



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:46 AM UTC

PDB ID : 8D8J / pdb_00008d8j
EMDB ID : EMD-27249
Title : Yeast mitochondrial small subunit assembly intermediate (State 1)
Authors : Burnside, C.; Harper, N.; Klinge, S.
Deposited on : 2022-06-08
Resolution : 3.80 Å (reported)
Based on initial model : 5MRC

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

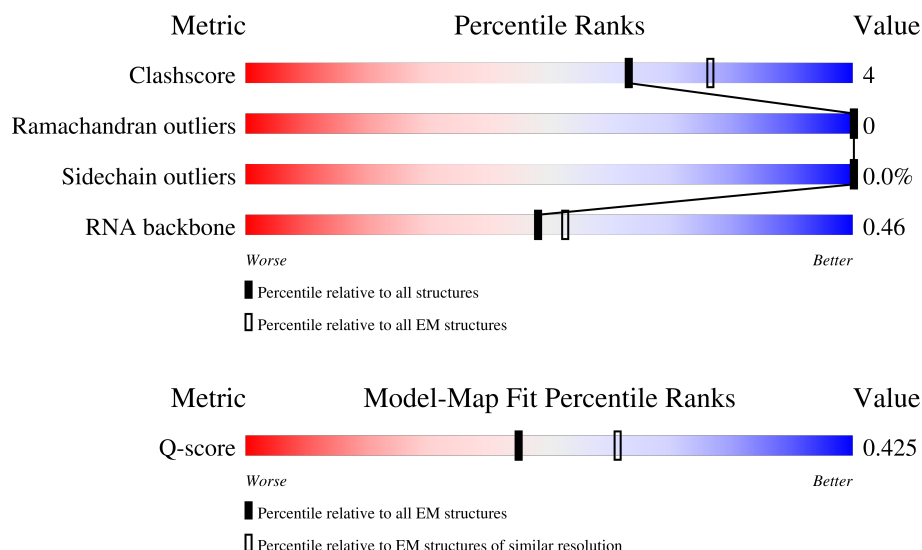
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



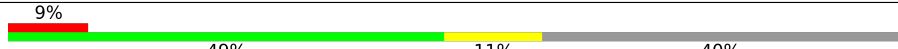
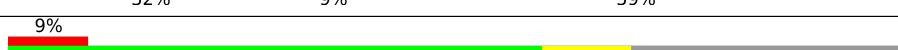
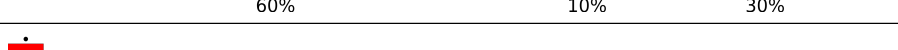
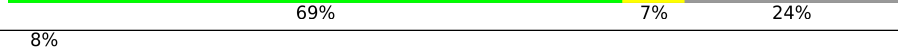
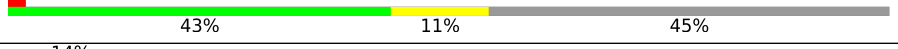
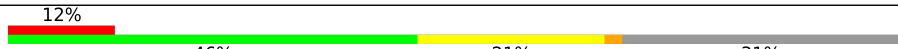
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	0	628	13% 77% 21%
2	5	339	59% 69% 11% 20%
3	d	864	38% 64% 12% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	O	286	
5	P	121	
6	Q	237	
7	R	138	
8	V	318	
9	2	130	
10	D	486	
11	E	307	
12	F	131	
13	6	345	
14	H	155	
15	a	1713	
16	L	153	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 51386 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 Probable S-adenosyl-L-methionine-dependent RNA methyltransferase RSM22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	493	Total	C	N	O	S	0	0
			2448	1458	493	493	4		

- Molecule 2 is a protein called 37S ribosomal protein MRP13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	270	Total	C	N	O	S	0	0
			2199	1426	375	394	4		

- Molecule 3 is a protein called Mitochondrial group I intron splicing factor CCM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	660	Total	C	N	O	S	0	0
			5497	3530	934	999	34		

- Molecule 4 is a protein called 37S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	210	Total	C	N	O	S	0	0
			1724	1079	318	319	8		

- Molecule 5 is a protein called 37S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	115	Total	C	N	O	S	0	0
			913	583	171	157	2		

- Molecule 6 is a protein called 37S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	143	Total	C	N	O	S	0	0
			1172	736	220	215	1		

- Molecule 7 is a protein called 37S ribosomal protein RSM18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	57	Total	C	N	O	S	0	0
			454	280	94	78	2		

- Molecule 8 is a protein called 37S ribosomal protein PET123, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	222	Total	C	N	O	S	0	0
			1787	1136	326	322	3		

- Molecule 9 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	99	Total	C	N	O	S	0	0
			833	530	156	146	1		

- Molecule 10 is a protein called 37S ribosomal protein NAM9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	308	Total	C	N	O	S	0	0
			2567	1677	452	434	4		

- Molecule 11 is a protein called 37S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	168	Total	C	N	O	S	0	0
			1334	850	243	234	7		

- Molecule 12 is a protein called 37S ribosomal protein MRP17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	131	Total	C	N	O	S	0	0
			1054	671	189	190	4		

- Molecule 13 is a protein called 37S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	6	250	Total	C	N	O	S	0	0
			2063	1318	374	365	6		

- Molecule 14 is a protein called 37S ribosomal protein S8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	155	Total	C	N	O	S	0	0
			1221	772	218	221	10		

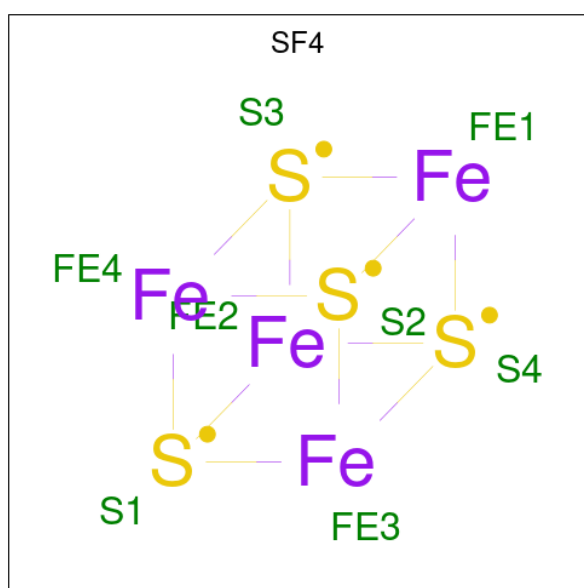
- Molecule 15 is a RNA chain called 15S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	1183	Total	C	N	O	P	0	0
			25157	11312	4468	8194	1183		

- Molecule 16 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	121	Total	C	N	O	S	0	0
			926	571	190	161	4		

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	0	1	Total	Fe	S	0
			8	4	4	

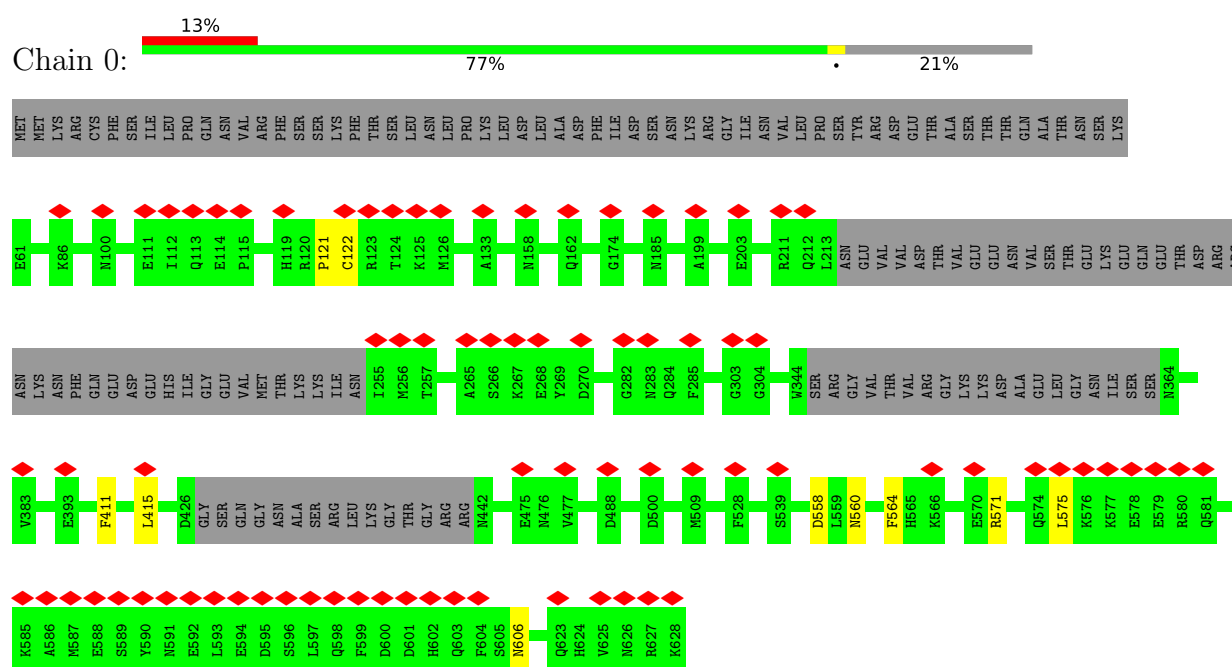
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

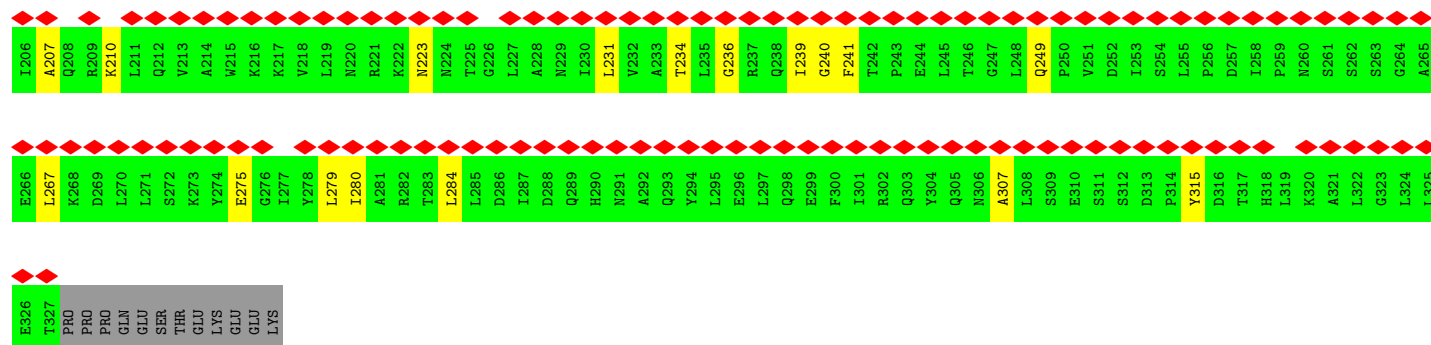
Mol	Chain	Residues	Atoms		AltConf
18	a	29	Total	Mg	0
			29	29	

3 Residue-property plots

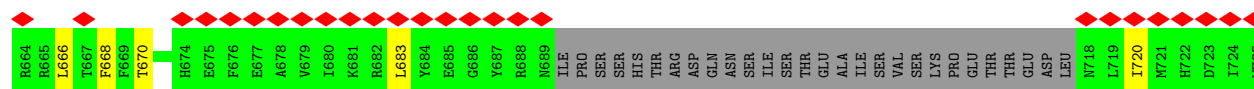
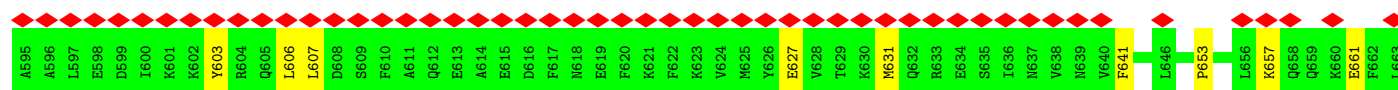
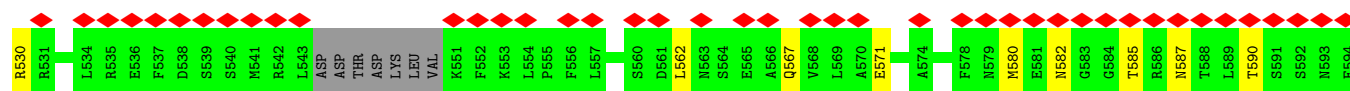
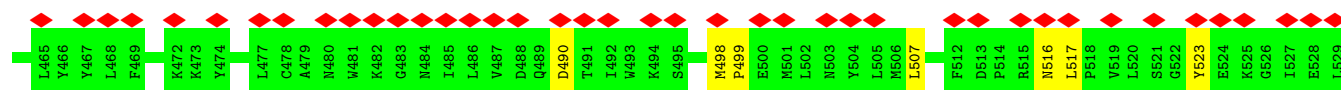
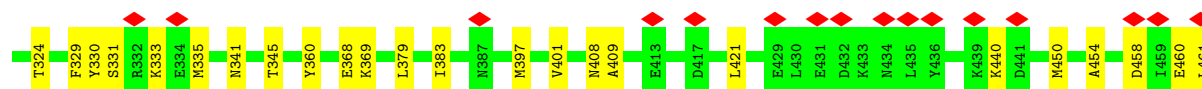
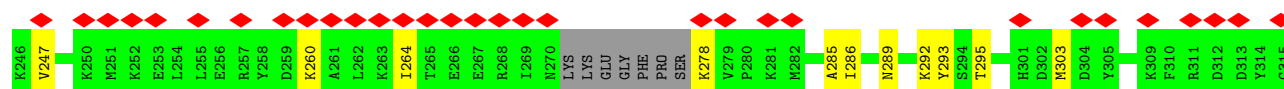
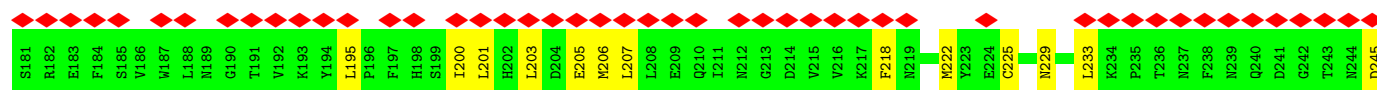
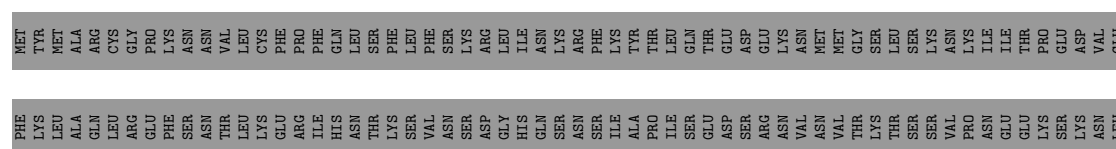
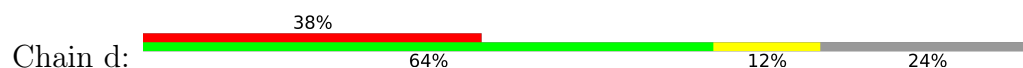
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

