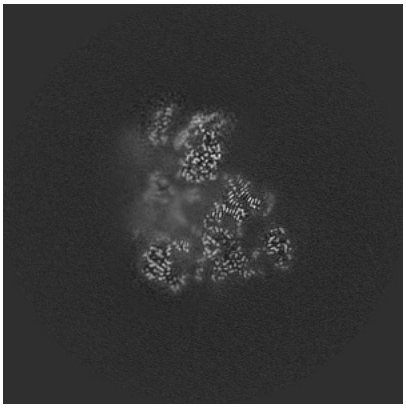


Y Index: 209

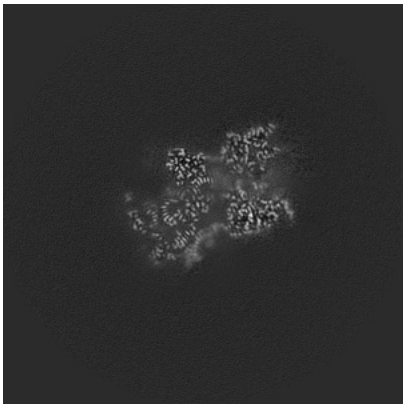


Z Index: 243

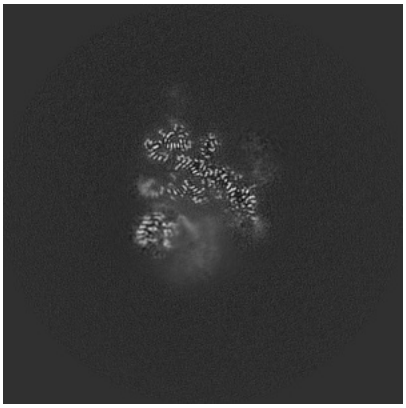
6.3.2 Raw map



X Index: 190



Y Index: 209

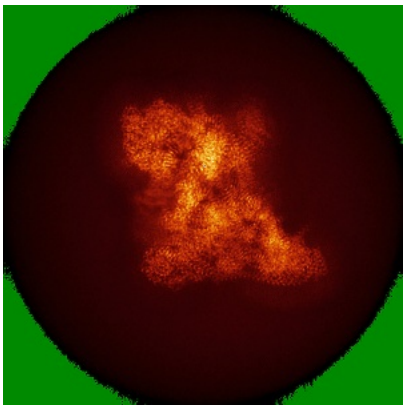


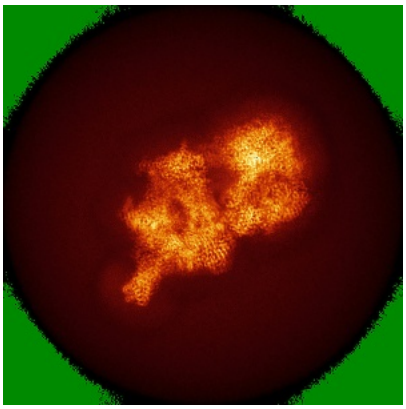
Z Index: 187

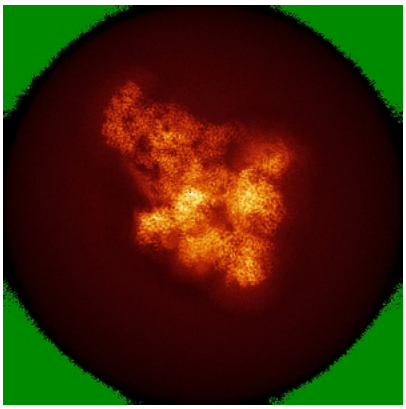
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

