



Full wwPDB EM Validation Report ⓘ

Feb 4, 2023 – 01:58 PM EST

PDB ID : 8D8K
EMDB ID : EMD-27250
Title : Yeast mitochondrial small subunit assembly intermediate (State 2)
Authors : Burnside, C.; Harper, N.J.; Klinge, S.
Deposited on : 2022-06-08
Resolution : 3.13 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:

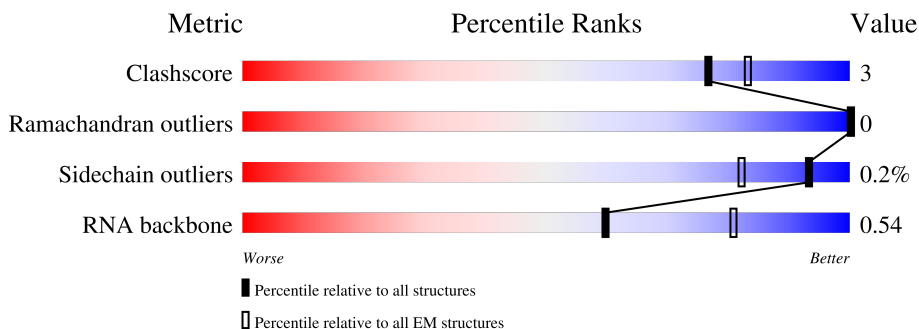
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

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 3.13 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">42%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">58%</div> <div style="text-align: center;">10%</div> <div style="text-align: center;">32%</div> </div>
2	5	339	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">75%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">70%</div> <div style="text-align: center;">9%</div> <div style="text-align: center;">20%</div> </div>
3	C	398	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">10%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">51%</div> <div style="text-align: center;">9%</div> <div style="text-align: center;">40%</div> </div>
4	d	864	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">33%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">76%</div> <div style="text-align: center;">24%</div> </div>
5	M	143	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">11%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">55%</div> <div style="text-align: center;">•</div> <div style="text-align: center;">42%</div> </div>
6	N	115	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">•</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">97%</div> <div style="text-align: center;">••</div> </div>
7	O	286	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">11%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">71%</div> <div style="text-align: center;">•</div> <div style="text-align: center;">27%</div> </div>

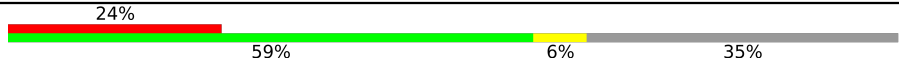
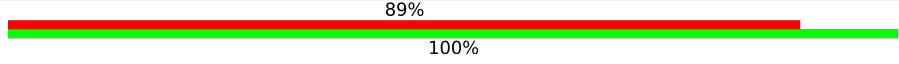

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Mol	Chain	Length	Quality of chain
8	P	121	12% 96%
9	Q	237	40% 77% 10% 14%
10	R	138	17% 61% 5% 34%
11	S	91	12% 78% 18%
12	T	177	16% 48% 48%
13	U	264	15% 79% 9% 12%
14	V	318	19% 68% 5% 27%
15	W	450	75% 13% 12%
16	X	110	5% 75% 11% 13%
17	Y	319	13% 70% 13% 18%
18	Z	95	55% 85% 12%
19	A	344	18% 54% 42%
20	B	394	10% 63% 5% 32%
21	2	130	18% 70% 6% 24%
22	3	266	32% 81% 11% 8%
23	D	486	14% 60% 37%
24	4	321	53% 78% 7% 16%
25	E	307	11% 88% 7% 5%
26	F	131	22% 92% 8%
27	6	345	7% 70% 27%
28	G	247	10% 54% 6% 40%
29	H	155	90% 10%
30	I	278	20% 68% 7% 25%
31	a	1713	18% 68% 21% 10%
32	J	203	67% 29%

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Mol	Chain	Length	Quality of chain
33	K	217	
34	c	94	
35	L	153	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 88977 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
			Total	C	N	O	S		
1	0	429	3471	2204	626	629	12	0	0

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

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

- Molecule 3 is a protein called Ribosomal protein VAR1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	239	2014	1275	348	364	27	0	0

- Molecule 4 is a protein called Mitochondrial group I intron splicing factor CCM1.

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

- Molecule 5 is a protein called 37S ribosomal protein SWS2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	83	645	417	111	112	5	0	0

- Molecule 6 is a protein called 37S ribosomal protein MRP2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	113	931	596	179	152	4	0	0

- Molecule 7 is a protein called 37S ribosomal protein S28, mitochondrial.

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

- Molecule 8 is a protein called 37S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	116	919	586	172	159	2	0	0

- Molecule 9 is a protein called 37S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Q	205	1690	1059	316	310	5	0	0

- Molecule 10 is a protein called 37S ribosomal protein RSM18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	R	91	738	463	143	128	4	0	0

- Molecule 11 is a protein called 37S ribosomal protein S19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	75	595	383	109	101	2	0	0

- Molecule 12 is a protein called 37S ribosomal protein MRP21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	92	760	475	150	130	5	0	0

- Molecule 13 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	U	233	1907	1211	331	358	7	0	0

- Molecule 14 is a protein called 37S ribosomal protein PET123, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	233	Total	C	N	O	S	0	0
			1872	1189	338	342	3		

- Molecule 15 is a protein called 37S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	395	Total	C	N	O	S	0	0
			3174	2047	531	588	8		

- Molecule 16 is a protein called Mitochondrial 37S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	96	Total	C	N	O	S	0	0
			774	496	140	135	3		

- Molecule 17 is a protein called 37S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	263	Total	C	N	O	S	0	0
			2208	1400	393	411	4		

- Molecule 18 is a protein called 37S ribosomal protein MRP10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	84	Total	C	N	O	S	0	0
			660	418	121	115	6		

- Molecule 19 is a protein called 37S ribosomal protein MRP51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	199	Total	C	N	O	S	0	0
			1585	1023	278	279	5		

- Molecule 20 is a protein called 37S ribosomal protein MRP4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	266	Total	C	N	O	S	0	0
			2085	1313	366	404	2		

- Molecule 21 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	99	Total	C	N	O	S	0	0
			833	530	156	146	1		

- Molecule 22 is a protein called 37S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3	244	Total	C	N	O	S	0	0
			1953	1261	328	359	5		

- Molecule 23 is a protein called 37S ribosomal protein NAM9, mitochondrial.

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

- Molecule 24 is a protein called 37S ribosomal protein MRP1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4	271	Total	C	N	O	S	0	0
			2182	1390	373	412	7		

- Molecule 25 is a protein called 37S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	E	291	Total	C	N	O	S	0	0
			2321	1479	411	423	8		

- Molecule 26 is a protein called 37S ribosomal protein MRP17, mitochondrial.

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

- Molecule 27 is a protein called 37S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	6	251	Total	C	N	O	S	0	0
			2071	1322	375	368	6		

- Molecule 28 is a protein called 37S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	148	Total	C	N	O	S	0	0
			1185	749	220	211	5		

- Molecule 29 is a protein called 37S ribosomal protein S8, mitochondrial.

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

- Molecule 30 is a protein called 37S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	I	208	Total	C	N	O	S	0	0
			1667	1067	299	297	4		

- Molecule 31 is a RNA chain called 15S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1538	Total	C	N	O	P	0	0
			32666	14691	5767	10670	1538		

- Molecule 32 is a protein called 37S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	144	Total	C	N	O	S	0	0
			1186	768	204	210	4		

- Molecule 33 is a protein called 37S ribosomal protein S18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	141	Total	C	N	O	S	0	0
			1113	711	194	202	6		

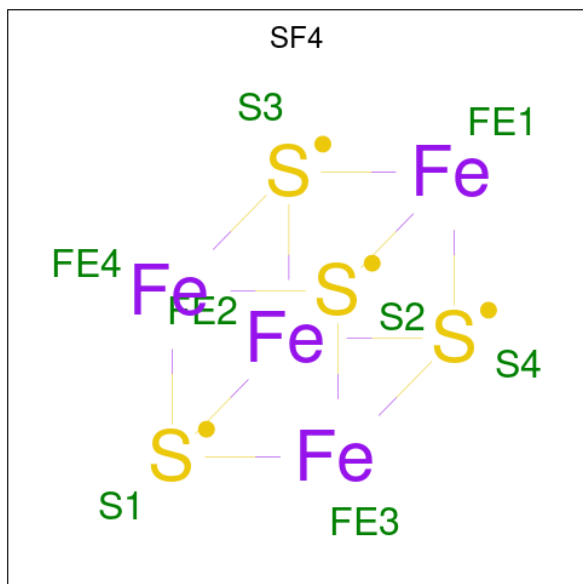
- Molecule 34 is a protein called unknown protein sequence.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	c	94	Total	C	N	O	0	0
			470	282	94	94		

- Molecule 35 is a protein called MRPS12 isoform 1.