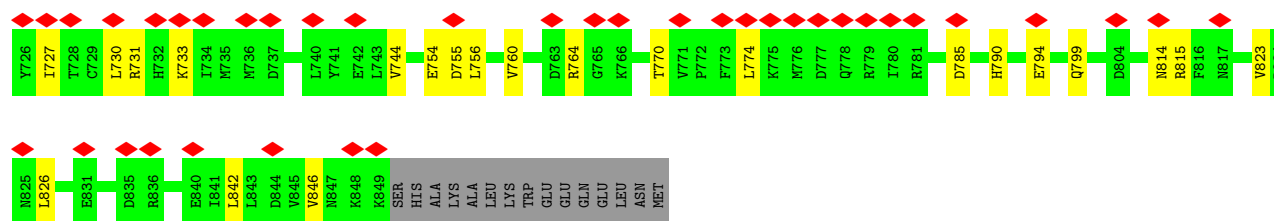
- Molecule 1: Probable S-adenosyl-L-methionine-dependent RNA methyltransferase RSM22, mitochondrial



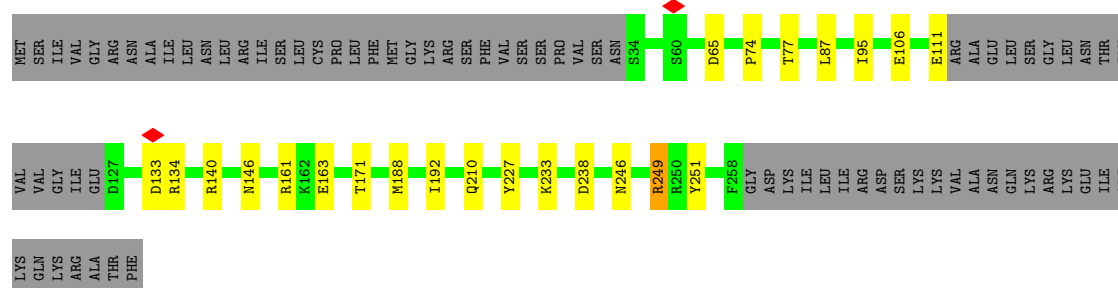


• Molecule 3: Mitochondrial group I intron splicing factor CCM1

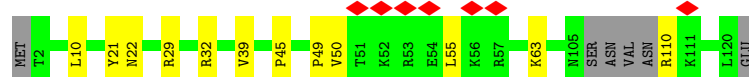
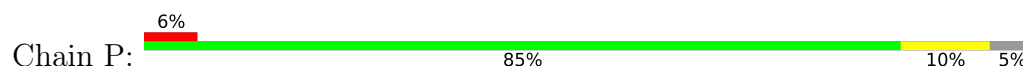




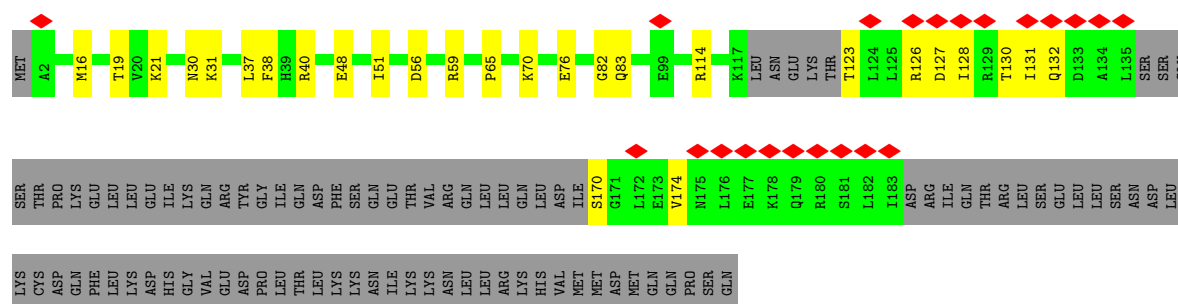
- Molecule 4: 37S ribosomal protein S28, mitochondrial



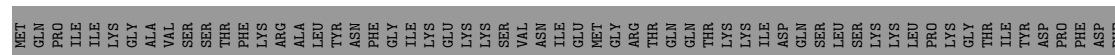
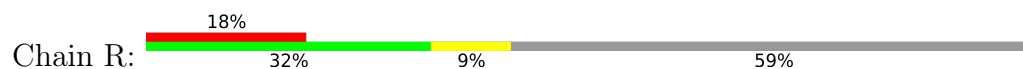
- Molecule 5: 37S ribosomal protein S16, mitochondrial

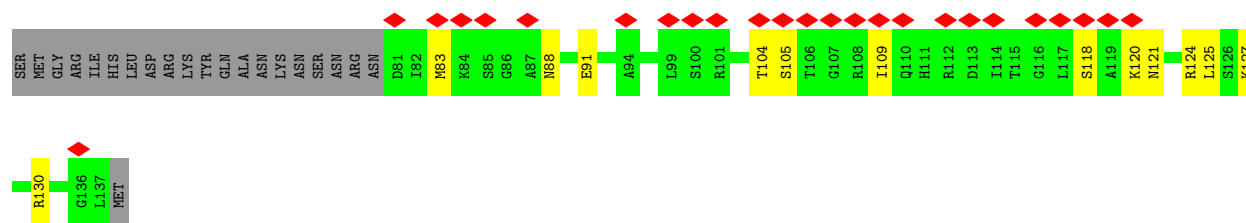


- Molecule 6: 37S ribosomal protein S17, mitochondrial

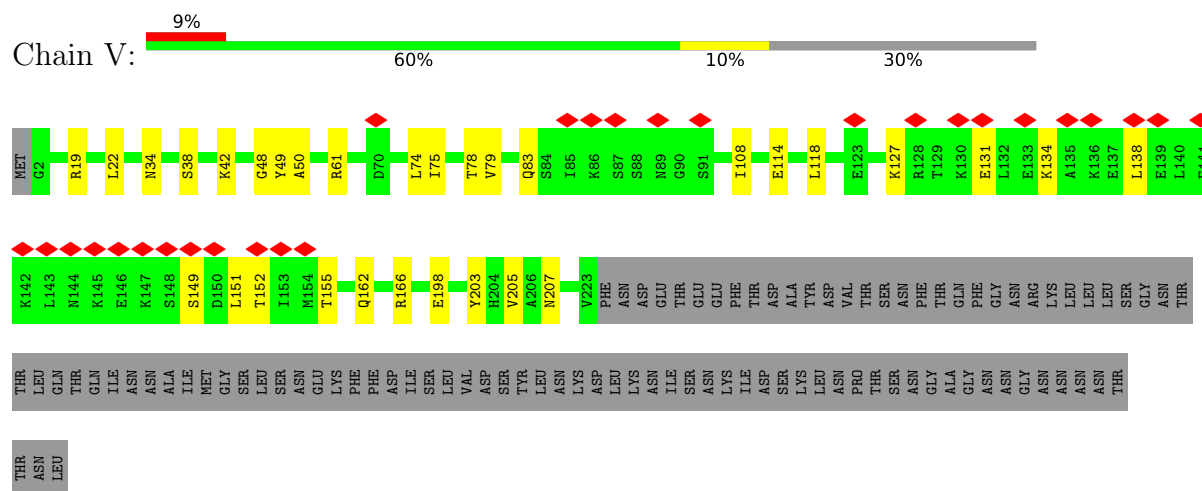


- Molecule 7: 37S ribosomal protein RSM18, mitochondrial

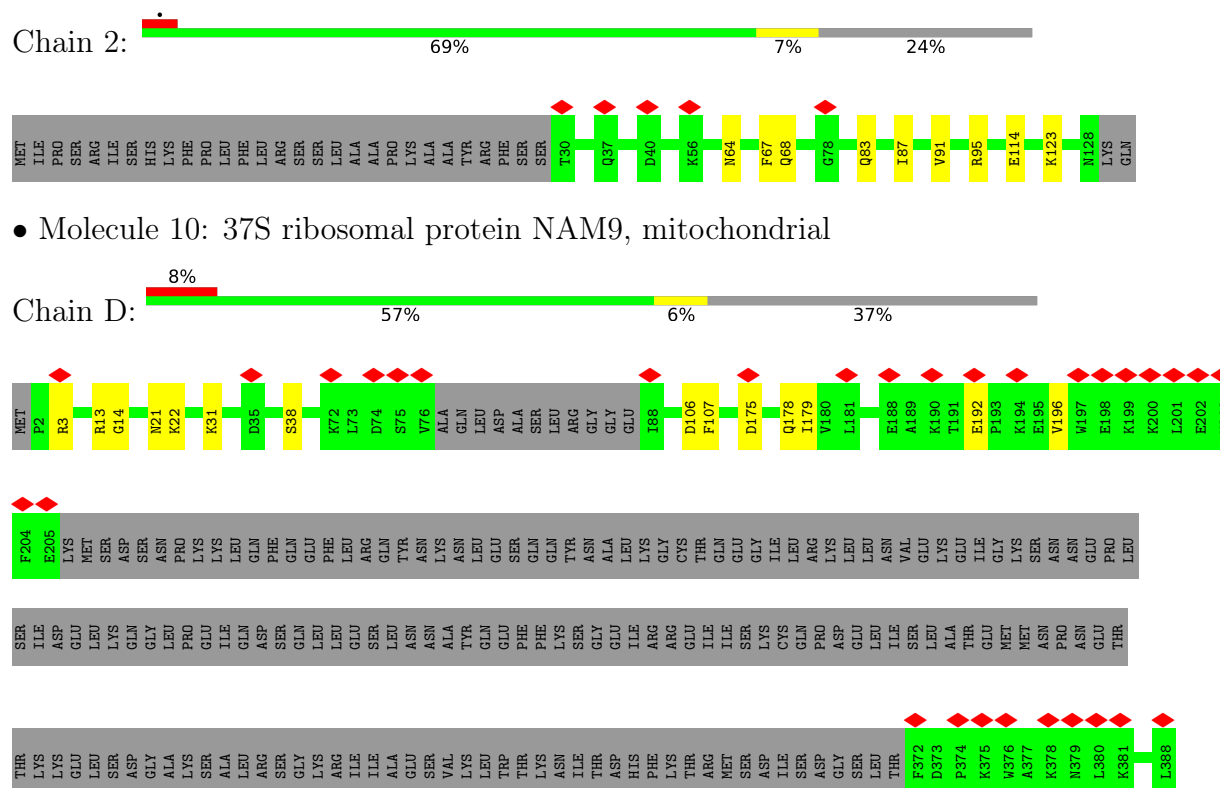




- Molecule 8: 37S ribosomal protein PET123, mitochondrial



- Molecule 9: Protein FYV4, mitochondrial

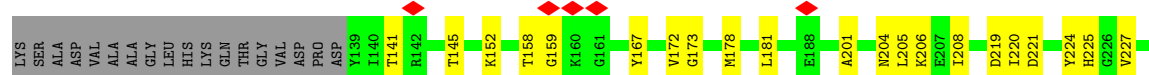
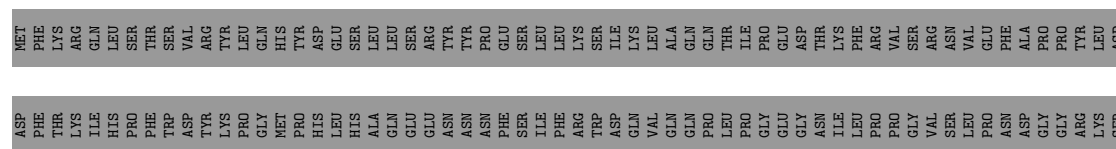


- Molecule 10: 37S ribosomal protein NAM9, mitochondrial



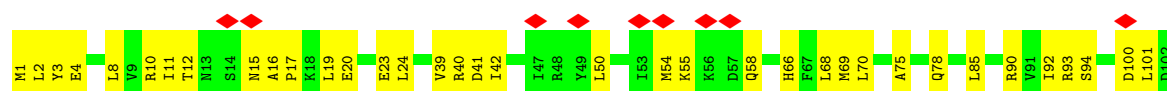
- Molecule 11: 37S ribosomal protein S5, mitochondrial

Chain E: 43% 11% 45%



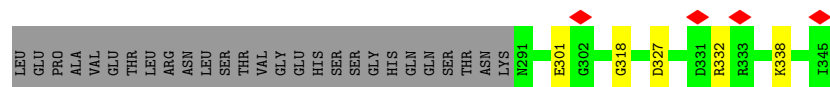
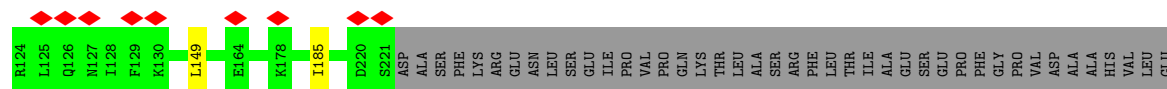
- Molecule 12: 37S ribosomal protein MRP17, mitochondrial