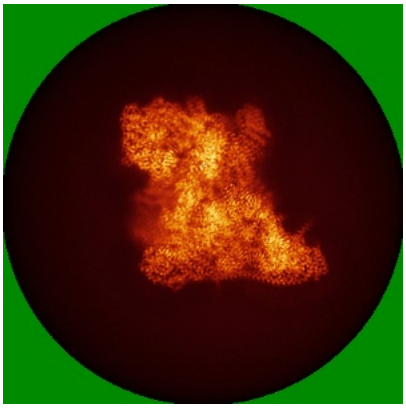
6.4.1 Primary map

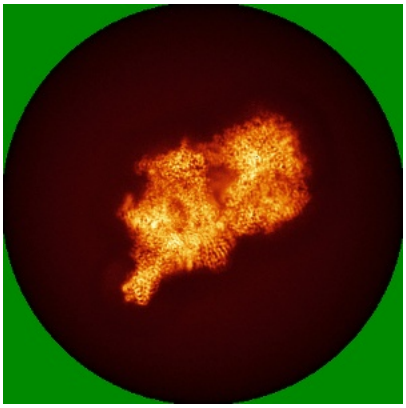

X

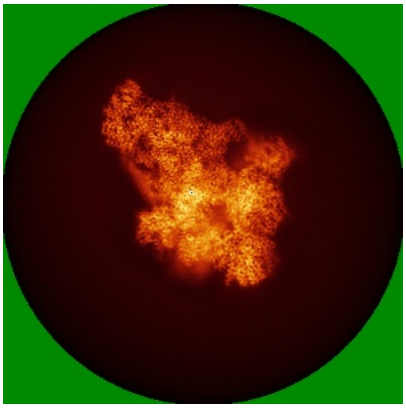

Y


Z

6.4.2 Raw map


X

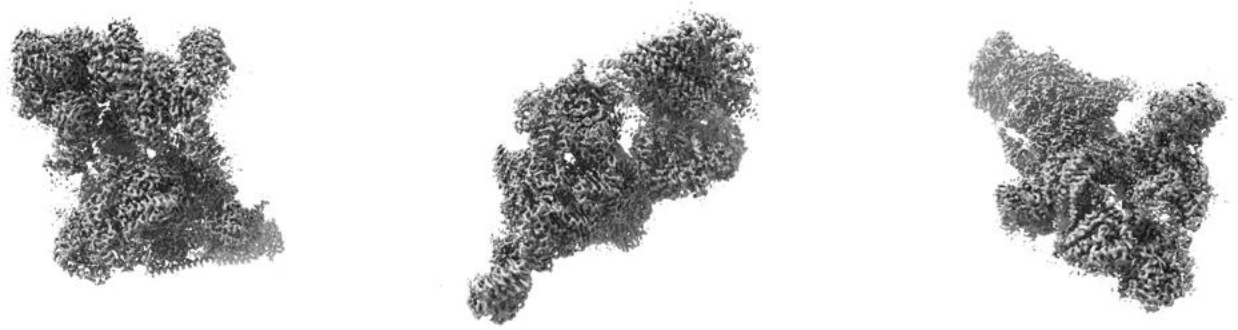

Y


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)

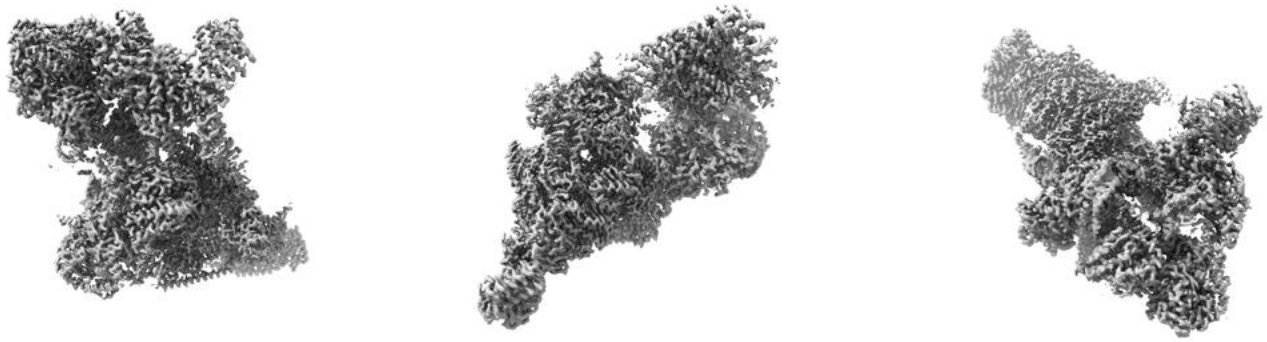
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 8.5. 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.

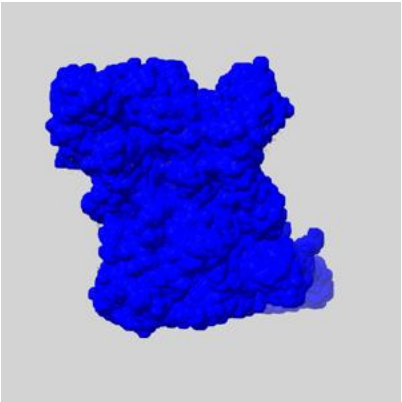
6.6 Mask visualisation (i)