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

- Molecule 36 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).

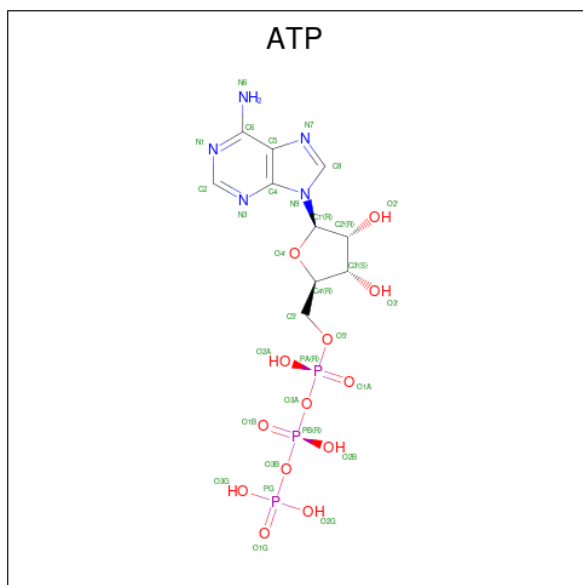


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
36	0	1	8	4	4	0

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	Q	1	Total	Mg	0
			1	1	
37	W	1	Total	Mg	0
			1	1	
37	B	1	Total	Mg	0
			1	1	
37	a	69	Total	Mg	0
			69	69	

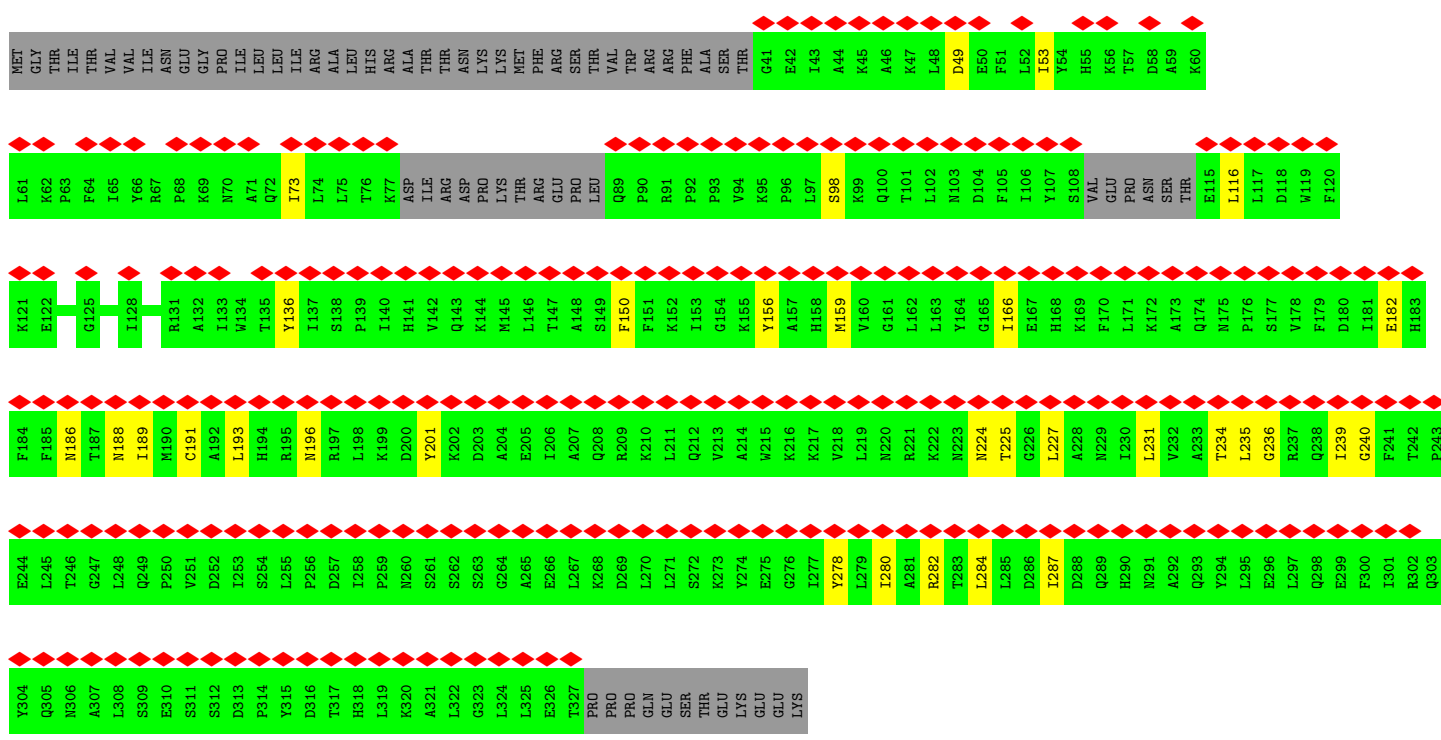
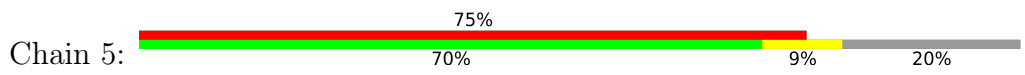
- Molecule 38 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



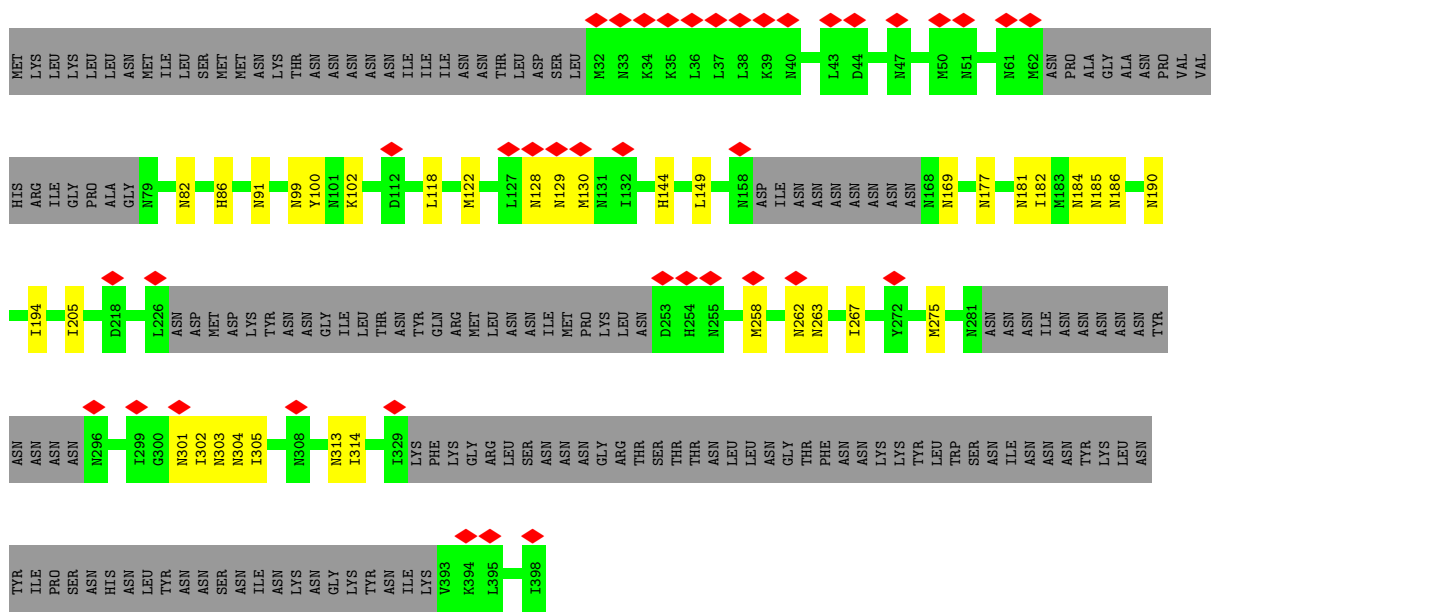
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	W	1	31	10	5	13	3	0

- Molecule 39 is water.