Chain F: 14% 65% 34%



- Molecule 13: 37S ribosomal protein S35, mitochondrial

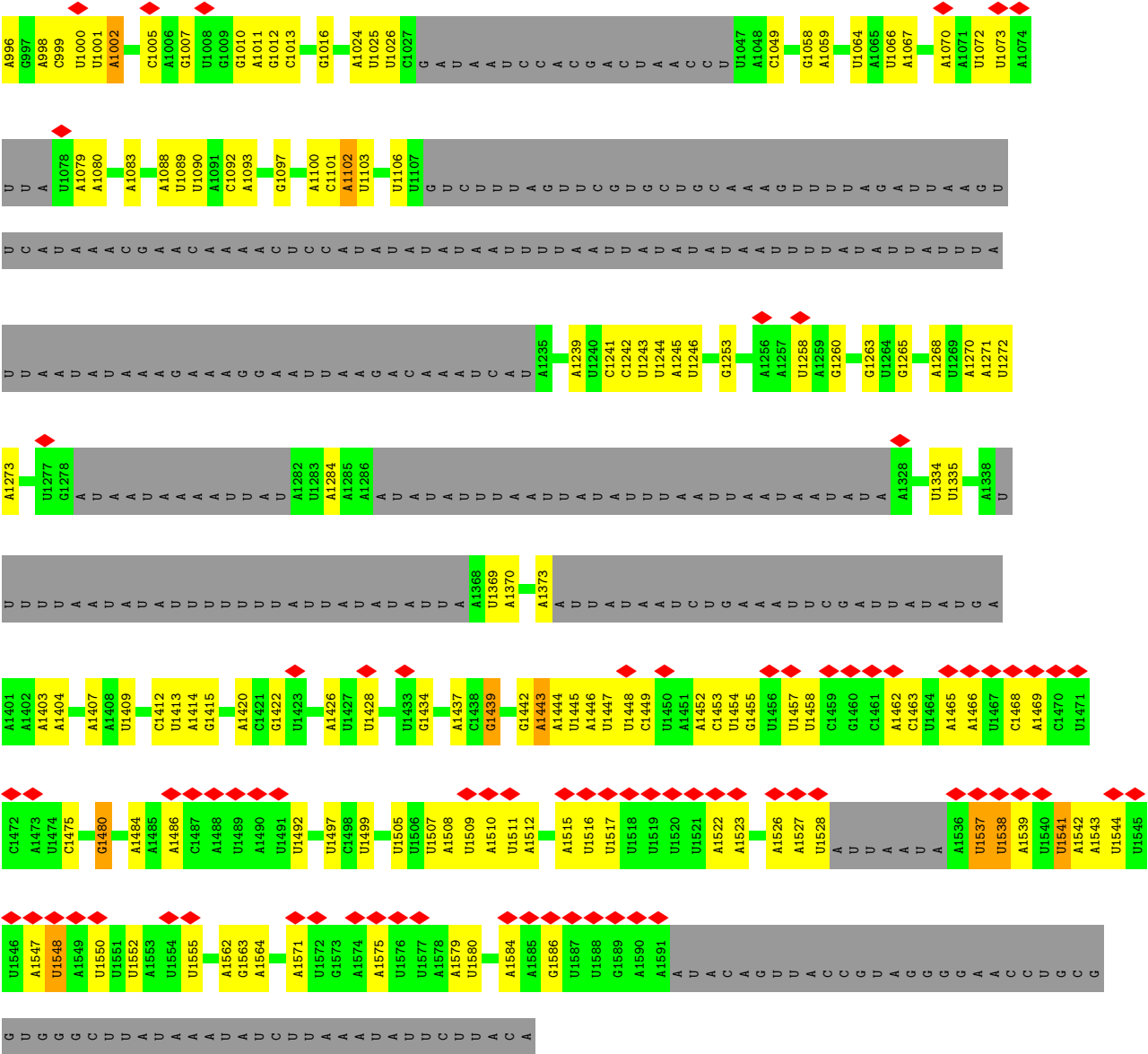
Chain 6: 6% 66% 6% 28%



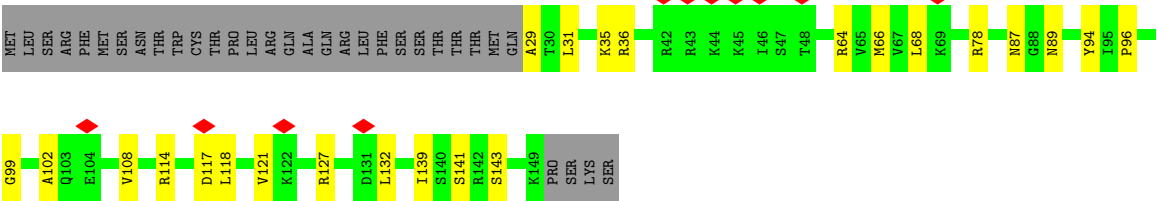
- Molecule 14: 37S ribosomal protein S8, mitochondrial

Chain H: 80% 20%





● Molecule 16: uS12m



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19720	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.73	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	27.063	Depositor
Minimum map value	-10.443	Depositor
Average map value	0.028	Depositor
Map value standard deviation	1.069	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	422.80002, 422.80002, 422.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	0	0.18	0/2447	0.48	0/3404
2	5	0.16	0/2249	0.37	0/3040
3	d	0.17	0/5612	0.38	0/7552
4	O	0.20	0/1746	0.41	0/2335
5	P	0.20	0/928	0.37	0/1252
6	Q	0.20	0/1181	0.41	0/1571
7	R	0.22	0/459	0.56	0/613
8	V	0.18	0/1813	0.41	0/2421
9	2	0.18	0/852	0.41	0/1142
10	D	0.18	0/2642	0.36	0/3561
11	E	0.19	0/1356	0.42	0/1812
12	F	0.21	0/1067	0.46	0/1430
13	6	0.17	0/2113	0.34	0/2845
14	H	0.19	0/1240	0.39	0/1670
15	a	0.16	0/28166	0.32	0/43793
16	L	0.19	0/940	0.41	0/1261
All	All	0.17	0/54811	0.36	0/79702

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
12	F	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
12	F	124	VAL	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	2448	0	1079	7	0
2	5	2199	0	2246	25	0
3	d	5497	0	5513	76	0
4	O	1724	0	1761	20	0
5	P	913	0	977	9	0
6	Q	1172	0	1226	20	0
7	R	454	0	480	11	0
8	V	1787	0	1915	26	0
9	2	833	0	839	6	0
10	D	2567	0	2630	19	0
11	E	1334	0	1392	24	0
12	F	1054	0	1129	33	0
13	6	2063	0	2095	19	0
14	H	1221	0	1289	22	0
15	a	25157	0	12624	116	0
16	L	926	0	980	22	0
17	0	8	0	0	0	0
18	a	29	0	0	0	0
All	All	51386	0	38175	371	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.