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

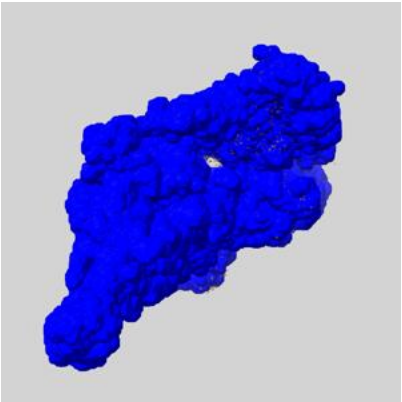
A mask typically either:

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

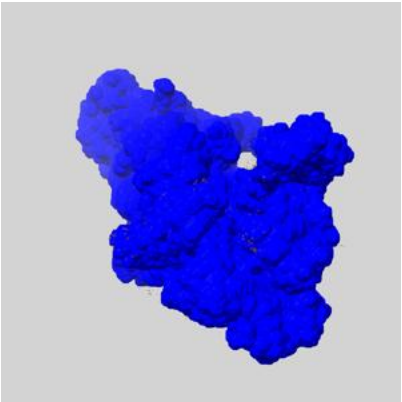
6.6.1 emd_26967_msk_1.map (i)



X



Y

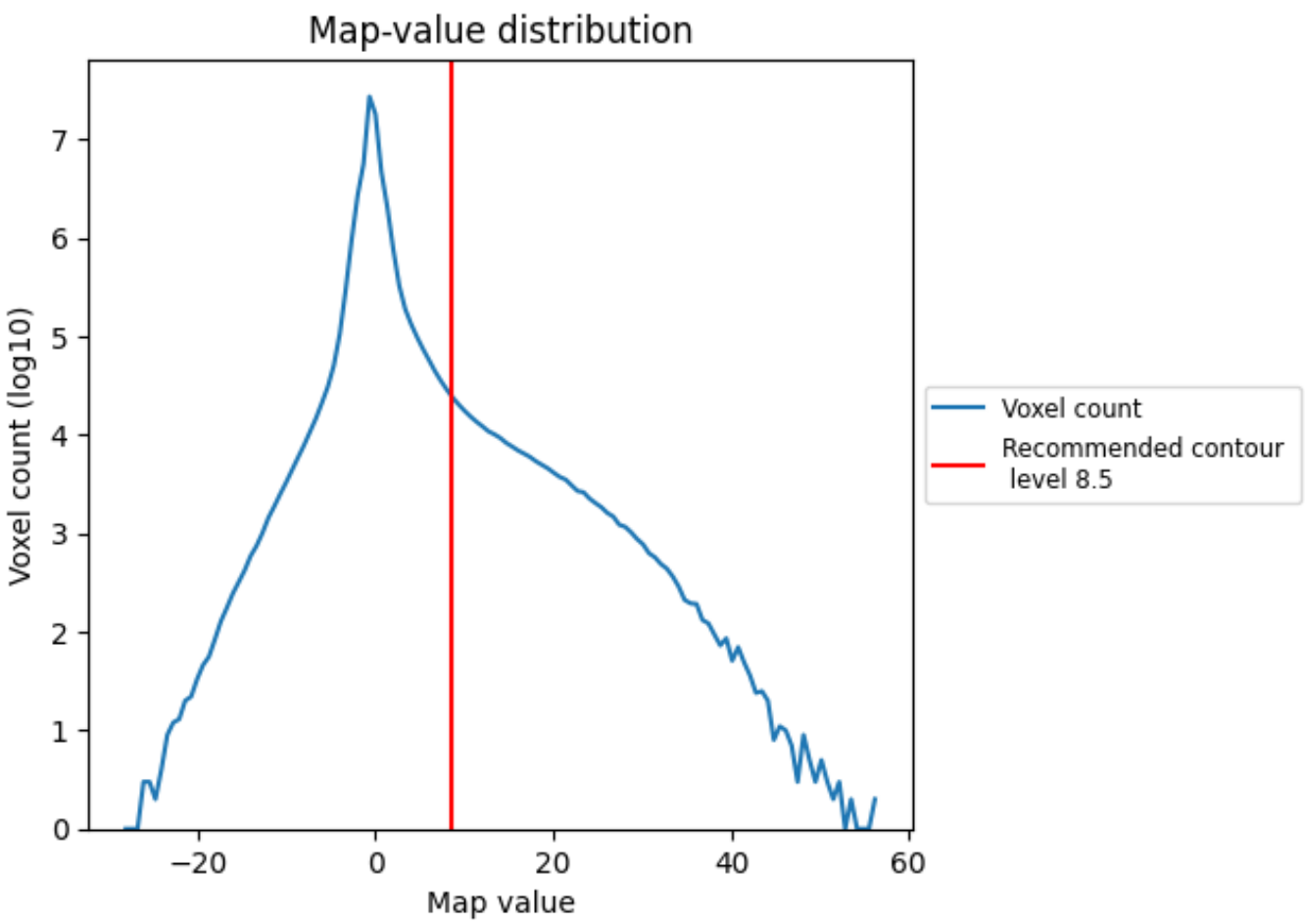


Z

7 Map analysis (i)

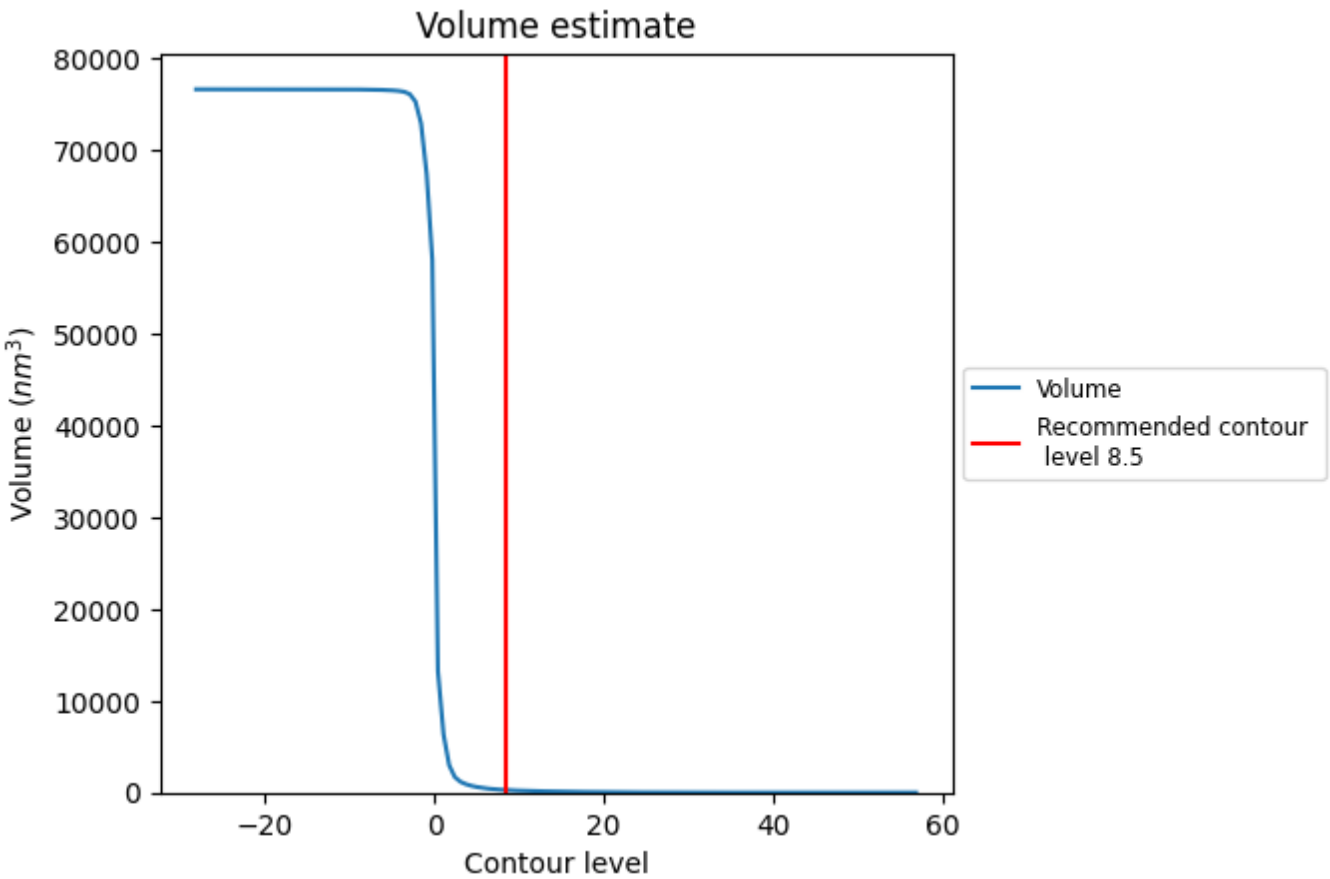
This section contains the results of statistical analysis of the map.

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.