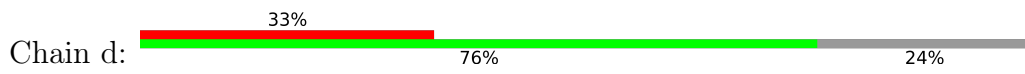
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	W	3	3	3	0

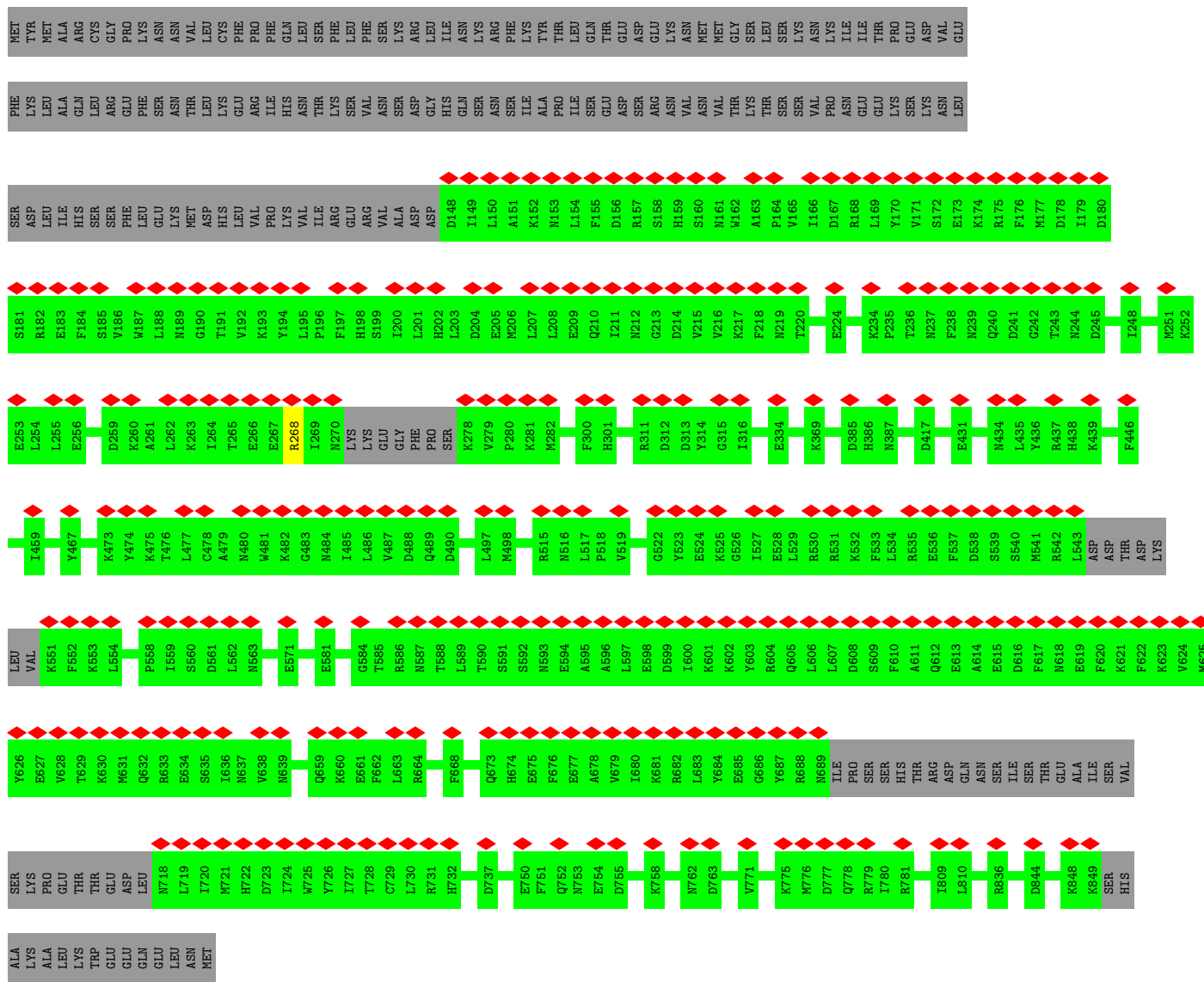


• Molecule 3: Ribosomal protein VAR1, mitochondrial

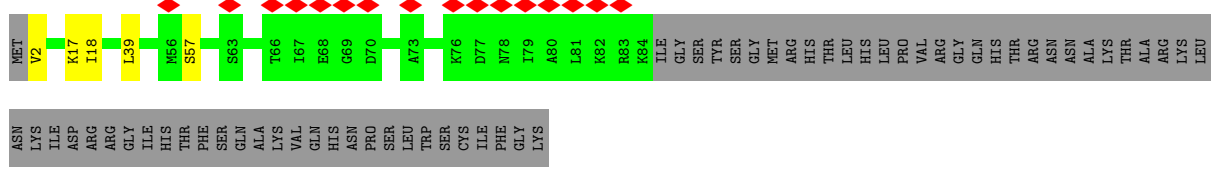


• Molecule 4: Mitochondrial group I intron splicing factor CCM1

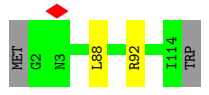




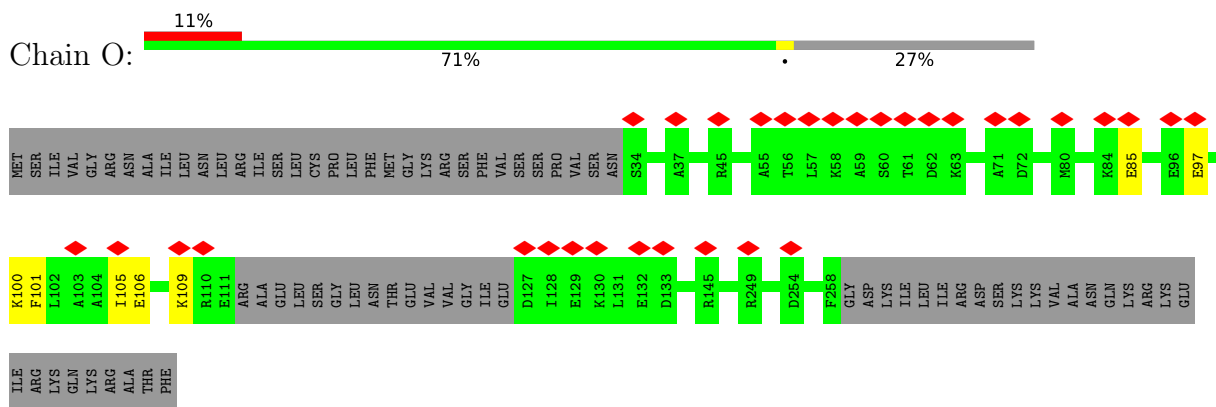
- Molecule 5: 37S ribosomal protein SWS2, mitochondrial



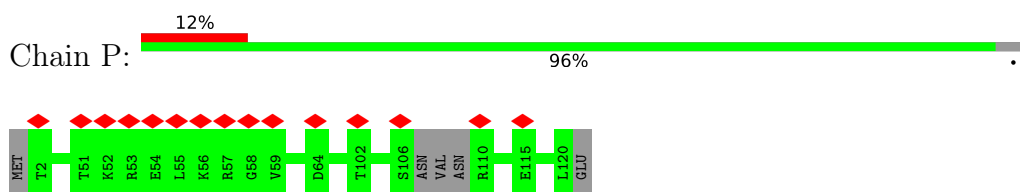
- Molecule 6: 37S ribosomal protein MRP2, mitochondrial



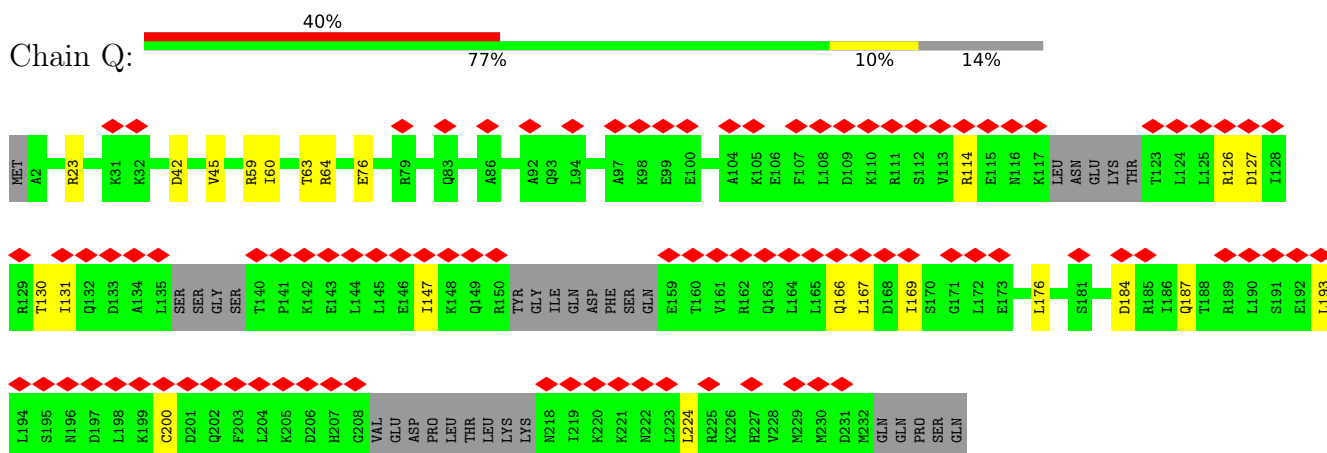
- Molecule 7: 37S ribosomal protein S28, mitochondrial