All (371) 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)
3:d:335:MET:SD	8:V:149:SER:OG	2.28	0.90
11:E:219:ASP:OD1	14:H:119:LYS:NZ	2.07	0.86
13:6:66:ASN:ND2	15:a:482:U:OP1	2.11	0.84
4:O:65:ASP:OD1	4:O:251:TYR:OH	1.98	0.82
12:F:103:LYS:NZ	15:a:726:A:OP2	2.13	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:100:ASP:O	12:F:107:ARG:NH1	2.14	0.81
7:R:127:LYS:NZ	15:a:801:U:OP1	2.12	0.81
4:O:140:ARG:O	4:O:146:ASN:ND2	2.16	0.79
9:2:114:GLU:OE2	15:a:107:G:N2	2.14	0.79
4:O:134:ARG:NH2	8:V:203:TYR:O	2.15	0.79
15:a:625:A:N1	15:a:654:G:O2'	2.15	0.78
15:a:1093:A:N6	15:a:1243:U:O2	2.17	0.77
4:O:106:GLU:OE2	8:V:203:TYR:OH	2.02	0.77
4:O:249:ARG:NH1	15:a:828:A:OP1	2.17	0.77
15:a:786:U:OP2	15:a:787:A:O2'	2.02	0.76
8:V:19:ARG:NH2	15:a:234:A:OP2	2.13	0.76
15:a:1284:A:N3	15:a:1439:G:O2'	2.17	0.75
15:a:384:G:N2	15:a:387:A:OP2	2.18	0.75
3:d:153:ASN:ND2	3:d:161:ASN:O	2.20	0.74
15:a:35:A:O2'	15:a:302:U:OP1	2.04	0.74
15:a:616:C:OP2	16:L:141:SER:OG	2.05	0.74
8:V:42:LYS:NZ	8:V:49:TYR:O	2.21	0.73
3:d:379:LEU:O	3:d:383:ILE:HD12	1.89	0.72
6:Q:59:ARG:NH2	8:V:48:GLY:O	2.23	0.72
16:L:108:VAL:HG12	16:L:132:LEU:HD23	1.69	0.72
14:H:99:ILE:HG21	14:H:118:ILE:HD11	1.71	0.72
3:d:498:MET:HE3	3:d:499:PRO:HD2	1.73	0.71
12:F:119:SER:OG	12:F:122:GLU:OE1	2.09	0.71
3:d:331:SER:O	3:d:369:LYS:NZ	2.23	0.71
2:5:129:ARG:NH2	15:a:154:U:OP2	2.22	0.70
16:L:102:ALA:HB2	16:L:132:LEU:HD21	1.73	0.70
4:O:87:LEU:O	6:Q:114:ARG:NH2	2.24	0.70
10:D:178:GLN:OE1	10:D:407:GLN:NE2	2.24	0.70
14:H:1:MET:N	15:a:699:A:OP1	2.23	0.70
8:V:34:ASN:O	8:V:38:SER:OG	2.05	0.70
8:V:79:VAL:O	15:a:143:A:O2'	2.09	0.70
2:5:53:ILE:O	2:5:57:THR:HG23	1.92	0.70
6:Q:31:LYS:NZ	15:a:307:G:OP1	2.20	0.68
3:d:562:LEU:HD11	3:d:571:GLU:OE1	1.94	0.68
7:R:118:SER:OG	7:R:121:ASN:OD1	2.07	0.68
7:R:130:ARG:NH2	15:a:800:U:O3'	2.26	0.68
8:V:166:ARG:NE	14:H:62:GLU:OE1	2.26	0.68
5:P:110:ARG:N	13:6:301:GLU:OE2	2.26	0.68
12:F:2:LEU:HD21	12:F:40:ARG:NH1	2.09	0.68
3:d:666:LEU:O	3:d:670:THR:OG1	2.05	0.67
1:O:558:ASP:N	15:a:1102:A:OP1	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:152:LYS:NZ	15:a:24:U:OP1	2.19	0.66
3:d:668:PHE:O	3:d:733:LYS:NZ	2.29	0.66
1:0:571:ARG:O	1:0:575:LEU:N	2.29	0.65
3:d:278:LYS:NZ	15:a:-15:U:OP2	2.17	0.65
4:O:161:ARG:HD2	4:O:171:THR:HG22	1.79	0.65
10:D:38:SER:O	13:6:27:PHE:N	2.29	0.65
15:a:1024:A:N1	15:a:1253:G:O2'	2.27	0.64
8:V:83:GLN:N	15:a:145:A:OP1	2.30	0.64
4:O:134:ARG:NH1	8:V:207:ASN:OD1	2.31	0.64
12:F:93:ARG:NH2	15:a:738:A:O3'	2.31	0.64
15:a:695:A:OP2	16:L:35:LYS:NZ	2.31	0.64
15:a:946:A:OP2	16:L:36:ARG:NH2	2.31	0.64
8:V:50:ALA:O	8:V:61:ARG:NH2	2.32	0.63
9:2:123:LYS:NZ	15:a:348:A:OP1	2.20	0.63
12:F:2:LEU:HD21	12:F:40:ARG:CZ	2.29	0.62
3:d:755:ASP:OD1	3:d:756:LEU:N	2.33	0.62
10:D:21:ASN:OD1	10:D:22:LYS:N	2.32	0.62
4:O:87:LEU:HB3	4:O:95:ILE:HD11	1.80	0.62
11:E:225:HIS:ND1	15:a:931:A:OP1	2.27	0.62
12:F:41:ASP:OD2	12:F:42:ILE:N	2.33	0.62
15:a:21:U:N3	15:a:24:U:OP2	2.33	0.62
6:Q:127:ASP:O	6:Q:131:ILE:HD12	2.01	0.61
3:d:245:ASP:OD2	3:d:247:VAL:N	2.34	0.60
3:d:490:ASP:OD1	3:d:582:ASN:ND2	2.35	0.60
3:d:823:VAL:HG21	3:d:846:VAL:HG21	1.83	0.60
15:a:1480:G:OP1	16:L:64:ARG:NH2	2.34	0.60
3:d:562:LEU:HD22	3:d:567:GLN:HB3	1.83	0.60
10:D:3:ARG:NH2	15:a:660:G:OP2	2.34	0.60
11:E:221:ASP:OD1	11:E:230:HIS:ND1	2.30	0.60
4:O:188:MET:O	4:O:192:ILE:HD12	2.02	0.59
12:F:1:MET:SD	12:F:3:TYR:OH	2.60	0.59
15:a:1415:G:N2	15:a:1443:A:OP2	2.36	0.59
9:2:83:GLN:O	9:2:87:ILE:HD12	2.03	0.59
15:a:58:A:N7	15:a:114:U:O2'	2.36	0.59
3:d:324:THR:OG1	15:a:-5:G:N2	2.28	0.58
15:a:639:U:OP1	16:L:114:ARG:NH2	2.36	0.58
2:5:124:THR:HG21	2:5:166:ILE:HD13	1.85	0.58
2:5:98:SER:O	2:5:101:THR:HG22	2.04	0.58
3:d:303:MET:HE3	3:d:329:PHE:CD1	2.38	0.58
14:H:96:ASN:ND2	15:a:943:U:OP1	2.34	0.57
3:d:260:LYS:O	3:d:264:ILE:HD12	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:49:PRO:O	13:6:338:LYS:NZ	2.19	0.57
6:Q:56:ASP:OD1	6:Q:82:GLY:N	2.37	0.57
15:a:731:U:P	15:a:798:U:HO2'	2.28	0.57
1:0:411:PHE:O	1:0:415:LEU:N	2.36	0.57
5:P:29:ARG:O	15:a:110:A:O2'	2.20	0.57
13:6:28:SER:OG	15:a:623:A:OP1	2.14	0.57
3:d:207:LEU:HD23	3:d:222:MET:HE3	1.88	0.56
3:d:440:LYS:NZ	15:a:-4:G:O3'	2.38	0.56
15:a:652:A:H4'	16:L:139:ILE:HD11	1.87	0.56
15:a:659:C:O2'	15:a:663:C:OP1	2.24	0.56
3:d:421:LEU:HD21	3:d:523:TYR:CE2	2.41	0.56
12:F:15:ASN:OD1	12:F:16:ALA:N	2.39	0.56
2:5:210:LYS:NZ	15:a:85:G:O3'	2.38	0.56
3:d:814:ASN:OD1	3:d:815:ARG:N	2.38	0.56
3:d:408:ASN:OD1	3:d:409:ALA:N	2.39	0.56
4:O:161:ARG:NH1	15:a:721:U:O2'	2.39	0.56
14:H:98:ARG:NH2	15:a:697:G:OP1	2.39	0.56
3:d:295:THR:HG23	3:d:303:MET:HE1	1.87	0.56
6:Q:51:ILE:O	6:Q:83:GLN:NE2	2.38	0.56
3:d:225:CYS:O	3:d:229:ASN:ND2	2.39	0.55
3:d:587:ASN:OD1	3:d:590:THR:OG1	2.15	0.55
12:F:85:LEU:HD23	12:F:94:SER:HB2	1.88	0.55
15:a:695:A:O2'	15:a:944:C:OP1	2.23	0.55
10:D:428:ARG:NH2	15:a:412:U:OP1	2.39	0.55
12:F:8:LEU:HD22	12:F:66:HIS:CD2	2.40	0.55
14:H:29:THR:OG1	14:H:32:GLN:OE1	2.24	0.55
6:Q:16:MET:HE3	15:a:281:C:H5'	1.88	0.55
15:a:1541:U:O4	15:a:1542:A:N6	2.40	0.55
1:0:560:ASN:O	1:0:564:PHE:N	2.37	0.55
15:a:1426:A:H2	15:a:1434:G:H22	1.55	0.55
5:P:22:ASN:OD1	5:P:39:VAL:HG13	2.07	0.55
6:Q:128:ILE:CG2	6:Q:132:GLN:HE22	2.20	0.55
12:F:39:VAL:O	12:F:39:VAL:HG13	2.07	0.54
3:d:661:GLU:OE2	3:d:661:GLU:N	2.40	0.54
15:a:366:G:N1	15:a:369:U:OP2	2.37	0.54
2:5:158:HIS:O	2:5:162:LEU:HD23	2.07	0.54
12:F:50:LEU:HD23	12:F:54:MET:SD	2.47	0.54
11:E:243:ASN:OD1	11:E:244:HIS:N	2.41	0.54
12:F:16:ALA:HB1	12:F:19:LEU:HD23	1.87	0.54
13:6:41:LYS:NZ	15:a:496:A:O4'	2.39	0.54
8:V:134:LYS:O	8:V:138:LEU:HD13	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:345:THR:HG21	8:V:155:THR:HA	1.89	0.54
3:d:333:LYS:CB	3:d:335:MET:HE2	2.38	0.54
10:D:192:GLU:O	10:D:196:VAL:HG23	2.07	0.53
14:H:19:VAL:HG23	14:H:21:VAL:HG13	1.90	0.53
11:E:167:TYR:CE2	11:E:269:MET:HE2	2.43	0.53
12:F:23:GLU:OE1	12:F:90:ARG:NH2	2.41	0.53
3:d:397:MET:O	3:d:401:VAL:HG23	2.07	0.53
3:d:631:MET:HE2	3:d:731:ARG:HD2	1.91	0.53
13:6:65:LYS:NZ	15:a:414:A:OP1	2.27	0.53
6:Q:19:THR:OG1	6:Q:70:LYS:NZ	2.41	0.53
15:a:731:U:OP1	15:a:798:U:O2'	2.22	0.53
12:F:124:VAL:O	12:F:124:VAL:HG23	2.09	0.53
16:L:118:LEU:HD22	16:L:121:VAL:HG23	1.89	0.53
2:5:189:ILE:HG21	2:5:231:LEU:HB3	1.90	0.53
3:d:368:GLU:HB2	3:d:401:VAL:HG22	1.89	0.53
14:H:87:SER:OG	14:H:155:LYS:O	2.26	0.52
16:L:96:PRO:O	16:L:127:ARG:NH1	2.42	0.52
11:E:167:TYR:HE2	11:E:269:MET:HE2	1.75	0.52
11:E:220:ILE:HG21	11:E:278:ALA:HB1	1.92	0.52
15:a:691:U:OP2	15:a:823:G:N1	2.40	0.52
2:5:48:LEU:HD23	2:5:97:LEU:HD21	1.92	0.52
3:d:440:LYS:HB3	15:a:-2:A:H61	1.74	0.52
15:a:299:U:O2'	15:a:313:A:N1	2.39	0.51
3:d:341:ASN:O	3:d:345:THR:HG23	2.11	0.51
4:O:74:PRO:O	4:O:77:THR:OG1	2.19	0.51
15:a:1445:U:O2'	15:a:1446:A:O4'	2.24	0.51
11:E:178:MET:HB3	11:E:205:LEU:HD11	1.92	0.51
12:F:2:LEU:HD22	12:F:70:LEU:HD21	1.92	0.51
6:Q:123:THR:HG22	6:Q:126:ARG:NH2	2.26	0.51
5:P:50:VAL:HG23	5:P:55:LEU:HD21	1.92	0.50
3:d:360:TYR:CD1	3:d:383:ILE:HD11	2.47	0.50
14:H:89:CYS:SG	14:H:154:VAL:HG12	2.52	0.50
14:H:15:ASN:O	14:H:19:VAL:HG22	2.12	0.50
3:d:330:TYR:HD1	3:d:335:MET:HE3	1.75	0.50
16:L:118:LEU:HD22	16:L:121:VAL:CG2	2.41	0.50
3:d:790:HIS:NE2	3:d:794:GLU:OE2	2.44	0.50
11:E:181:LEU:HD12	11:E:276:ILE:HG21	1.94	0.50
14:H:92:ILE:HD12	14:H:150:VAL:HG22	1.94	0.50
3:d:421:LEU:HD21	3:d:523:TYR:HE2	1.76	0.50
11:E:219:ASP:OD2	11:E:220:ILE:N	2.45	0.50
15:a:38:A:O2'	15:a:55:A:N6	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:275:GLU:O	2:5:279:LEU:HD23	2.12	0.49
4:O:210:GLN:OE1	15:a:689:C:O2'	2.26	0.49
12:F:11:ILE:HD12	12:F:17:PRO:CB	2.42	0.49
2:5:234:THR:HG21	2:5:284:LEU:HD11	1.93	0.49
3:d:176:PHE:CZ	3:d:206:MET:HE3	2.47	0.49
8:V:205:VAL:HG21	12:F:120:ILE:HG13	1.94	0.49
15:a:303:G:N2	15:a:306:A:OP2	2.43	0.49
15:a:955:G:O2'	15:a:971:G:O6	2.27	0.49
2:5:236:GLY:O	2:5:240:GLY:N	2.46	0.49
6:Q:127:ASP:O	6:Q:130:THR:OG1	2.23	0.49
10:D:13:ARG:NH1	15:a:657:G:OP2	2.45	0.49
13:6:58:MET:HE3	13:6:62:LEU:HD11	1.95	0.49
5:P:45:PRO:O	5:P:63:LYS:NZ	2.38	0.49
1:O:122:CYS:C	15:a:1468:C:H41	2.21	0.49
3:d:285:ALA:O	3:d:289:ASN:ND2	2.46	0.49
2:5:97:LEU:HD23	2:5:136:TYR:CZ	2.48	0.49
3:d:292:LYS:O	3:d:295:THR:OG1	2.30	0.49
13:6:34:TYR:OH	15:a:498:A:OP1	2.27	0.49
13:6:327:ASP:OD2	15:a:50:A:O2'	2.30	0.49
13:6:53:ASN:ND2	15:a:495:U:O2	2.45	0.49
15:a:963:G:N2	15:a:966:A:OP2	2.33	0.49
13:6:110:ARG:NH2	13:6:114:THR:OG1	2.46	0.49
14:H:99:ILE:HG21	14:H:118:ILE:CD1	2.41	0.49
2:5:48:LEU:CD2	2:5:97:LEU:HD21	2.43	0.48
3:d:450:MET:O	3:d:454:ALA:N	2.42	0.48
3:d:461:LEU:HD11	3:d:530:ARG:HG3	1.95	0.48
12:F:16:ALA:HB1	12:F:19:LEU:CD2	2.43	0.48
16:L:68:LEU:HB2	16:L:118:LEU:HD11	1.95	0.48
10:D:459:ARG:NH1	10:D:464:GLU:OE2	2.42	0.48
11:E:271:ILE:O	11:E:275:THR:OG1	2.15	0.48
3:d:460:GLU:OE1	3:d:530:ARG:NH2	2.42	0.48
3:d:292:LYS:NZ	15:a:-6:A:O3'	2.38	0.48
11:E:208:ILE:HD11	11:E:279:PHE:CD1	2.49	0.48
13:6:332:ARG:NH2	15:a:50:A:N3	2.60	0.48
15:a:1005:C:O2'	15:a:1444:A:N3	2.43	0.48
2:5:189:ILE:HB	2:5:231:LEU:HD23	1.95	0.48
3:d:516:ASN:OD1	3:d:517:LEU:N	2.47	0.48
3:d:756:LEU:O	3:d:760:VAL:HG13	2.14	0.48
10:D:484:ASN:ND2	15:a:35:A:OP1	2.46	0.47
11:E:172:VAL:HG22	11:E:201:ALA:HB1	1.96	0.47
12:F:55:LYS:NZ	12:F:58:GLN:O	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:145:THR:HG22	11:E:173:GLY:O	2.13	0.47
8:V:74:LEU:O	8:V:78:THR:OG1	2.21	0.47
7:R:109:ILE:HD12	15:a:785:A:C2	2.49	0.47
2:5:73:ILE:HD12	2:5:73:ILE:H	1.80	0.47
3:d:580:MET:HE1	3:d:641:PHE:HB2	1.96	0.47
3:d:727:ILE:HA	3:d:730:LEU:HD12	1.95	0.47
3:d:764:ARG:NH2	3:d:785:ASP:OD2	2.47	0.47
4:O:133:ASP:OD1	4:O:134:ARG:N	2.48	0.47
4:O:210:GLN:NE2	4:O:246:ASN:OD1	2.48	0.47
10:D:175:ASP:OD1	10:D:407:GLN:NE2	2.47	0.47
12:F:12:THR:HG22	12:F:20:GLU:OE1	2.15	0.47
15:a:677:G:O6	16:L:29:ALA:HB2	2.15	0.47
10:D:106:ASP:OD1	10:D:107:PHE:N	2.48	0.47
13:6:52:THR:HG22	15:a:498:A:N7	2.30	0.47
16:L:87:ASN:OD1	16:L:89:ASN:ND2	2.48	0.47
2:5:140:ILE:HD12	2:5:140:ILE:H	1.80	0.47
3:d:160:SER:OG	3:d:162:TRP:NE1	2.48	0.46
14:H:31:LEU:CD1	14:H:135:ILE:HD11	2.45	0.46
3:d:744:VAL:HG12	3:d:760:VAL:HG11	1.96	0.46
7:R:88:ASN:HB3	7:R:91:GLU:HG3	1.97	0.46
14:H:7:ALA:HB2	14:H:91:LEU:HD12	1.96	0.46
4:O:163:GLU:OE2	4:O:233:LYS:NZ	2.48	0.46
16:L:66:MET:HE2	16:L:68:LEU:HD21	1.96	0.46
10:D:416:ASP:H	10:D:423:THR:HG21	1.79	0.46
14:H:106:MET:HE1	14:H:146:LEU:O	2.15	0.46
15:a:1537:U:H2'	15:a:1538:U:C6	2.51	0.46
3:d:176:PHE:CE1	3:d:206:MET:HE3	2.51	0.46
11:E:158:THR:HG22	11:E:159:GLY:N	2.31	0.46
3:d:218:PHE:CD1	3:d:222:MET:HE2	2.51	0.46
12:F:20:GLU:O	12:F:24:LEU:HD23	2.16	0.46
3:d:200:ILE:HD12	3:d:233:LEU:HD11	1.98	0.45
12:F:4:GLU:OE2	12:F:110:SER:N	2.49	0.45
13:6:51:ASP:OD1	13:6:52:THR:N	2.46	0.45
15:a:1453:C:H2'	15:a:1454:U:O4'	2.17	0.45
15:a:989:C:N4	15:a:990:G:O6	2.49	0.45
2:5:223:ASN:ND2	2:5:249:GLN:O	2.49	0.45
3:d:607:LEU:CD2	3:d:683:LEU:HD13	2.46	0.45
6:Q:65:PRO:O	15:a:268:G:O2'	2.30	0.45
3:d:498:MET:HE3	3:d:499:PRO:CD	2.44	0.45
9:2:67:PHE:O	9:2:95:ARG:NH2	2.45	0.45
12:F:115:LEU:HD23	12:F:115:LEU:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:38:PHE:O	15:a:694:A:O2'	2.30	0.45
6:Q:59:ARG:NH1	6:Q:76:GLU:OE1	2.50	0.45
15:a:1334:U:H2'	15:a:1335:U:C6	2.52	0.45
15:a:1499:U:H3	15:a:1562:A:H61	1.63	0.45
3:d:286:ILE:HD12	3:d:286:ILE:H	1.81	0.44
6:Q:21:LYS:NZ	15:a:282:C:OP2	2.36	0.44
7:R:91:GLU:OE1	12:F:113:ARG:HB3	2.17	0.44
11:E:244:HIS:O	11:E:248:GLU:OE1	2.35	0.44
15:a:412:U:H3	15:a:505:A:H61	1.65	0.44
15:a:730:A:HO2'	15:a:731:U:C5'	2.29	0.44
3:d:606:LEU:HD11	3:d:627:GLU:OE1	2.17	0.44
15:a:606:U:H2'	15:a:607:U:O4'	2.17	0.44
2:5:186:ASN:HB3	2:5:280:ILE:HD13	1.99	0.44
8:V:151:LEU:O	8:V:152:THR:OG1	2.30	0.44
8:V:166:ARG:HG2	8:V:166:ARG:HH11	1.83	0.44
10:D:419:LYS:HD2	10:D:423:THR:HG23	1.99	0.44
12:F:101:LEU:HD23	12:F:101:LEU:H	1.82	0.44
3:d:458:ASP:OD2	3:d:461:LEU:HD12	2.17	0.44
5:P:39:VAL:HG11	13:6:318:GLY:HA3	2.00	0.44
5:P:32:ARG:NH1	15:a:379:U:O2	2.48	0.44
7:R:120:LYS:HG3	7:R:124:ARG:HH22	1.83	0.44
2:5:59:ALA:N	15:a:154:U:OP1	2.51	0.43
3:d:653:PRO:O	3:d:657:LYS:N	2.50	0.43
11:E:204:ASN:O	11:E:206:LYS:NZ	2.49	0.43
11:E:224:TYR:O	11:E:227:VAL:HG22	2.18	0.43
12:F:68:LEU:HD23	12:F:69:MET:N	2.32	0.43
15:a:93:A:O2'	15:a:214:A:OP2	2.15	0.43
15:a:132:A:N3	15:a:267:A:O2'	2.36	0.43
15:a:1547:A:O2'	15:a:1548:U:OP2	2.31	0.43
14:H:9:THR:HG23	14:H:26:ILE:HG21	2.00	0.43
4:O:95:ILE:HD12	6:Q:114:ARG:HH22	1.83	0.43
7:R:104:THR:HG22	7:R:105:SER:N	2.33	0.43
10:D:175:ASP:O	10:D:179:ILE:HG13	2.18	0.43
16:L:31:LEU:H	16:L:31:LEU:HD12	1.83	0.43
11:E:158:THR:HG22	11:E:159:GLY:H	1.82	0.43
16:L:94:TYR:HB2	16:L:121:VAL:HG11	2.00	0.43
6:Q:48:GLU:N	6:Q:48:GLU:OE1	2.51	0.43
4:O:249:ARG:H	4:O:249:ARG:HE	1.67	0.43
15:a:709:A:O2'	15:a:710:U:P	2.77	0.43
12:F:85:LEU:HD23	12:F:94:SER:CB	2.49	0.43
2:5:207:ALA:HB3	2:5:239:ILE:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:455:ASP:O	10:D:457:VAL:HG13	2.18	0.43
2:5:239:ILE:HD11	2:5:241:PHE:CE1	2.54	0.43
6:Q:170:SER:O	6:Q:174:VAL:HG23	2.18	0.43
12:F:11:ILE:HD12	12:F:17:PRO:HB2	2.01	0.43
7:R:83:MET:SD	7:R:125:LEU:HD13	2.59	0.43
3:d:770:THR:O	3:d:774:LEU:HD12	2.19	0.42
16:L:99:GLY:O	16:L:127:ARG:NH2	2.52	0.42
3:d:245:ASP:OD1	3:d:293:TYR:OH	2.21	0.42
4:O:227:TYR:OH	4:O:238:ASP:OD1	2.35	0.42
1:O:121:PRO:CB	15:a:1468:C:H42	2.32	0.42
2:5:267:LEU:HD21	2:5:307:ALA:CB	2.49	0.42
10:D:472:PRO:HA	10:D:475:GLU:HG2	2.02	0.42
10:D:478:TYR:CE2	10:D:482:LEU:HD11	2.53	0.42
13:6:149:LEU:CD1	13:6:185:ILE:HD11	2.49	0.42
7:R:104:THR:HG22	7:R:105:SER:H	1.84	0.42
6:Q:30:ASN:HB2	6:Q:37:LEU:HD22	2.01	0.42
8:V:162:GLN:O	14:H:30:LYS:NZ	2.40	0.42
14:H:12:HIS:HD1	15:a:891:C:H4'	1.84	0.42
15:a:822:U:OP1	15:a:887:A:O2'	2.37	0.42
12:F:10:ARG:HB3	12:F:92:ILE:HD11	2.01	0.42
15:a:615:C:OP1	16:L:143:SER:OG	2.13	0.42
3:d:333:LYS:HB2	3:d:335:MET:HE2	2.02	0.42
3:d:826:LEU:HD23	3:d:842:LEU:HD22	2.00	0.42
5:P:10:LEU:HD22	5:P:21:TYR:HB3	2.02	0.42
8:V:198:GLU:HG2	12:F:105:LEU:HD13	2.01	0.42
9:2:64:ASN:O	9:2:68:GLN:HG2	2.19	0.42
16:L:66:MET:CE	16:L:68:LEU:HD21	2.49	0.42
16:L:78:ARG:NH2	16:L:117:ASP:OD1	2.52	0.42
3:d:603:TYR:OH	3:d:631:MET:HE3	2.19	0.42
15:a:616:C:O2'	15:a:623:A:N1	2.43	0.42
3:d:207:LEU:HD23	3:d:222:MET:CE	2.50	0.42
3:d:720:ILE:H	3:d:720:ILE:HD12	1.85	0.42
3:d:754:GLU:OE1	3:d:799:GLN:NE2	2.53	0.42
10:D:14:GLY:O	10:D:31:LYS:NZ	2.40	0.42
7:R:130:ARG:NH1	15:a:801:U:OP1	2.41	0.42
9:2:87:ILE:O	9:2:91:VAL:HG23	2.20	0.42
15:a:375:A:H2'	15:a:376:C:O4'	2.20	0.42
15:a:991:G:H3'	15:a:992:U:H5'	2.02	0.42
11:E:297:LEU:HA	11:E:300:VAL:HG12	2.02	0.41
15:a:147:A:O2'	15:a:199:A:N1	2.52	0.41
15:a:1001:U:N3	15:a:1002:A:N7	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:114:GLU:OE2	8:V:118:LEU:HD11	2.20	0.41
13:6:149:LEU:HD11	13:6:185:ILE:HD11	2.02	0.41
3:d:201:LEU:O	3:d:205:GLU:OE1	2.38	0.41
3:d:490:ASP:CB	3:d:585:THR:HG21	2.51	0.41
6:Q:40:ARG:NH1	15:a:694:A:N7	2.69	0.41
8:V:22:LEU:HD12	8:V:114:GLU:OE1	2.21	0.41
14:H:2:SER:OG	15:a:698:A:O5'	2.38	0.41
14:H:119:LYS:HD2	14:H:120:PRO:HD2	2.02	0.41
15:a:1415:G:H22	15:a:1442:G:H3'	1.86	0.41
2:5:58:ASP:OD1	2:5:59:ALA:N	2.53	0.41
8:V:75:ILE:HG23	8:V:108:ILE:HG12	2.02	0.41
15:a:377:A:O2'	15:a:522:A:N7	2.54	0.41
15:a:1579:A:H2'	15:a:1580:U:O4'	2.21	0.41
11:E:244:HIS:CE1	11:E:245:VAL:HG23	2.56	0.41
2:5:67:ARG:NE	15:a:1543:A:OP1	2.52	0.41
14:H:21:VAL:O	14:H:79:TYR:OH	2.27	0.41
15:a:637:A:H61	16:L:117:ASP:CG	2.28	0.41
4:O:111:GLU:N	4:O:111:GLU:OE2	2.54	0.41
1:0:606:ASN:HA	11:E:141:THR:HG21	2.03	0.40
8:V:205:VAL:HG22	8:V:205:VAL:O	2.21	0.40
13:6:32:ILE:O	13:6:34:TYR:N	2.55	0.40
15:a:285:C:H3'	15:a:286:G:H5'	2.03	0.40
15:a:1001:U:C2	15:a:1002:A:C8	3.09	0.40
2:5:279:LEU:HD13	2:5:315:TYR:HD1	1.87	0.40
3:d:218:PHE:CE1	3:d:222:MET:HE2	2.56	0.40
3:d:507:LEU:HD12	15:a:0:A:H4'	2.03	0.40
10:D:399:ARG:NH1	10:D:415:GLN:O	2.48	0.40
15:a:415:U:O2'	15:a:416:A:OP1	2.34	0.40
15:a:492:G:O2'	15:a:497:A:N1	2.45	0.40
3:d:195:LEU:O	3:d:233:LEU:HD21	2.21	0.40
3:d:330:TYR:CZ	8:V:151:LEU:HD12	2.56	0.40
12:F:75:ALA:O	12:F:78:GLN:HG2	2.21	0.40
15:a:1241:C:N4	15:a:1242:C:H41	2.19	0.40
3:d:203:LEU:O	3:d:207:LEU:HD13	2.22	0.40
3:d:607:LEU:HD23	3:d:683:LEU:HD13	2.04	0.40
8:V:127:LYS:O	8:V:131:GLU:OE1	2.39	0.40
11:E:244:HIS:O	11:E:247:PHE:HB3	2.21	0.40
15:a:1012:G:H2'	15:a:1013:C:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	485/628 (77%)	466 (96%)	19 (4%)	0	100	100
2	5	264/339 (78%)	261 (99%)	3 (1%)	0	100	100
3	d	652/864 (76%)	643 (99%)	9 (1%)	0	100	100
4	O	206/286 (72%)	203 (98%)	3 (2%)	0	100	100
5	P	111/121 (92%)	110 (99%)	1 (1%)	0	100	100
6	Q	137/237 (58%)	135 (98%)	2 (2%)	0	100	100
7	R	55/138 (40%)	53 (96%)	2 (4%)	0	100	100
8	V	220/318 (69%)	215 (98%)	5 (2%)	0	100	100
9	2	97/130 (75%)	95 (98%)	2 (2%)	0	100	100
10	D	302/486 (62%)	297 (98%)	5 (2%)	0	100	100
11	E	166/307 (54%)	162 (98%)	4 (2%)	0	100	100
12	F	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
13	6	246/345 (71%)	243 (99%)	3 (1%)	0	100	100
14	H	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
16	L	119/153 (78%)	114 (96%)	5 (4%)	0	100	100
All	All	3342/4638 (72%)	3270 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	7/564 (1%)	7 (100%)	0	100	100
2	5	239/303 (79%)	239 (100%)	0	100	100
3	d	610/803 (76%)	610 (100%)	0	100	100
4	O	183/250 (73%)	182 (100%)	1 (0%)	81	81
5	P	100/106 (94%)	100 (100%)	0	100	100
6	Q	127/218 (58%)	127 (100%)	0	100	100
7	R	48/121 (40%)	48 (100%)	0	100	100
8	V	200/287 (70%)	200 (100%)	0	100	100
9	2	90/117 (77%)	90 (100%)	0	100	100
10	D	277/437 (63%)	277 (100%)	0	100	100
11	E	141/266 (53%)	141 (100%)	0	100	100
12	F	120/120 (100%)	120 (100%)	0	100	100
13	6	229/312 (73%)	229 (100%)	0	100	100
14	H	142/142 (100%)	142 (100%)	0	100	100
16	L	100/131 (76%)	100 (100%)	0	100	100
All	All	2613/4177 (63%)	2612 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
4	O	249	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	5	175	ASN
2	5	212	GLN
3	d	289	ASN
3	d	639	ASN
3	d	752	GLN
4	O	146	ASN
4	O	151	ASN
5	P	81	GLN
6	Q	5	ASN
6	Q	102	GLN
8	V	73	ASN
8	V	183	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	192	HIS
8	V	204	HIS
9	2	61	ASN
9	2	82	GLN
9	2	83	GLN
10	D	133	ASN
10	D	183	ASN
11	E	156	ASN
11	E	244	HIS
13	6	46	HIS
13	6	83	HIS
14	H	139	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	a	1161/1713 (67%)	290 (24%)	0