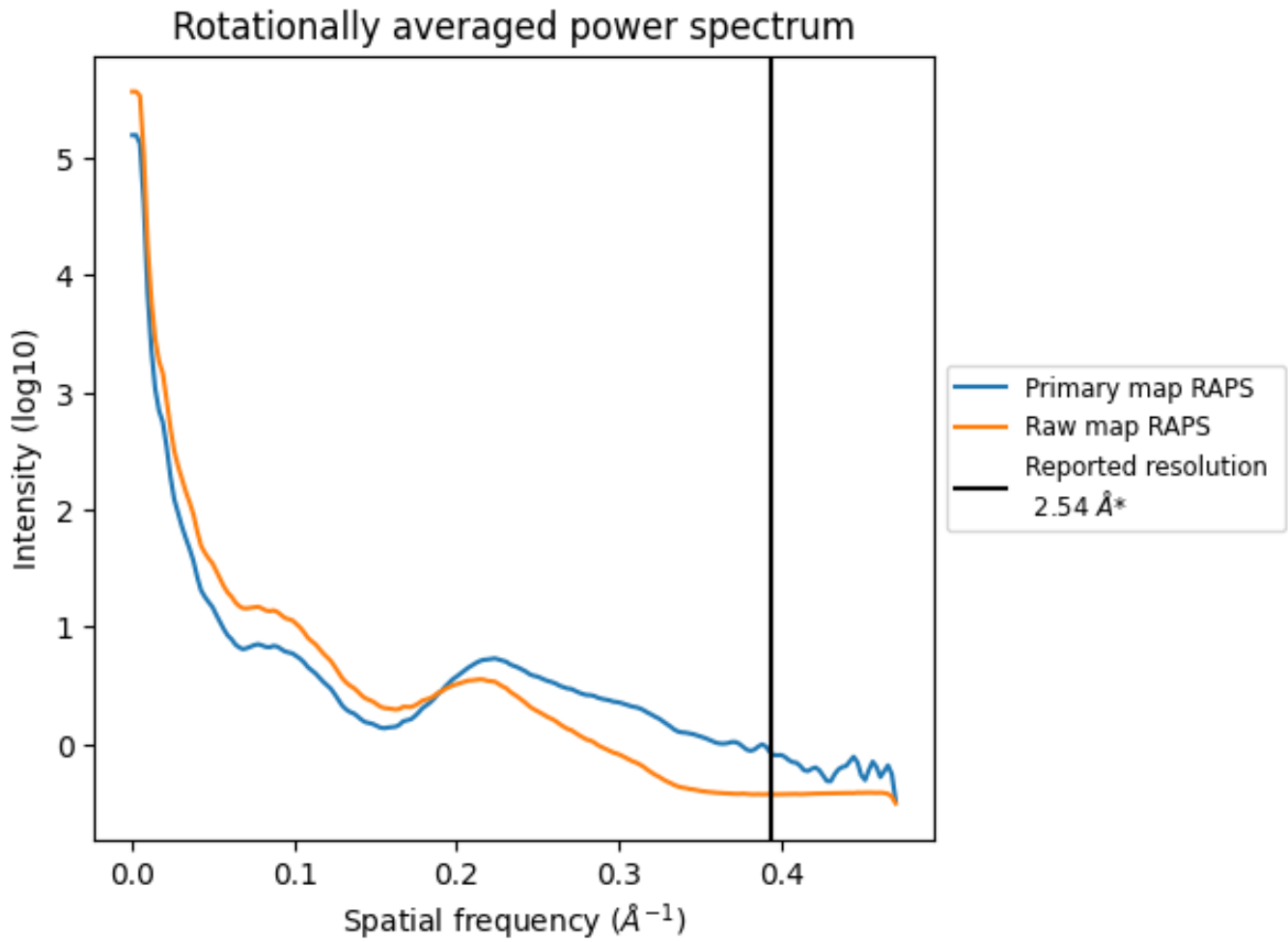
7.2 Volume estimate (i)



The volume at the recommended contour level is 276 nm^3; this corresponds to an approximate mass of 249 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 (i)