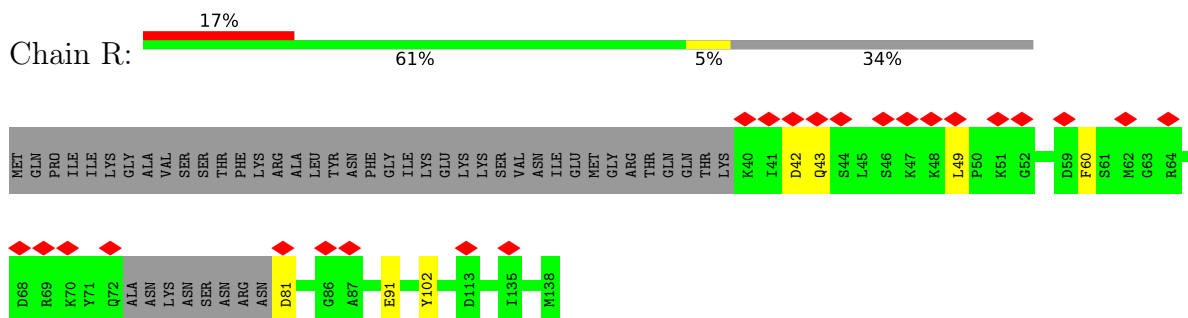
- Molecule 8: 37S ribosomal protein S16, mitochondrial



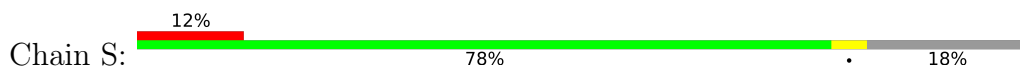
- Molecule 9: 37S ribosomal protein S17, mitochondrial

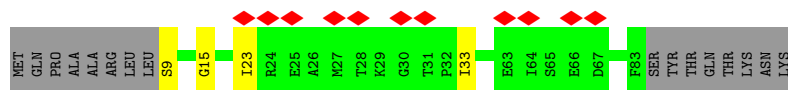


- Molecule 10: 37S ribosomal protein RSM18, mitochondrial

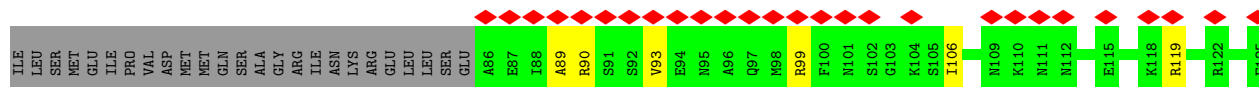


- Molecule 11: 37S ribosomal protein S19, mitochondrial

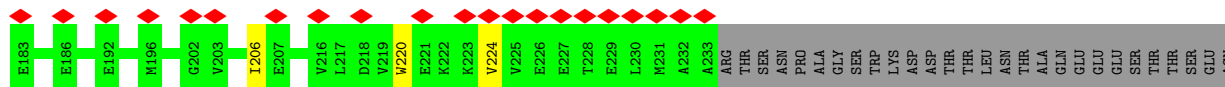
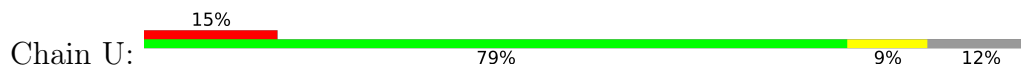




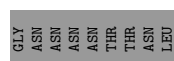
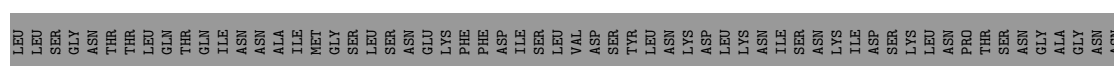
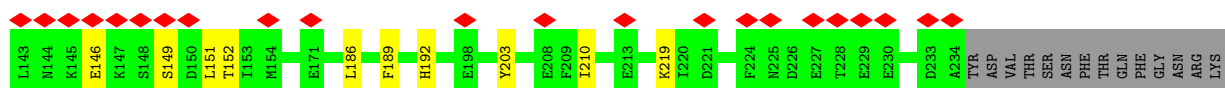
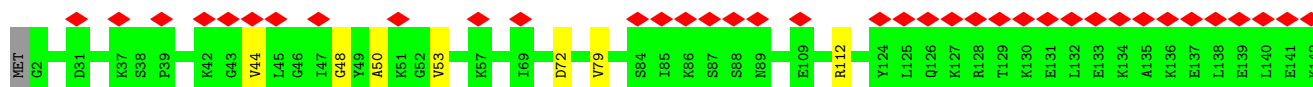
- Molecule 12: 37S ribosomal protein MRP21, mitochondrial



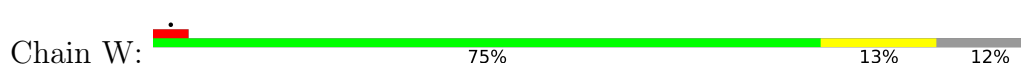
- Molecule 13: 37S ribosomal protein S25, mitochondrial

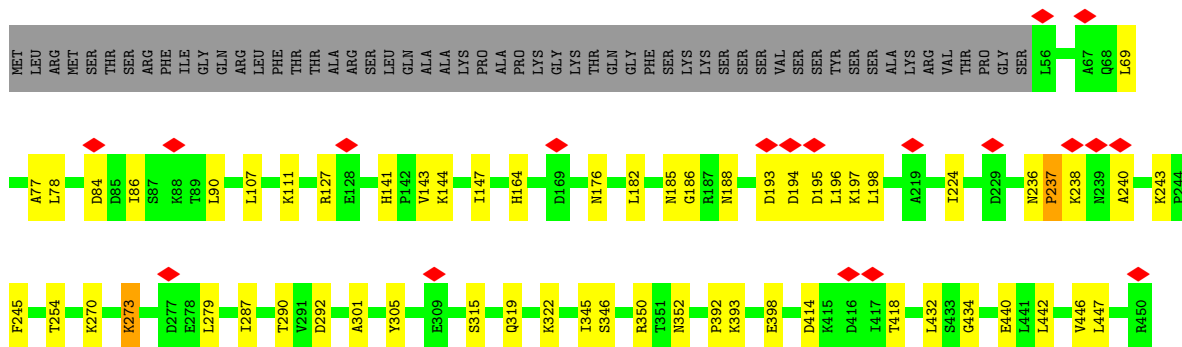


- Molecule 14: 37S ribosomal protein PET123, mitochondrial



- Molecule 15: 37S ribosomal protein S23, mitochondrial

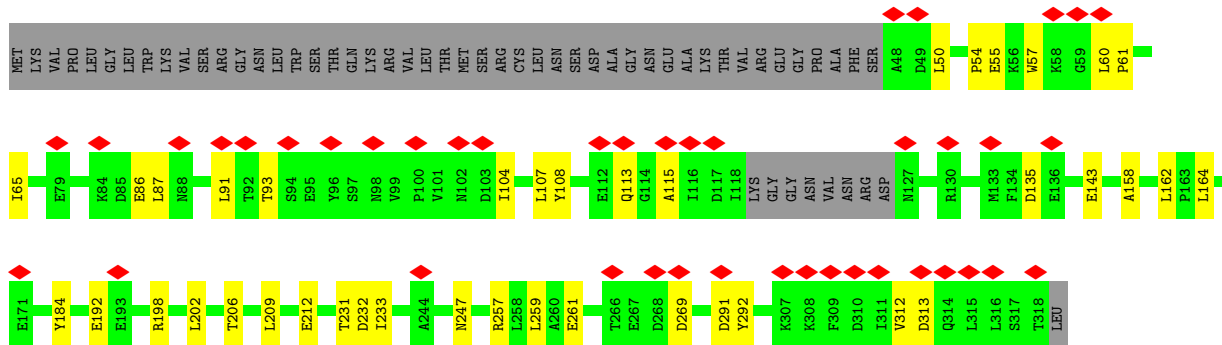




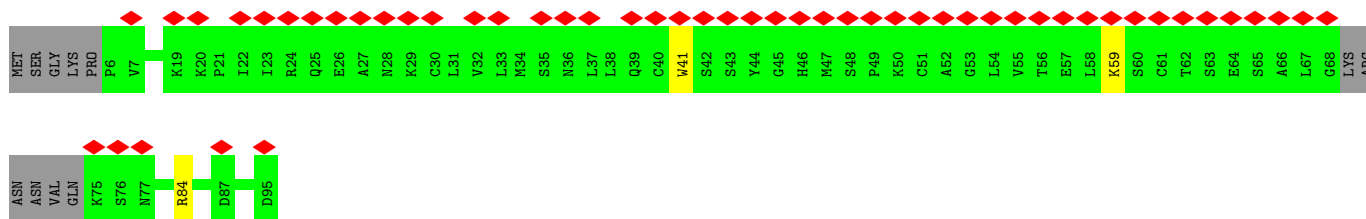
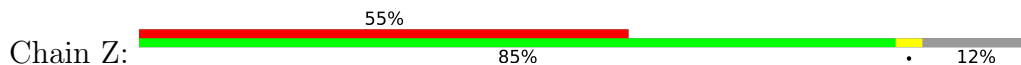
• Molecule 16: Mitochondrial 37S ribosomal protein S27