All (290) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	a	-7	A
15	a	-5	G
15	a	-4	G
15	a	-3	A
15	a	-2	A
15	a	-1	A
15	a	11	U
15	a	14	A
15	a	16	G
15	a	20	A
15	a	29	G
15	a	39	A
15	a	46	A
15	a	54	C
15	a	55	A
15	a	58	A
15	a	73	A
15	a	76	U
15	a	78	U
15	a	85	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	a	90	G
15	a	97	A
15	a	101	U
15	a	102	G
15	a	109	A
15	a	119	A
15	a	120	A
15	a	121	U
15	a	122	U
15	a	128	A
15	a	129	G
15	a	132	A
15	a	136	A
15	a	139	A
15	a	141	C
15	a	143	A
15	a	145	A
15	a	146	G
15	a	151	A
15	a	154	U
15	a	155	A
15	a	156	A
15	a	159	A
15	a	161	U
15	a	175	U
15	a	176	A
15	a	178	A
15	a	180	A
15	a	184	A
15	a	185	A
15	a	192	U
15	a	194	A
15	a	195	U
15	a	196	A
15	a	197	A
15	a	202	G
15	a	204	U
15	a	205	A
15	a	208	U
15	a	209	A
15	a	216	A
15	a	218	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	a	222	U
15	a	224	A
15	a	235	A
15	a	250	A
15	a	251	G
15	a	254	A
15	a	255	G
15	a	261	U
15	a	270	G
15	a	271	U
15	a	272	U
15	a	286	G
15	a	294	A
15	a	304	A
15	a	331	A
15	a	334	U
15	a	336	U
15	a	347	U
15	a	350	A
15	a	351	A
15	a	352	G
15	a	356	C
15	a	370	A
15	a	371	U
15	a	372	U
15	a	376	C
15	a	393	A
15	a	401	A
15	a	409	G
15	a	414	A
15	a	416	A
15	a	479	A
15	a	480	U
15	a	481	A
15	a	485	A
15	a	486	U
15	a	488	A
15	a	495	U
15	a	496	A
15	a	498	A
15	a	501	U
15	a	503	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	a	514	U
15	a	516	A
15	a	517	U
15	a	527	G
15	a	528	A
15	a	538	C
15	a	540	A
15	a	542	A
15	a	551	U
15	a	552	A
15	a	557	G
15	a	560	A
15	a	604	A
15	a	606	U
15	a	611	U
15	a	612	A
15	a	621	U
15	a	624	U
15	a	625	A
15	a	635	G
15	a	641	G
15	a	644	G
15	a	645	U
15	a	646	A
15	a	661	A
15	a	668	A
15	a	673	A
15	a	674	A
15	a	677	G
15	a	682	A
15	a	688	C
15	a	694	A
15	a	698	A
15	a	704	A
15	a	709	A
15	a	710	U
15	a	716	A
15	a	728	A
15	a	729	U
15	a	731	U
15	a	749	A
15	a	777	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	a	780	G
15	a	788	U
15	a	799	A
15	a	820	A
15	a	828	A
15	a	835	C
15	a	837	A
15	a	838	G
15	a	839	A
15	a	840	G
15	a	874	G
15	a	878	U
15	a	879	A
15	a	886	G
15	a	894	U
15	a	898	U
15	a	912	A
15	a	913	U
15	a	914	A
15	a	915	U
15	a	916	A
15	a	920	A
15	a	924	U
15	a	931	A
15	a	936	A
15	a	937	A
15	a	938	A
15	a	939	G
15	a	954	A
15	a	989	C
15	a	990	G
15	a	991	G
15	a	992	U
15	a	994	A
15	a	996	A
15	a	998	A
15	a	999	C
15	a	1000	U
15	a	1002	A
15	a	1007	G
15	a	1010	G
15	a	1011	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	a	1016	G
15	a	1025	U
15	a	1026	U
15	a	1049	C
15	a	1058	G
15	a	1059	A
15	a	1064	U
15	a	1066	U
15	a	1067	A
15	a	1070	A
15	a	1072	U
15	a	1073	U
15	a	1079	A
15	a	1080	A
15	a	1083	A
15	a	1088	A
15	a	1089	U
15	a	1090	U
15	a	1092	C
15	a	1097	G
15	a	1100	A
15	a	1101	C
15	a	1102	A
15	a	1103	U
15	a	1106	U
15	a	1239	A
15	a	1244	U
15	a	1245	A
15	a	1246	U
15	a	1258	U
15	a	1260	G
15	a	1263	G
15	a	1265	G
15	a	1268	A
15	a	1270	A
15	a	1271	A
15	a	1272	U
15	a	1273	A
15	a	1369	U
15	a	1370	A
15	a	1373	A
15	a	1403	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	a	1404	A
15	a	1407	A
15	a	1409	U
15	a	1412	C
15	a	1413	U
15	a	1414	A
15	a	1420	A
15	a	1422	G
15	a	1428	U
15	a	1437	A
15	a	1439	G
15	a	1443	A
15	a	1447	U
15	a	1448	U
15	a	1449	C
15	a	1452	A
15	a	1455	G
15	a	1457	U
15	a	1458	U
15	a	1462	A
15	a	1463	C
15	a	1465	A
15	a	1466	A
15	a	1469	A
15	a	1475	C
15	a	1480	G
15	a	1484	A
15	a	1486	A
15	a	1492	U
15	a	1497	U
15	a	1505	U
15	a	1507	U
15	a	1508	A
15	a	1509	U
15	a	1510	A
15	a	1511	U
15	a	1512	A
15	a	1515	A
15	a	1516	U
15	a	1517	U
15	a	1522	A
15	a	1523	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	a	1526	A
15	a	1527	A
15	a	1528	U
15	a	1537	U
15	a	1538	U
15	a	1539	A
15	a	1541	U
15	a	1544	U
15	a	1548	U
15	a	1550	U
15	a	1552	U
15	a	1555	U
15	a	1563	G
15	a	1564	A
15	a	1571	A
15	a	1575	A
15	a	1584	A
15	a	1586	G

There are no RNA pucker outliers to report.