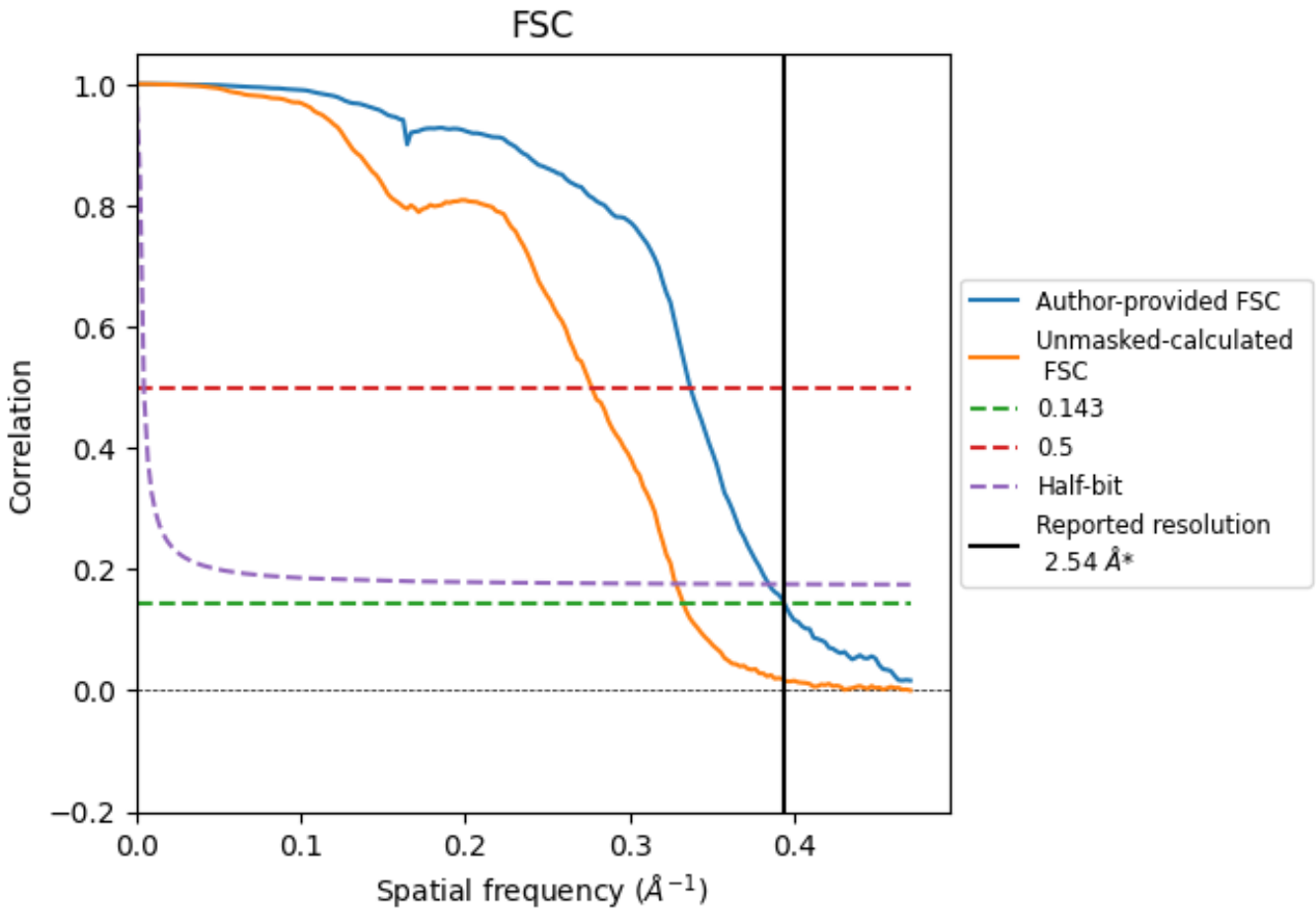


*Reported resolution corresponds to spatial frequency of 0.394 Å^{-1}

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 0.394 Å^{-1}

8.2 Resolution estimates (i)

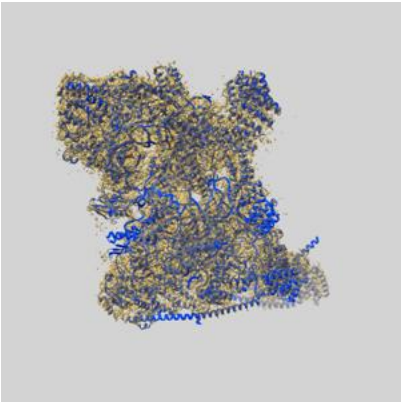
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.54	2.97	2.60
Unmasked-calculated*	3.00	3.61	3.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.54 by more than 10 %

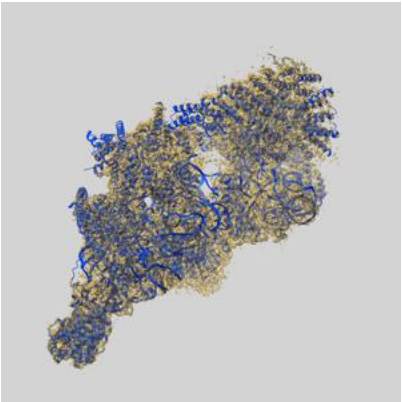
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26967 and PDB model 8CSQ. Per-residue inclusion information can be found in section 3 on page 13.