• Molecule 17: 37S ribosomal protein S24, mitochondrial

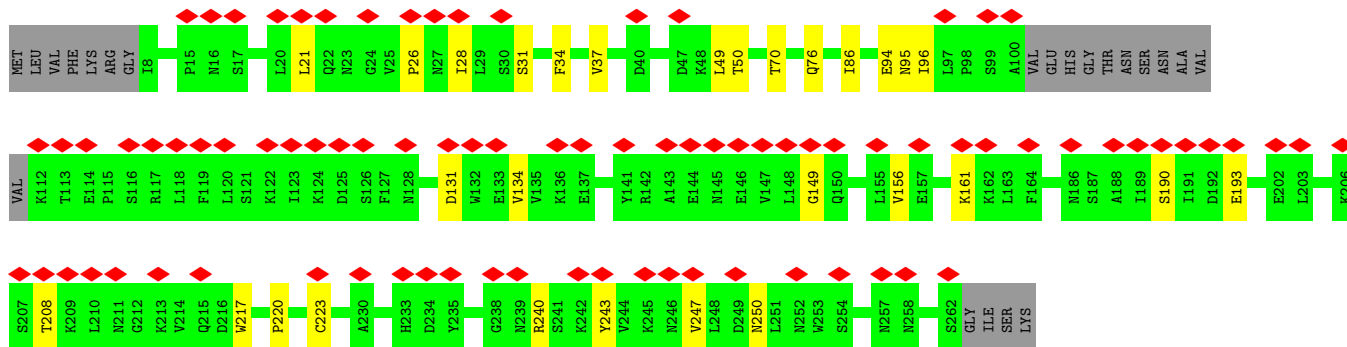


• Molecule 18: 37S ribosomal protein MRP10, mitochondrial

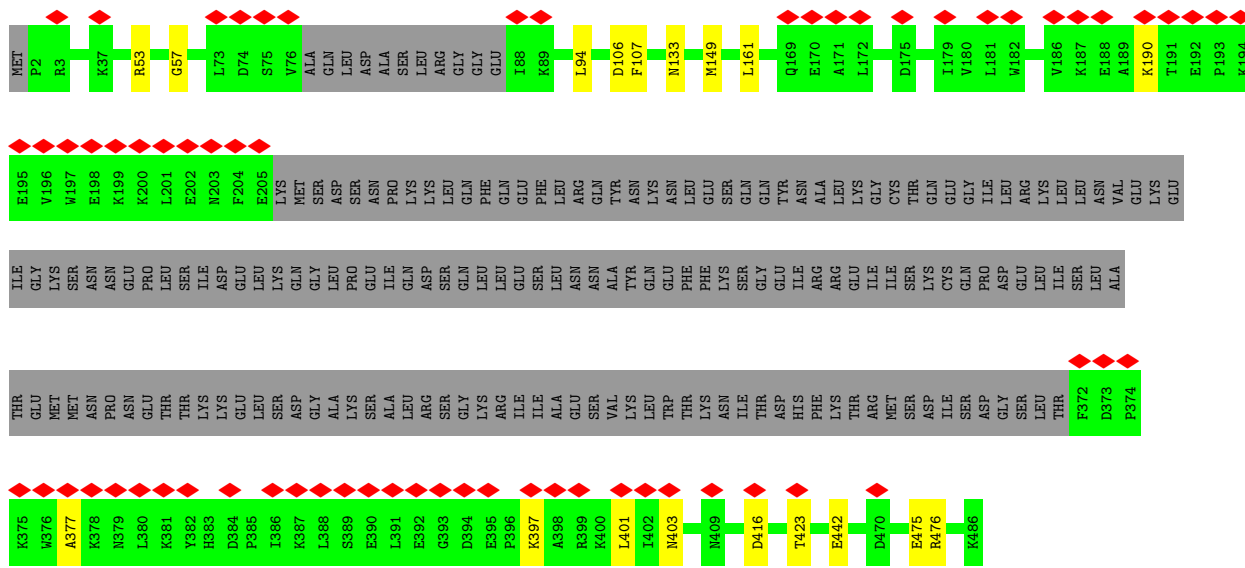


• Molecule 19: 37S ribosomal protein MRP51, mitochondrial

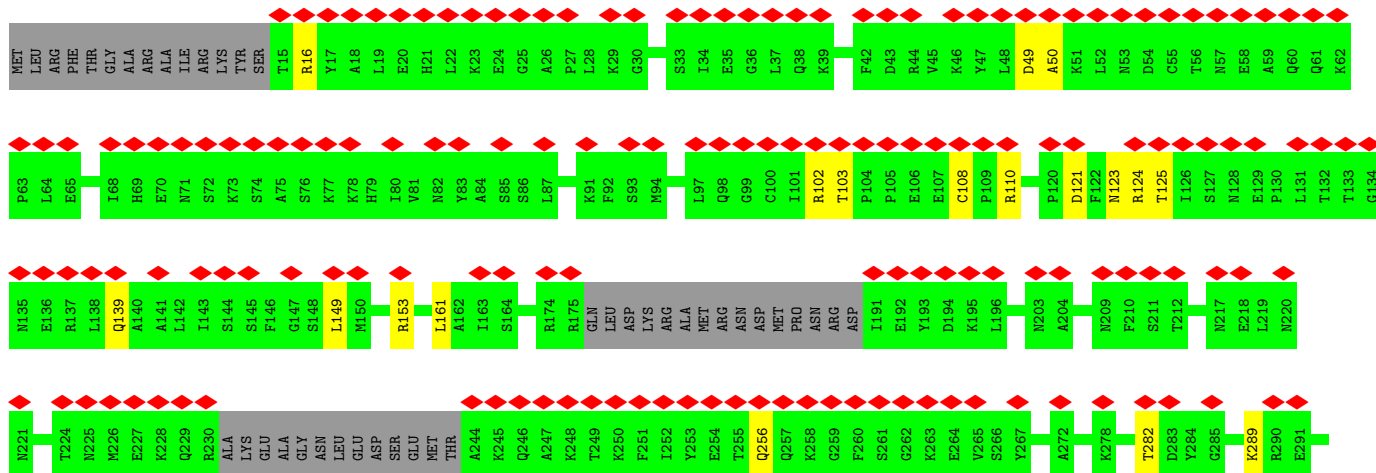
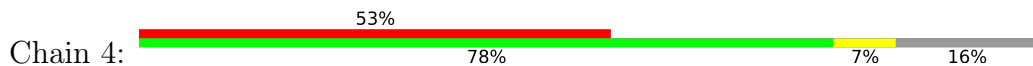