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 30 ligands modelled in this entry, 29 are monoatomic - leaving 1 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
17	SF4	0	701	1	0,12,12	-	-	-		

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
17	SF4	0	701	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

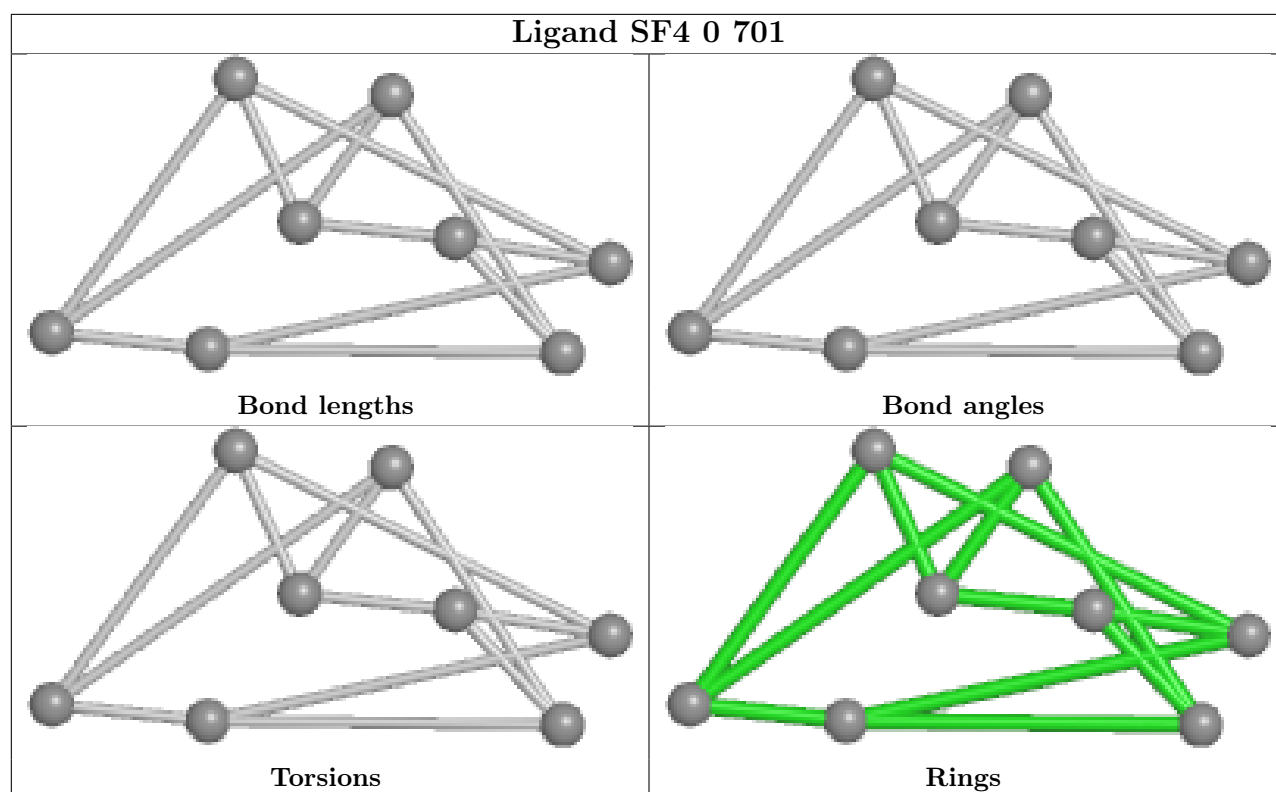
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

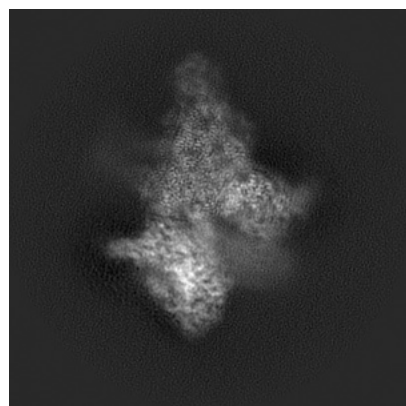
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27249. These allow visual inspection of the internal detail of the map and identification of artifacts.

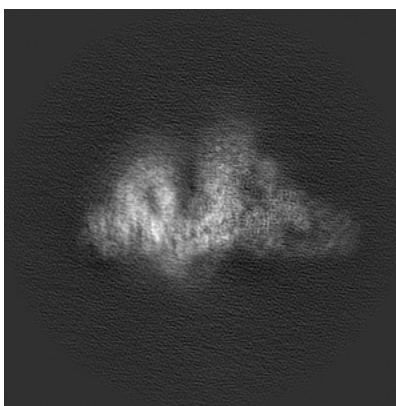
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

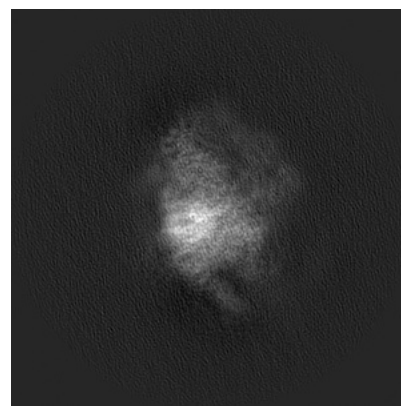
6.1.1 Primary map



X

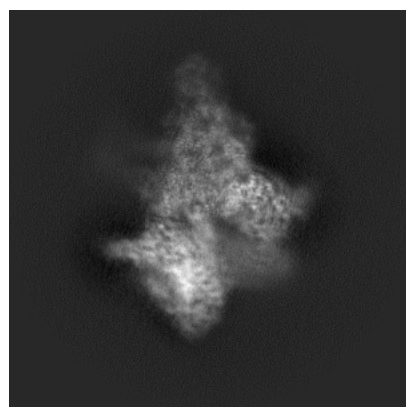


Y

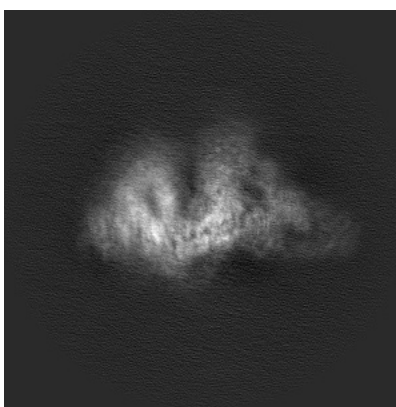


Z

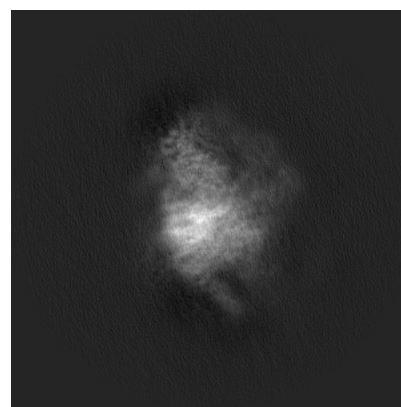
6.1.2 Raw map



X



Y

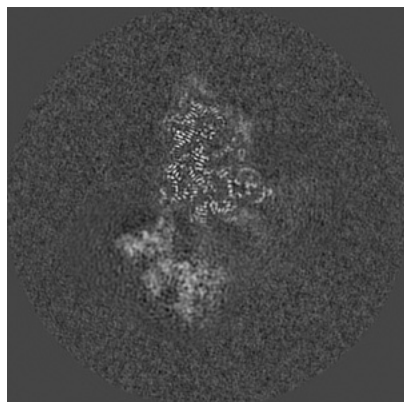


Z

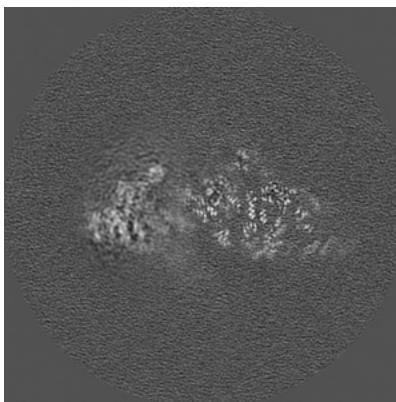
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

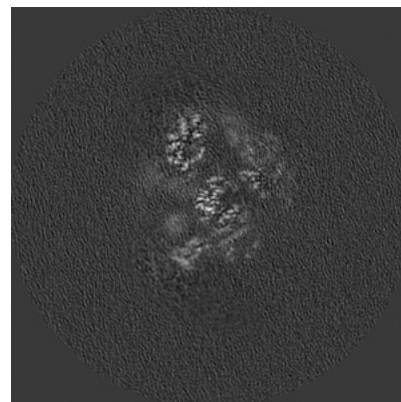
6.2.1 Primary map



X Index: 200

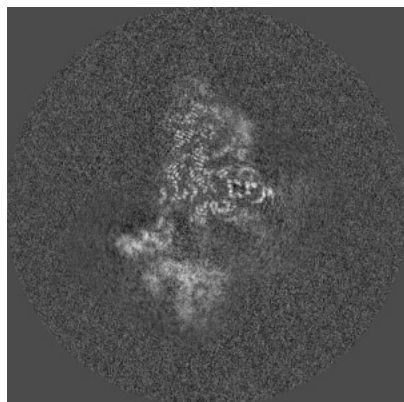


Y Index: 200

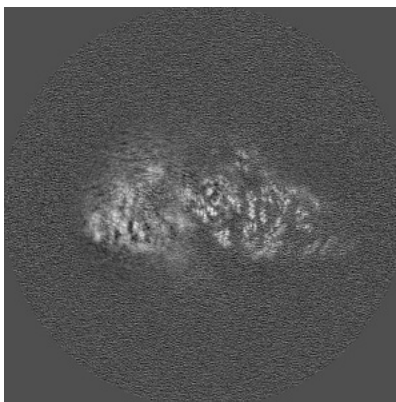


Z Index: 200

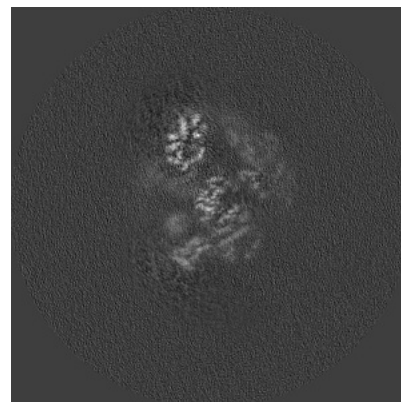
6.2.2 Raw map



X Index: 200



Y Index: 200

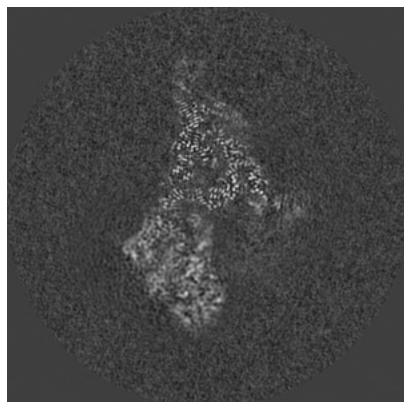


Z Index: 200

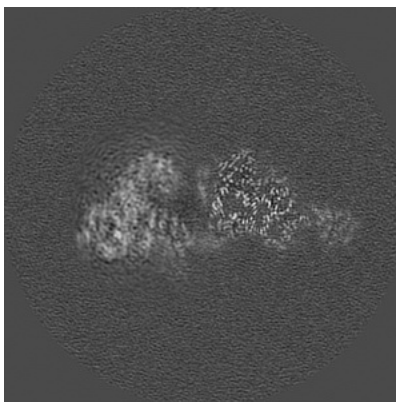
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

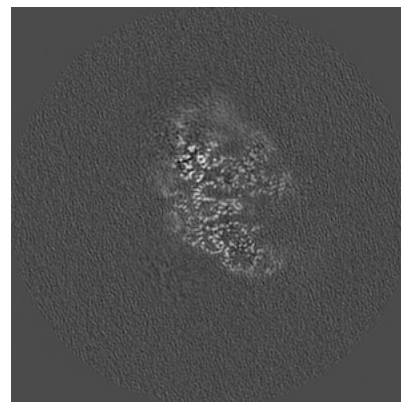
6.3.1 Primary map



X Index: 188

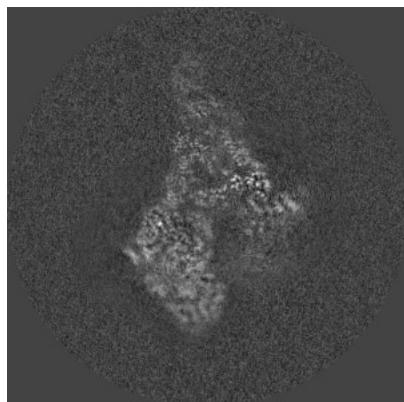


Y Index: 177

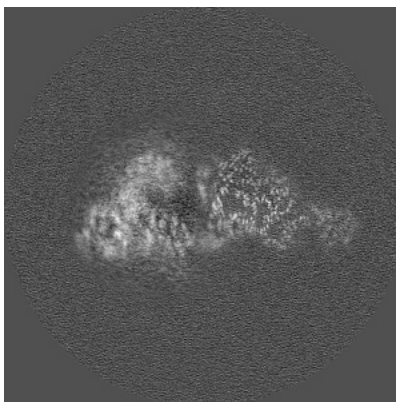


Z Index: 216

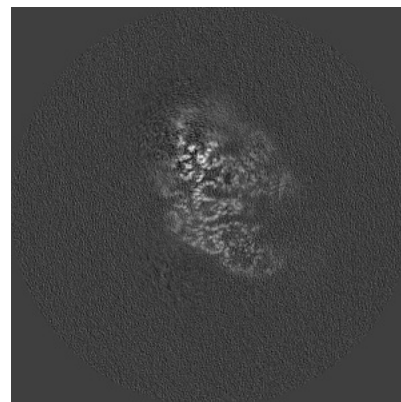
6.3.2 Raw map



X Index: 184



Y Index: 177

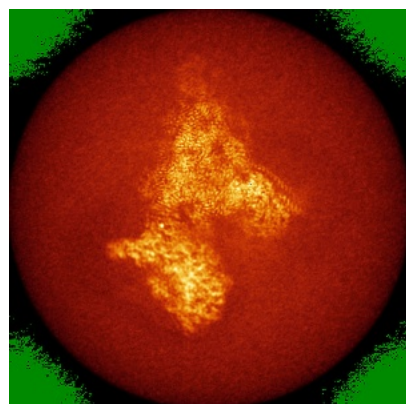


Z Index: 216

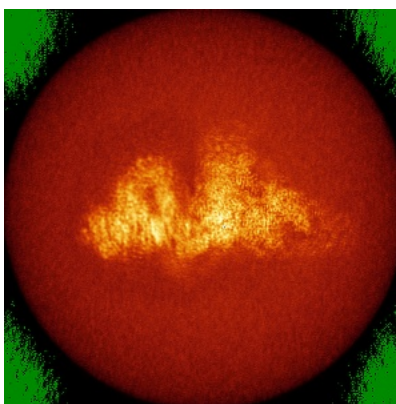
The images above show the largest variance slices of the map in three orthogonal directions.