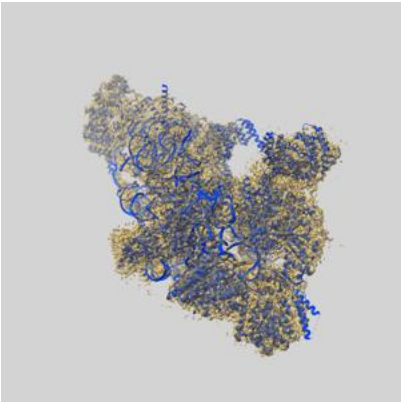
9.1 Map-model overlay (i)



X



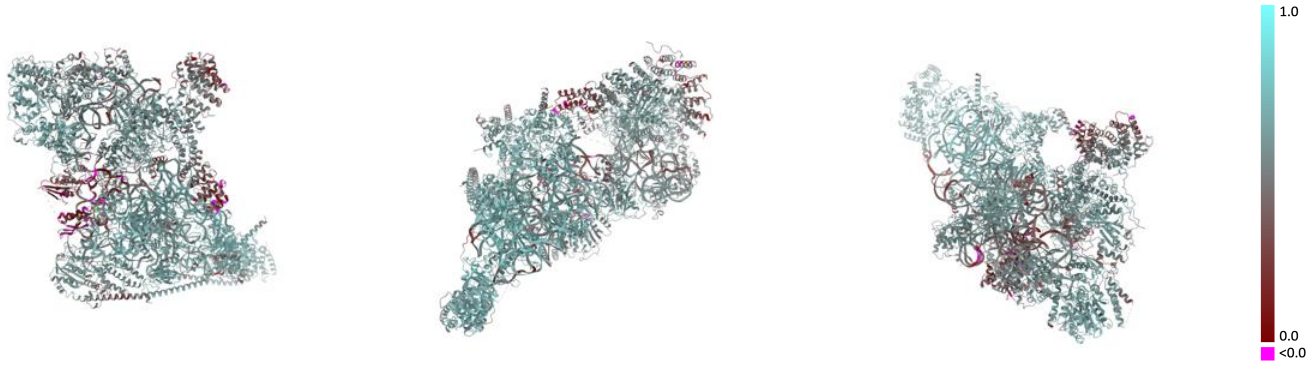
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.5 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.

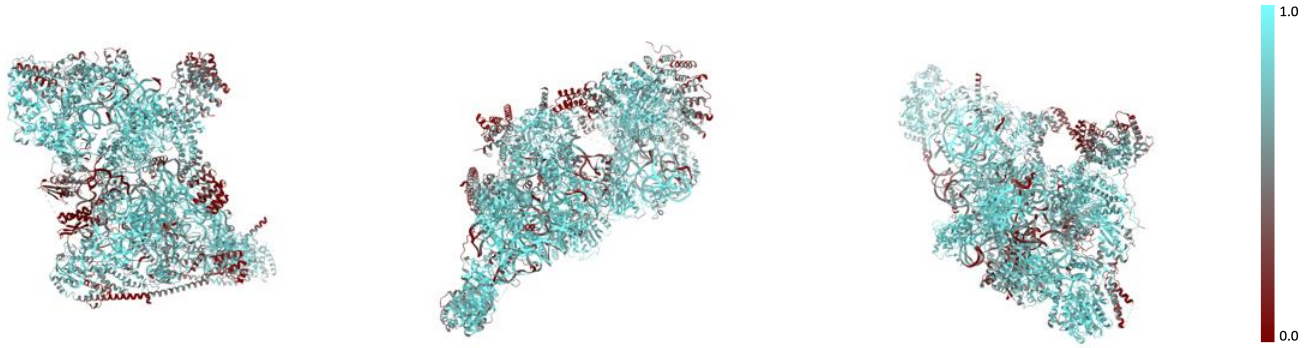
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