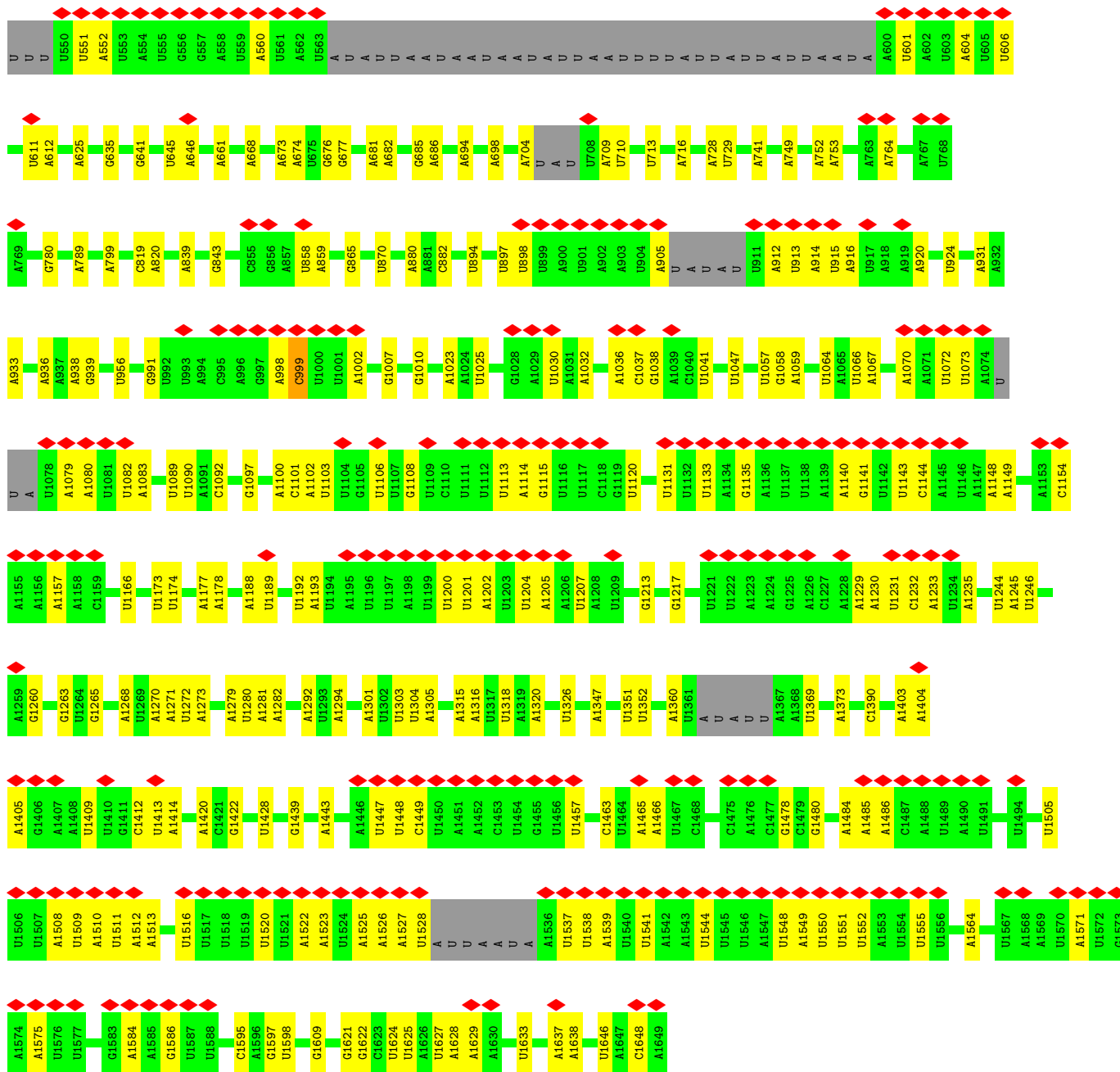


• Molecule 23: 37S ribosomal protein NAM9, mitochondrial

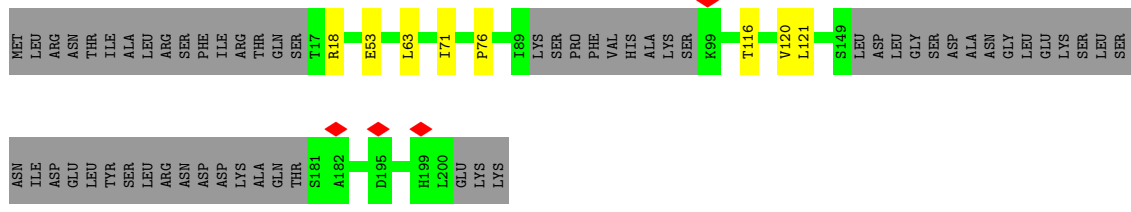


• Molecule 24: 37S ribosomal protein MRP1, mitochondrial

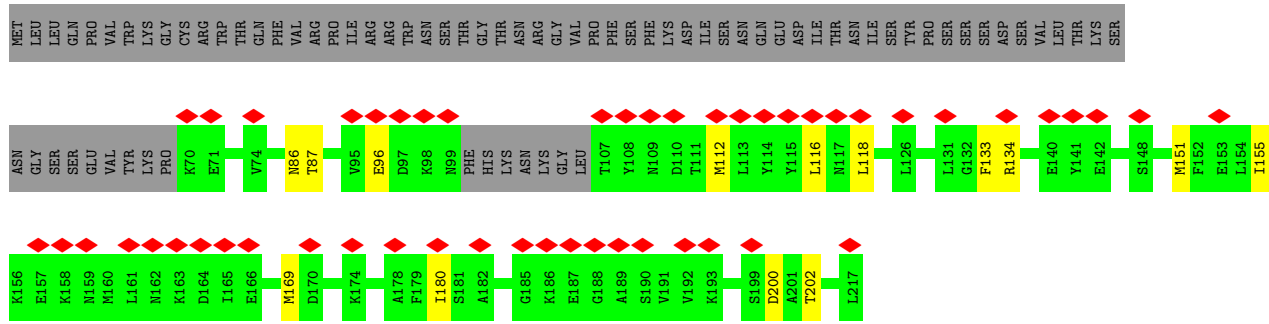




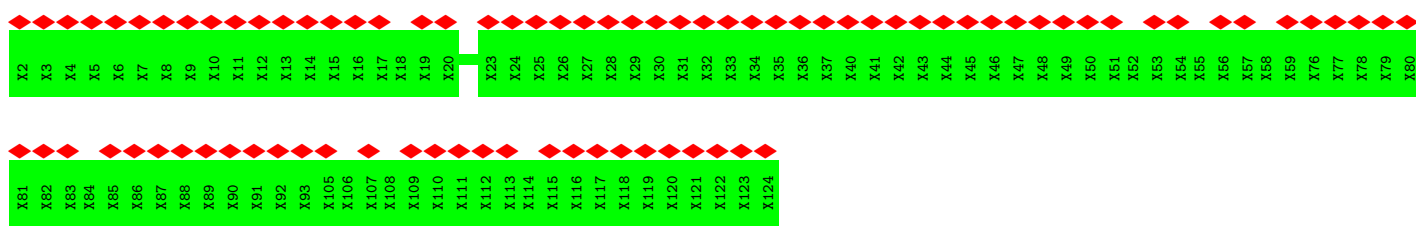
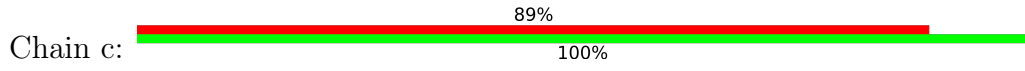
• Molecule 32: 37S ribosomal protein S10, mitochondrial



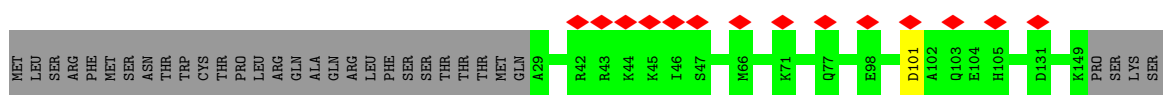
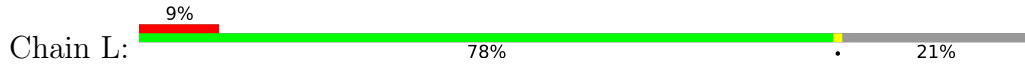
• Molecule 33: 37S ribosomal protein S18, mitochondrial



• Molecule 34: unknown protein sequence



• Molecule 35: MRPS12 isoform 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54519	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	24.070	Depositor
Minimum map value	-11.921	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.048	Depositor
Recommended contour level	4.5	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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, ATP

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	0.27	0/3544	0.55	0/4778
2	5	0.27	0/2249	0.52	0/3040
3	C	0.26	0/2040	0.46	0/2735
4	d	0.27	0/5612	0.51	0/7552
5	M	0.25	0/655	0.49	0/874
6	N	0.26	0/948	0.56	0/1267
7	O	0.25	0/1746	0.54	0/2335
8	P	0.26	0/934	0.60	0/1260
9	Q	0.27	0/1701	0.58	0/2262
10	R	0.25	0/749	0.58	0/998
11	S	0.26	0/610	0.55	0/824
12	T	0.26	0/771	0.56	0/1019
13	U	0.26	0/1950	0.51	0/2636
14	V	0.28	0/1900	0.53	0/2540
15	W	0.26	0/3239	0.49	1/4379 (0.0%)
16	X	0.27	0/788	0.53	0/1052
17	Y	0.27	0/2263	0.55	0/3053
18	Z	0.26	0/674	0.49	0/908
19	A	0.26	0/1621	0.55	0/2186
20	B	0.24	0/2128	0.51	0/2892
21	2	0.26	0/852	0.48	0/1142
22	3	0.26	0/2002	0.48	0/2721
23	D	0.26	0/2642	0.51	0/3561
24	4	0.40	2/2228 (0.1%)	0.63	3/3009 (0.1%)
25	E	0.25	0/2375	0.52	0/3201
26	F	0.26	0/1067	0.55	0/1430
27	6	0.26	0/2121	0.52	0/2856
28	G	0.25	0/1206	0.51	0/1630
29	H	0.25	0/1240	0.52	0/1670
30	I	0.25	0/1698	0.54	0/2287
31	a	0.22	0/36577	0.79	2/56897 (0.0%)
32	J	0.26	0/1216	0.52	0/1646