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

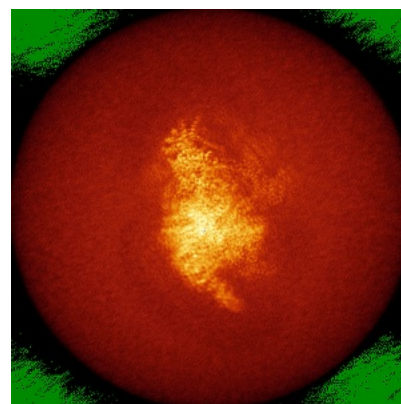
6.4.1 Primary map



X

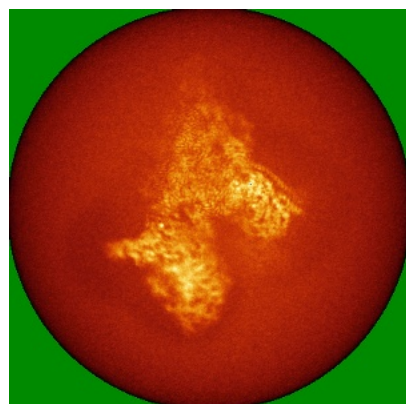


Y

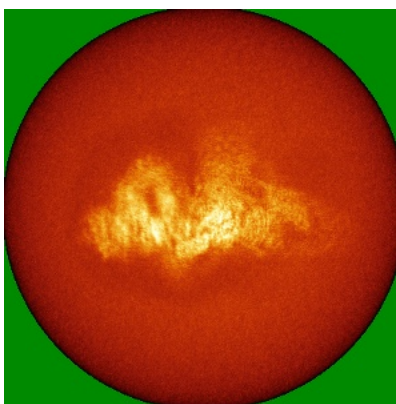


Z

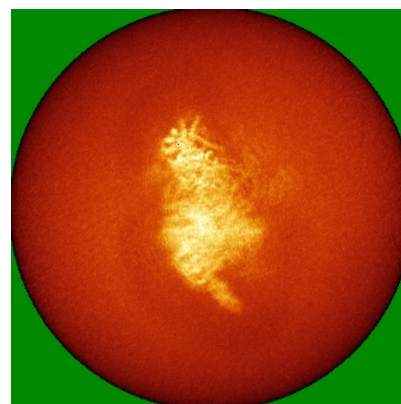
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

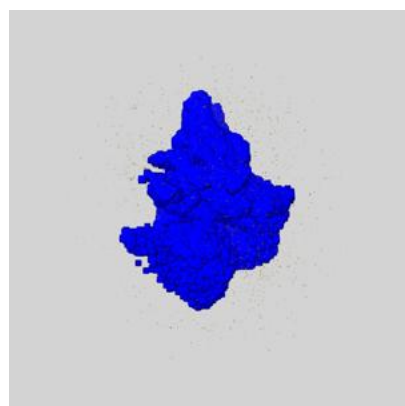
6.6 Mask visualisation [i](#)

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

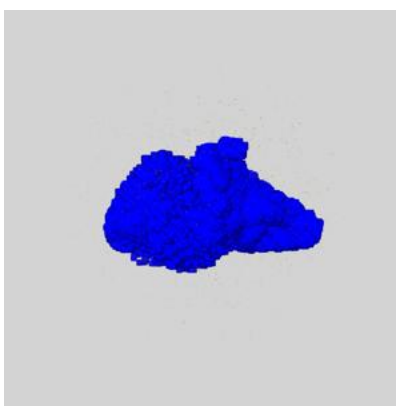
A mask typically either:

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

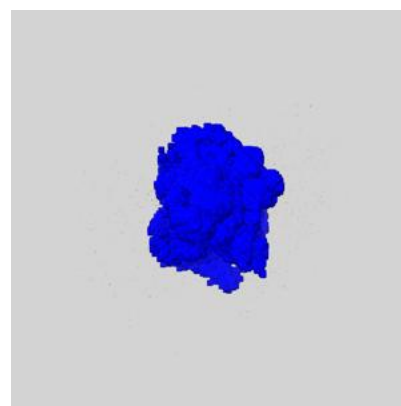
6.6.1 emd_27249_msk_1.map [i](#)



X



Y

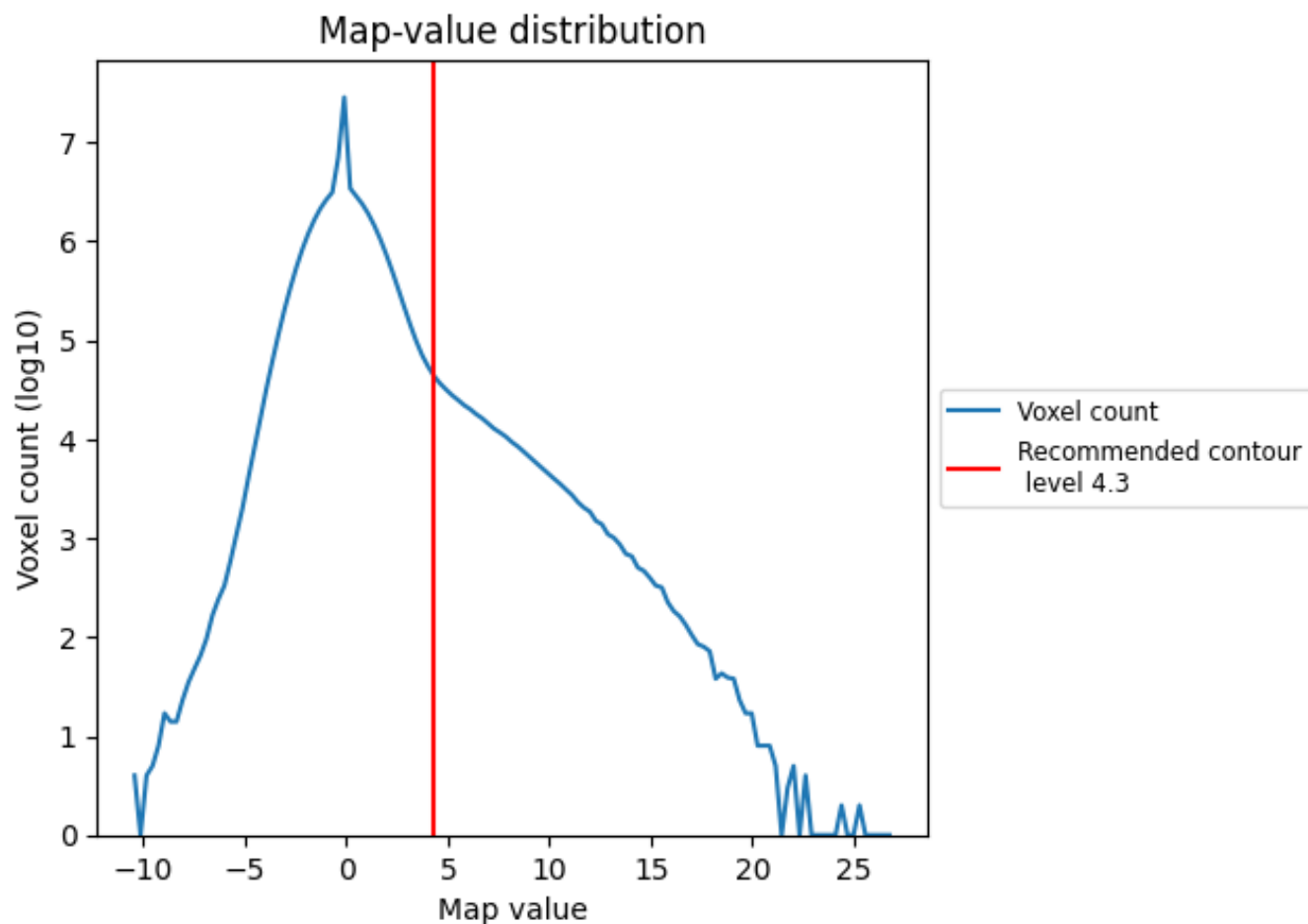


Z

7 Map analysis [i](#)

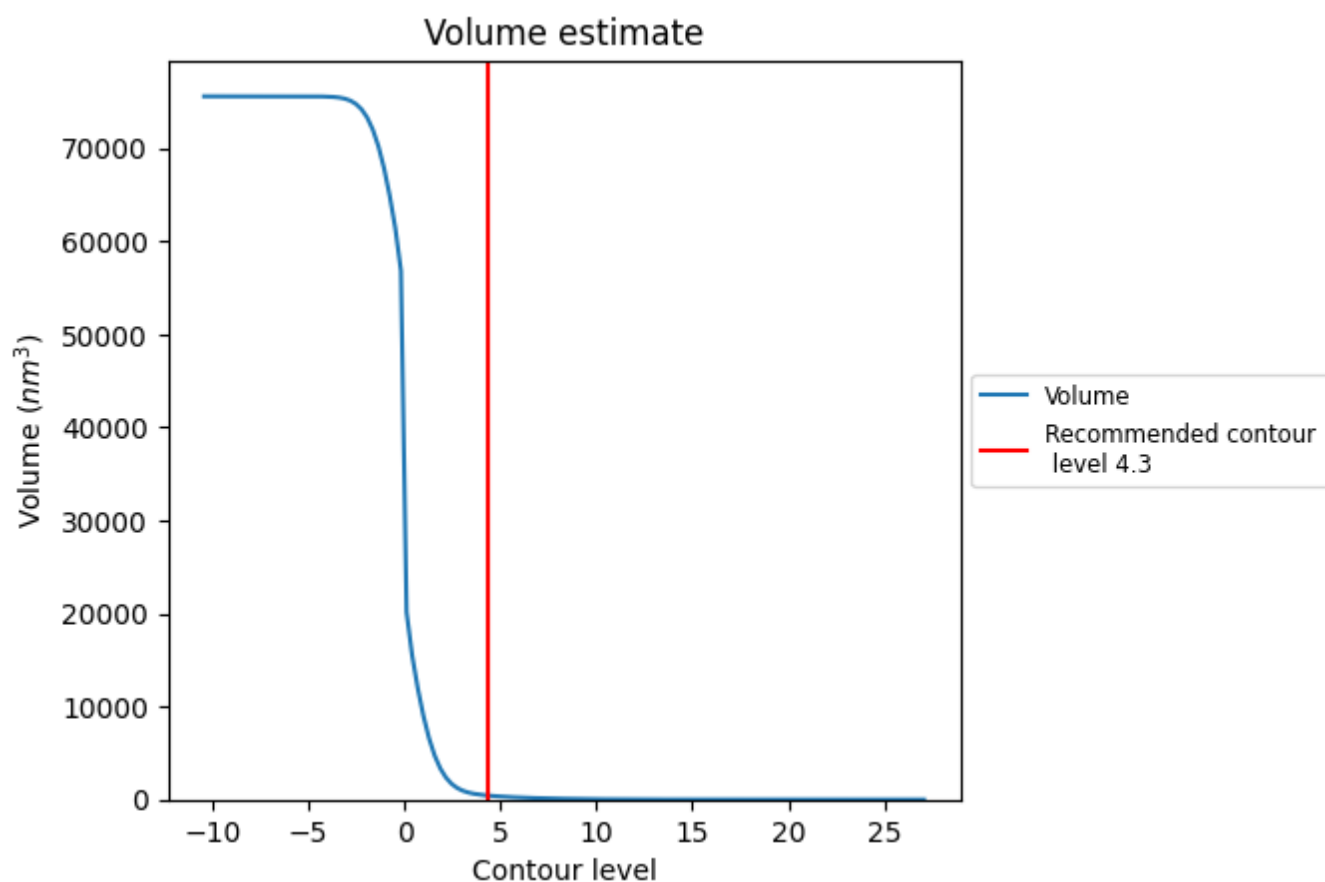
This section contains the results of statistical analysis of the map.

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.