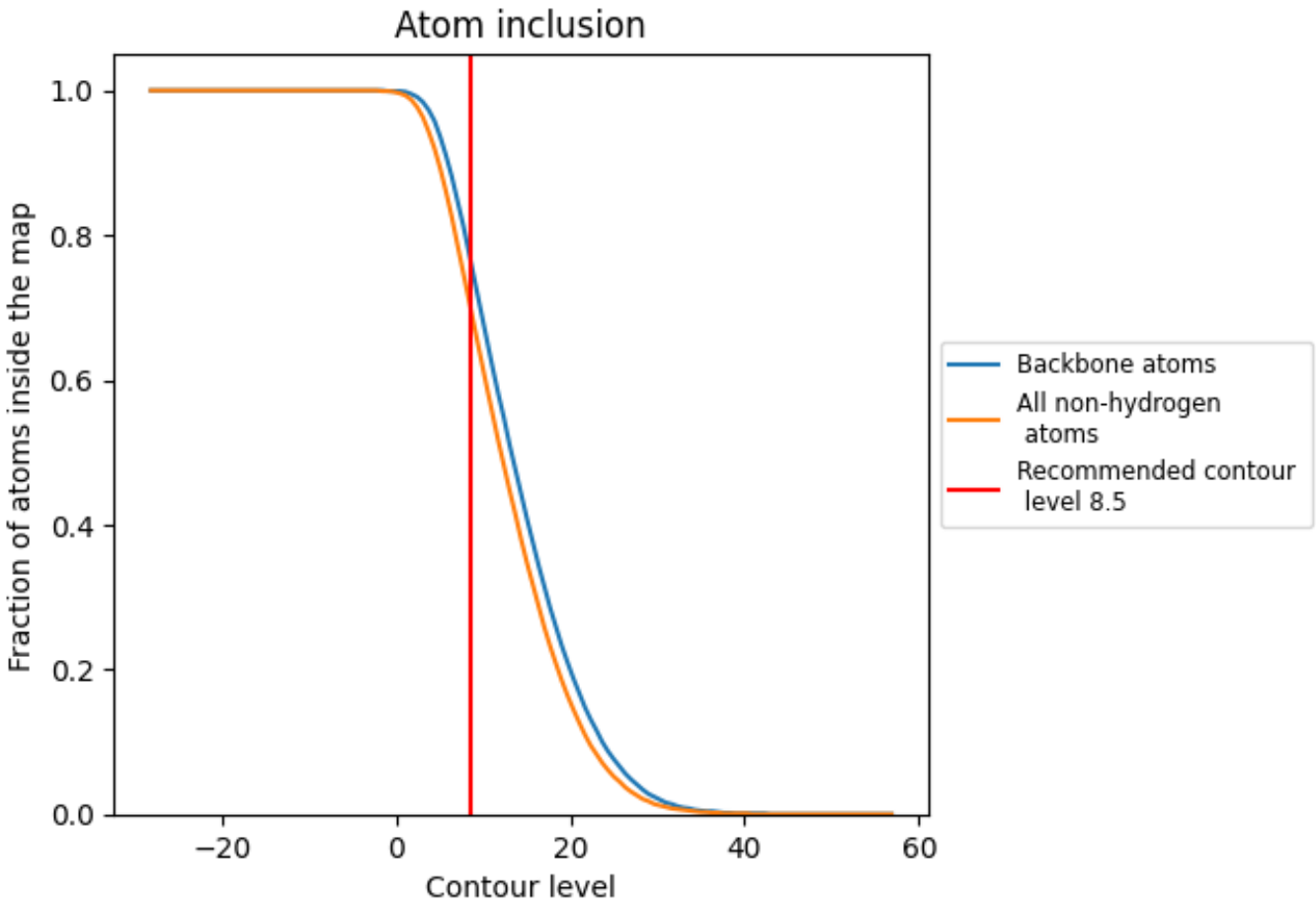
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (8.5).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (8.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7040	0.5660
0	0.7090	0.6480
1	0.6900	0.5720
3	0.3080	0.5310
4	0.5180	0.4430
5	0.8620	0.5610
7	0.8540	0.5890
8	0.7350	0.5270
A	0.7240	0.5480
B	0.8950	0.6560
C	0.8380	0.5970
D	0.7590	0.6490
E	0.7200	0.5810
F	0.7250	0.5560
G	0.7310	0.5670
H	0.7700	0.5830
J	0.6920	0.6440
K	0.6060	0.5080
L	0.6360	0.5900
M	0.8390	0.6840
N	0.7390	0.6670
O	0.7420	0.6640
P	0.6460	0.5430
Q	0.3330	0.6070
R	0.5870	0.6350
S	0.6410	0.5750
T	0.6930	0.6460
U	0.5090	0.5730
V	0.7510	0.6260
W	0.7170	0.6060
X	0.8390	0.6290
Y	0.6570	0.5390
Z	0.5560	0.4550
a	0.2340	0.2380