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	K	0.26	0/1128	0.56	0/1504
35	L	0.24	0/940	0.61	0/1261
All	All	0.25	2/93414 (0.0%)	0.66	6/133405 (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
1	0	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	310	PRO	CG-CD	-12.78	1.08	1.50
24	4	310	PRO	N-CD	5.91	1.56	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	310	PRO	N-CD-CG	-13.95	82.27	103.20
24	4	310	PRO	CA-N-CD	-9.38	98.37	111.50
24	4	310	PRO	CA-CB-CG	-7.73	89.32	104.00
31	a	999	C	C6-N1-C2	-6.31	117.78	120.30
15	W	237	PRO	CA-N-CD	-6.10	102.95	111.50
31	a	819	C	C2-N1-C1'	5.50	124.85	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	310	GLU	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	3471	0	3510	40	0
2	5	2199	0	2246	19	0
3	C	2014	0	2038	23	0
4	d	5497	0	5513	0	0
5	M	645	0	691	3	0
6	N	931	0	985	1	0
7	O	1724	0	1761	6	0
8	P	919	0	982	0	0
9	Q	1690	0	1776	23	0
10	R	738	0	771	4	0
11	S	595	0	618	2	0
12	T	760	0	791	4	0
13	U	1907	0	1898	16	0
14	V	1872	0	1978	14	0
15	W	3174	0	3270	38	0
16	X	774	0	823	14	0
17	Y	2208	0	2177	30	0
18	Z	660	0	684	3	0
19	A	1585	0	1618	11	0
20	B	2085	0	2094	13	0
21	2	833	0	839	4	0
22	3	1953	0	1913	18	0
23	D	2567	0	2630	12	0
24	4	2182	0	2172	11	0
25	E	2321	0	2327	15	0
26	F	1054	0	1129	8	0
27	6	2071	0	2099	6	0
28	G	1185	0	1234	10	0
29	H	1221	0	1289	10	0
30	I	1667	0	1719	11	0
31	a	32666	0	16387	0	0
32	J	1186	0	1193	7	0
33	K	1113	0	1161	9	0
34	c	470	0	103	0	0
35	L	926	0	980	1	0
36	0	8	0	0	0	0
37	B	1	0	0	0	0
37	Q	1	0	0	0	0
37	W	1	0	0	0	0
37	a	69	0	0	0	0
38	W	31	0	12	1	0
39	W	3	0	0	1	0
All	All	88977	0	73411	330	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 (330) 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)
1:0:149:GLU:OE2	1:0:153:ARG:NH1	2.02	0.91
1:0:300:LEU:O	1:0:458:ARG:NH1	2.09	0.85
24:4:125:THR:O	24:4:153:ARG:NH2	2.10	0.85
13:U:145:ASP:O	13:U:148:SER:OG	1.98	0.81
15:W:350:ARG:NH1	15:W:352:ASN:OD1	2.17	0.77
18:Z:59:LYS:NZ	28:G:158:ASP:OD1	2.18	0.77
15:W:393:LYS:NZ	15:W:434:GLY:O	2.14	0.75
20:B:139:LYS:O	22:3:161:LYS:NZ	2.20	0.75
2:5:196:ASN:ND2	2:5:201:TYR:O	2.19	0.75
22:3:21:LEU:O	22:3:31:SER:OG	2.04	0.75
2:5:98:SER:O	2:5:136:TYR:OH	2.03	0.74
24:4:103:THR:OG1	24:4:108:CYS:SG	2.44	0.73
17:Y:135:ASP:OD2	25:E:104:ASN:ND2	2.20	0.73
17:Y:86:GLU:OE2	17:Y:108:TYR:OH	2.07	0.72
15:W:182:LEU:O	15:W:188:ASN:ND2	2.21	0.72
29:H:125:GLU:OE1	29:H:153:ARG:NH2	2.23	0.72
33:K:151:MET:O	33:K:155:ILE:HD12	1.89	0.72
2:5:182:GLU:O	2:5:186:ASN:ND2	2.24	0.71
1:0:324:ARG:NH2	1:0:377:ARG:O	2.23	0.71
3:C:91:ASN:ND2	17:Y:143:GLU:OE1	2.23	0.70
15:W:414:ASP:O	15:W:418:THR:HG22	1.91	0.70
9:Q:127:ASP:O	9:Q:131:ILE:HD12	1.93	0.69
20:B:315:VAL:HG11	30:I:39:PRO:HD3	1.73	0.69
9:Q:59:ARG:NH1	14:V:48:GLY:O	2.26	0.68
7:O:106:GLU:OE1	14:V:203:TYR:OH	2.12	0.68
29:H:13:LEU:HD23	29:H:86:LEU:HD21	1.76	0.68
25:E:200:ASP:OD1	25:E:204:ASN:ND2	2.27	0.68
3:C:263:ASN:O	3:C:267:ILE:HD12	1.93	0.68
15:W:196:LEU:HD11	15:W:273:LYS:HG2	1.78	0.66
29:H:67:ASN:HD22	29:H:71:ARG:HH11	1.42	0.65
19:A:214:LEU:HD12	19:A:221:VAL:HG13	1.79	0.65
38:W:501:ATP:O1A	39:W:601:HOH:O	2.14	0.65
1:0:320:ILE:HG23	1:0:454:LEU:HG	1.77	0.65
15:W:224:ILE:O	15:W:254:THR:OG1	2.12	0.64
11:S:9:SER:N	11:S:15:GLY:O	2.30	0.63
3:C:100:TYR:N	17:Y:192:GLU:OE1	2.32	0.63
16:X:18:ILE:O	17:Y:257:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:X:14:LEU:HD21	17:Y:261:GLU:OE2	1.98	0.63
19:A:51:LYS:NZ	20:B:364:ASP:OD1	2.32	0.63
16:X:7:ARG:NH2	17:Y:269:ASP:O	2.33	0.62
13:U:152:ARG:NH1	13:U:175:GLU:OE1	2.33	0.62
20:B:294:GLU:OE1	20:B:304:ARG:NE	2.33	0.61
22:3:95:ASN:ND2	22:3:223:CYS:O	2.34	0.61
13:U:144:LEU:O	13:U:180:ARG:NH2	2.32	0.61
17:Y:54:PRO:HA	17:Y:57:TRP:CZ3	2.36	0.61
22:3:70:THR:HG22	22:3:76:GLN:NE2	2.17	0.60
3:C:194:ILE:HG21	16:X:54:LEU:HD12	1.84	0.60
17:Y:209:LEU:HD22	17:Y:259:LEU:HD21	1.82	0.60
9:Q:187:GLN:NE2	13:U:67:PRO:O	2.35	0.59
3:C:82:ASN:O	3:C:86:HIS:ND1	2.35	0.59
15:W:197:LYS:C	15:W:198:LEU:HD12	2.23	0.58
16:X:7:ARG:NH2	17:Y:269:ASP:OD1	2.35	0.58
2:5:156:TYR:OH	2:5:188:ASN:OD1	2.20	0.58
3:C:303:ASN:OD1	3:C:304:ASN:N	2.37	0.58
2:5:278:TYR:OH	2:5:282:ARG:NH1	2.37	0.57
9:Q:45:VAL:HG21	9:Q:60:ILE:HG21	1.85	0.57
17:Y:212:GLU:OE2	17:Y:212:GLU:N	2.36	0.57
1:0:161:PRO:O	1:0:186:TYR:OH	2.16	0.57
1:0:128:VAL:HG13	1:0:201:MET:CE	2.35	0.57
15:W:111:LYS:NZ	15:W:292:ASP:OD2	2.35	0.57
19:A:18:ASN:ND2	19:A:32:THR:O	2.38	0.57
15:W:127:ARG:NH2	15:W:392:PRO:O	2.37	0.57
15:W:193:ASP:OD2	15:W:270:LYS:NZ	2.37	0.57
11:S:23:ILE:HA	11:S:33:ILE:HD11	1.87	0.56
15:W:147:ILE:HD11	15:W:345:ILE:HD11	1.86	0.56
15:W:243:LYS:NZ	15:W:245:PHE:O	2.33	0.56
23:D:53:ARG:NH1	23:D:57:GLY:O	2.39	0.56
25:E:21:LEU:HD13	25:E:33:ILE:HG21	1.87	0.56
33:K:112:MET:O	33:K:116:LEU:HD12	2.05	0.56