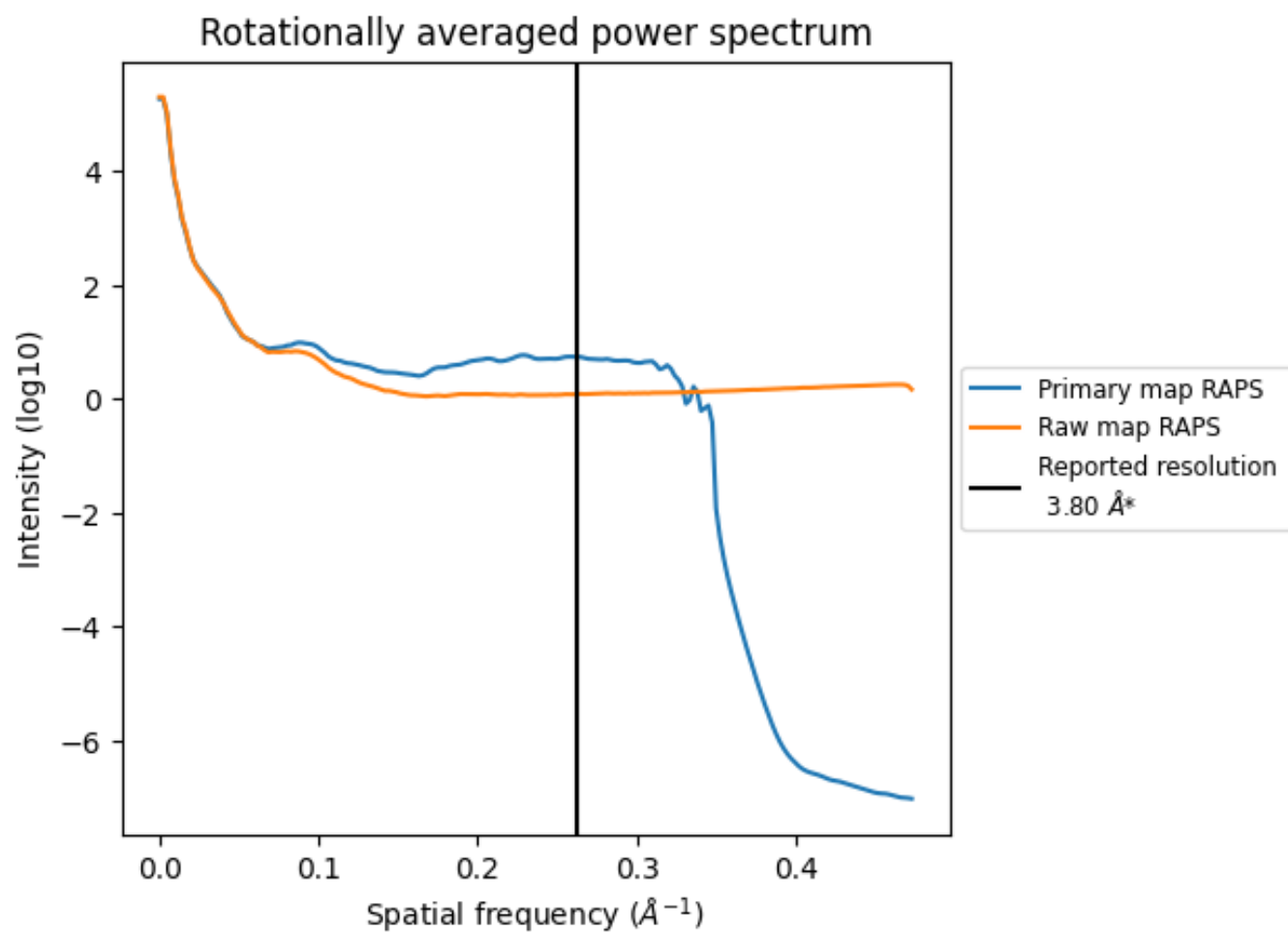
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 440 nm³; this corresponds to an approximate mass of 397 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 ⓘ

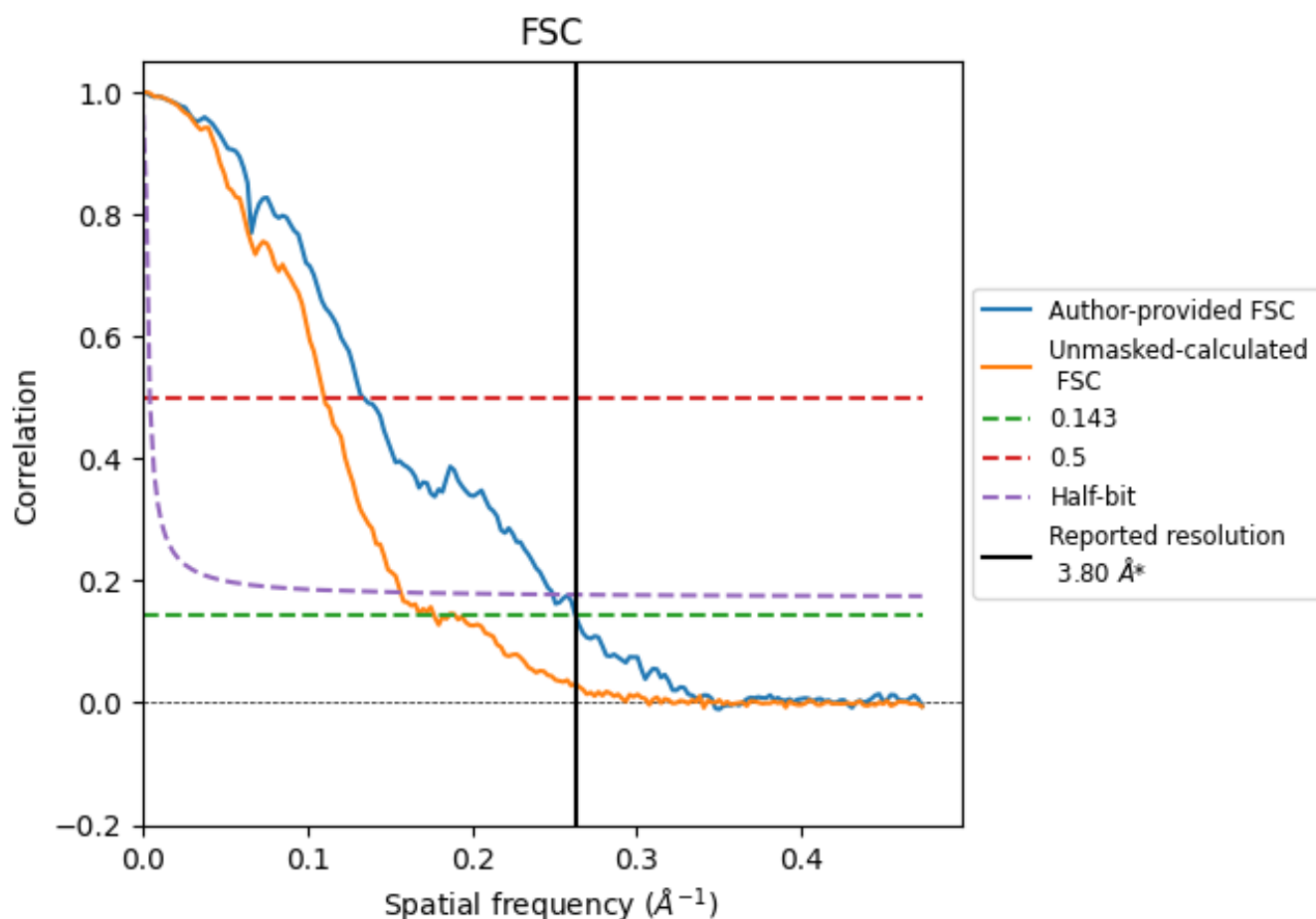


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	7.47	4.02
Unmasked-calculated*	5.65	9.07	6.38

*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 5.65 differs from the reported value 3.8 by more than 10 %

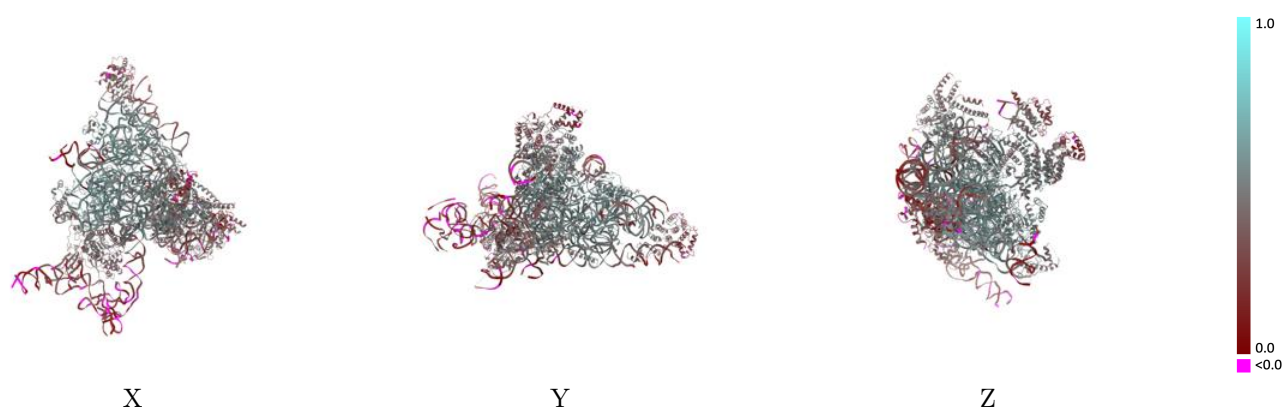
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-27249 and PDB model 8D8J. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

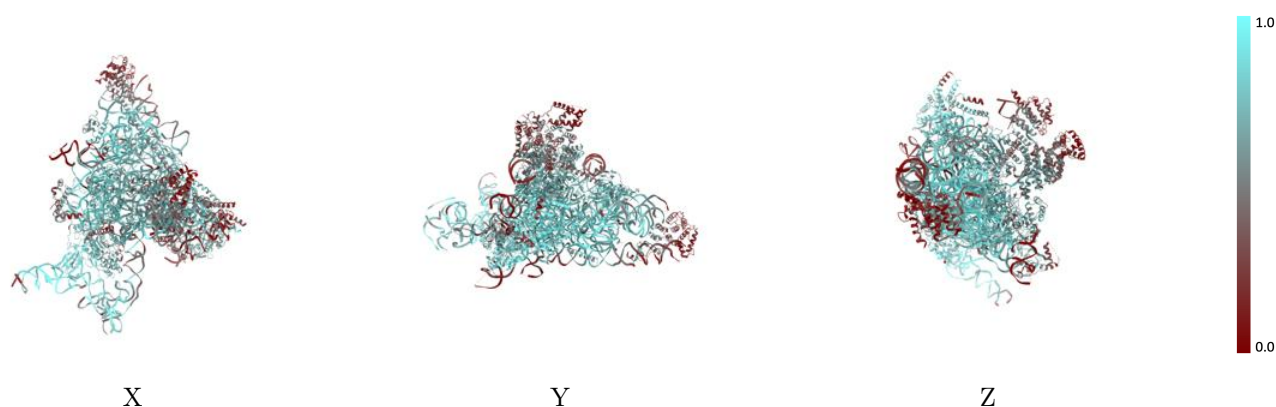
This section was not generated.

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



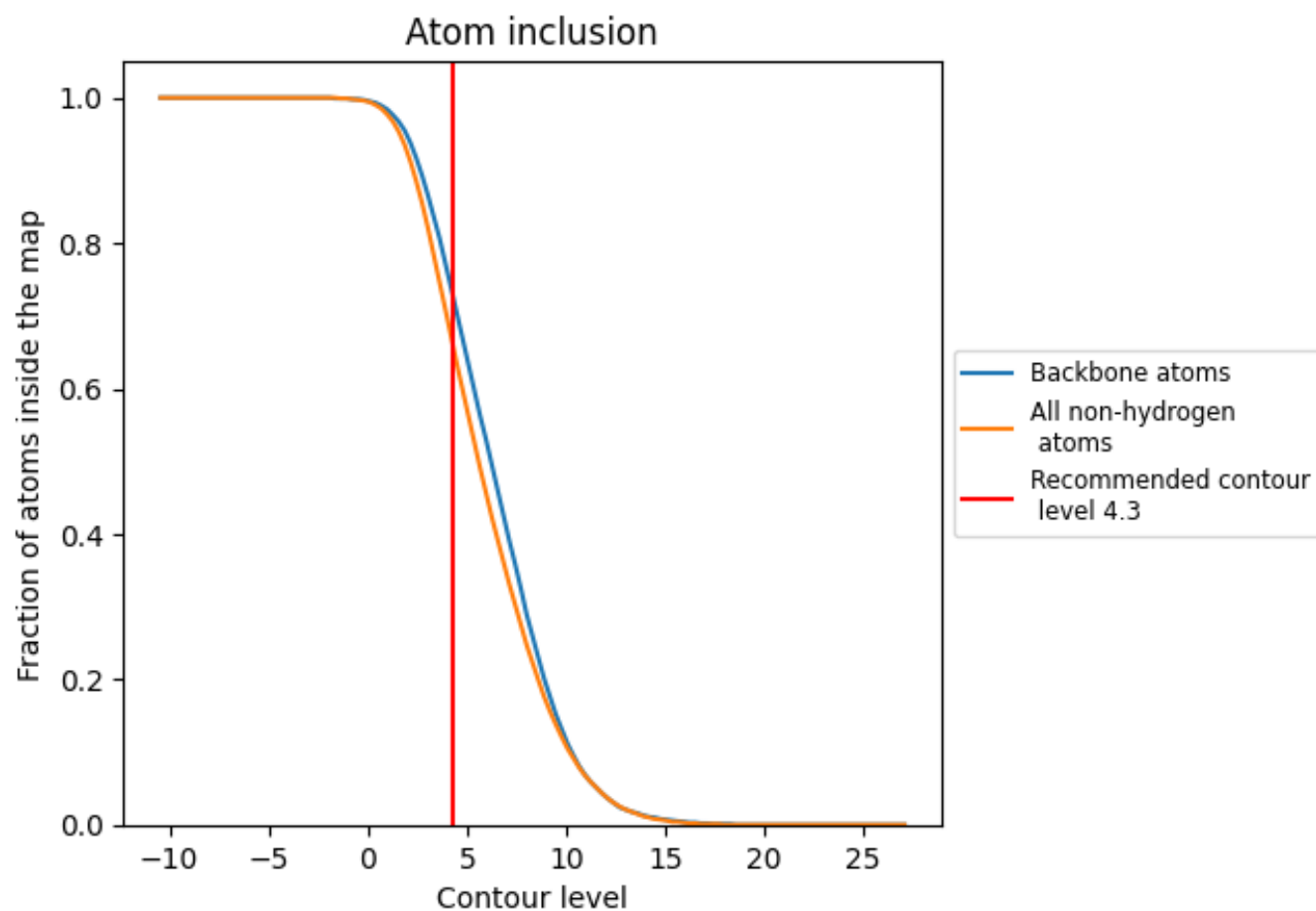
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 66% 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 (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6590	0.4250
0	0.7450	0.3530
2	0.6990	0.5360
5	0.2640	0.3280
6	0.6910	0.5520
D	0.6950	0.5470
E	0.7130	0.5090
F	0.6620	0.3840
H	0.7150	0.5390
L	0.6560	0.5490
O	0.8210	0.4800
P	0.7420	0.5580
Q	0.6760	0.4770
R	0.5110	0.3720
V	0.6300	0.4810
a	0.7150	0.3910
d	0.4150	0.4060

1.0

0.0

<0.0