2:5:193:LEU:HD23	2:5:235:LEU:HD13	1.87	0.56
9:Q:59:ARG:NH2	14:V:44:VAL:HA	2.21	0.56
19:A:231:ILE:HD13	19:A:245:ALA:HB2	1.88	0.56
16:X:22:ASN:O	16:X:22:ASN:ND2	2.38	0.56
1:0:274:LEU:HD21	1:0:296:TYR:CD2	2.40	0.56
2:5:150:PHE:CD2	2:5:191:CYS:HB3	2.41	0.56
3:C:184:ASN:ND2	3:C:205:ILE:O	2.35	0.56
1:0:316:GLY:O	1:0:320:ILE:HD12	2.05	0.55
13:U:138:LEU:CD1	13:U:179:LEU:HD13	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:189:ILE:HG21	2:5:231:LEU:HB3	1.88	0.55
3:C:86:HIS:NE2	32:J:53:GLU:OE2	2.34	0.55
13:U:146:GLY:O	13:U:150:ILE:HD12	2.06	0.55
20:B:321:VAL:HG12	20:B:343:ILE:HB	1.89	0.55
20:B:299:ASP:OD1	20:B:387:ARG:NH2	2.40	0.54
1:0:297:LEU:HD21	1:0:365:TYR:CZ	2.43	0.54
22:3:131:ASP:OD1	22:3:134:VAL:HG23	2.08	0.54
15:W:440:GLU:OE2	30:I:193:ARG:NH2	2.40	0.54
2:5:116:LEU:HD22	2:5:159:MET:SD	2.48	0.54
12:T:90:ARG:O	12:T:93:VAL:HG22	2.08	0.54
22:3:95:ASN:OD1	22:3:96:ILE:HG23	2.07	0.53
33:K:169:MET:SD	33:K:180:ILE:HD11	2.48	0.53
27:6:52:THR:O	27:6:56:THR:HG23	2.09	0.53
15:W:69:LEU:O	28:G:146:ARG:NH2	2.40	0.53
15:W:86:ILE:O	15:W:90:LEU:N	2.42	0.53
17:Y:61:PRO:O	17:Y:65:ILE:HD12	2.08	0.53
1:0:320:ILE:HG23	1:0:454:LEU:CG	2.39	0.53
3:C:177:ASN:O	3:C:181:ASN:ND2	2.42	0.53
12:T:177:TYR:O	18:Z:84:ARG:NH2	2.41	0.52
30:I:200:LEU:HD23	30:I:235:LEU:HD11	1.91	0.52
30:I:54:ARG:NH1	30:I:92:ILE:O	2.42	0.52
1:0:104:VAL:HG23	1:0:130:ALA:HB2	1.92	0.52
17:Y:93:THR:HG22	17:Y:93:THR:O	2.10	0.52
15:W:237:PRO:HD2	15:W:238:LYS:H	1.75	0.52
22:3:26:PRO:O	22:3:28:ILE:HD12	2.10	0.52
6:N:88:LEU:O	6:N:92:ARG:N	2.42	0.52
21:2:113:GLY:O	21:2:117:ARG:N	2.43	0.52
22:3:49:LEU:HD22	22:3:86:ILE:HD12	1.91	0.52
7:O:101:PHE:CE2	7:O:105:ILE:HD11	2.45	0.51
1:0:128:VAL:HG13	1:0:201:MET:HE1	1.92	0.51
9:Q:76:GLU:HB3	14:V:50:ALA:HB2	1.92	0.51
9:Q:176:LEU:HD21	14:V:186:LEU:HA	1.92	0.51
19:A:222:ILE:HG23	24:4:256:GLN:HE21	1.75	0.51
17:Y:87:LEU:O	17:Y:91:LEU:HD23	2.10	0.51
17:Y:91:LEU:HA	17:Y:104:ILE:HD11	1.92	0.51
1:0:150:LEU:HB2	1:0:455:ILE:HD13	1.92	0.51
33:K:96:GLU:OE1	33:K:118:LEU:HD22	2.11	0.50
2:5:49:ASP:O	2:5:53:ILE:HD12	2.11	0.50
13:U:206:ILE:HD13	19:A:89:ARG:HG2	1.91	0.50
1:0:143:ILE:HG21	1:0:174:GLY:HA2	1.93	0.50
3:C:122:MET:SD	16:X:59:LEU:HD21	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:55:GLU:N	17:Y:55:GLU:OE2	2.45	0.50
17:Y:50:LEU:HD21	17:Y:60:LEU:HD21	1.92	0.50
12:T:89:ALA:HB1	33:K:112:MET:CE	2.41	0.50
18:Z:41:TRP:HB2	28:G:238:ILE:HD11	1.93	0.50
33:K:133:PHE:O	33:K:134:ARG:NH1	2.44	0.50
28:G:228:GLU:OE2	28:G:228:GLU:N	2.45	0.50
1:0:112:ILE:O	1:0:117:SER:OG	2.30	0.49
25:E:112:LEU:HD23	25:E:115:ASP:HB2	1.94	0.49
15:W:164:HIS:NE2	15:W:290:THR:HG21	2.27	0.49
3:C:118:LEU:HD21	16:X:54:LEU:HD22	1.95	0.49
5:M:2:VAL:HG22	5:M:2:VAL:O	2.13	0.49
9:Q:169:ILE:HD13	14:V:192:HIS:HD2	1.77	0.49
15:W:196:LEU:O	15:W:198:LEU:N	2.46	0.49
17:Y:164:LEU:HD22	25:E:31:LYS:HE3	1.95	0.49
2:5:236:GLY:O	2:5:240:GLY:N	2.44	0.49
9:Q:184:ASP:OD1	13:U:75:TYR:OH	2.30	0.49
20:B:273:THR:HG21	30:I:52:GLU:OE2	2.13	0.49
29:H:67:ASN:ND2	29:H:71:ARG:HH11	2.10	0.49
1:0:274:LEU:HD13	1:0:306:ILE:HD11	1.94	0.48
13:U:47:ARG:NH2	20:B:207:GLN:O	2.41	0.48
15:W:185:ASN:OD1	15:W:186:GLY:N	2.46	0.48
22:3:149:GLY:O	22:3:240:ARG:NH1	2.46	0.48
29:H:1:MET:HA	29:H:31:LEU:HD22	1.95	0.48
13:U:166:VAL:HG22	19:A:196:PHE:CE1	2.48	0.48
7:O:85:GLU:OE2	9:Q:114:ARG:NH2	2.47	0.48
14:V:72:ASP:OD2	14:V:112:ARG:NH2	2.47	0.48
32:J:71:ILE:HG23	32:J:116:THR:HG21	1.94	0.48
3:C:186:ASN:O	3:C:190:ASN:ND2	2.43	0.48
9:Q:76:GLU:HA	14:V:53:VAL:HG21	1.96	0.48
9:Q:193:LEU:HD13	9:Q:224:LEU:HD11	1.95	0.48
15:W:194:ASP:OD1	15:W:195:ASP:N	2.47	0.48
15:W:301:ALA:O	15:W:315:SER:OG	2.28	0.48
25:E:63:THR:HG23	25:E:64:LYS:HG2	1.94	0.48
28:G:142:TYR:O	28:G:146:ARG:N	2.38	0.48
2:5:193:LEU:HD22	2:5:287:ILE:HD11	1.95	0.47
15:W:279:LEU:HD23	15:W:287:ILE:HD12	1.96	0.47
20:B:160:LEU:HD22	22:3:94:GLU:OE2	2.14	0.47
26:F:24:LEU:HD11	26:F:91:VAL:HG22	1.95	0.47
10:R:42:ASP:OD2	10:R:43:GLN:N	2.48	0.47
17:Y:65:ILE:HD12	17:Y:65:ILE:H	1.80	0.47
26:F:15:ASN:OD1	26:F:16:ALA:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:341:PRO:O	1:0:473:ARG:NH1	2.43	0.47
9:Q:131:ILE:HD11	9:Q:147:ILE:HG21	1.97	0.47
17:Y:198:ARG:O	17:Y:247:ASN:ND2	2.47	0.47
27:6:337:ASN:OD1	27:6:338:LYS:N	2.45	0.47
7:O:100:LYS:NZ	9:Q:166:GLN:O	2.39	0.47
16:X:56:PHE:HA	16:X:59:LEU:HD12	1.96	0.47
3:C:258:MET:O	3:C:262:ASN:ND2	2.44	0.47
3:C:128:ASN:OD1	17:Y:113:GLN:NE2	2.48	0.47
3:C:275:MET:SD	3:C:305:ILE:HG23	2.55	0.47
21:2:31:ILE:HG22	21:2:32:PRO:O	2.15	0.47
19:A:227:VAL:HG22	19:A:280:ILE:HD11	1.96	0.46
25:E:286:LEU:HD21	29:H:123:PRO:HB2	1.98	0.46
29:H:99:ILE:HG21	29:H:118:ILE:HD11	1.97	0.46
32:J:116:THR:HG23	32:J:121:LEU:CD2	2.45	0.46
19:A:214:LEU:HD12	19:A:221:VAL:CG1	2.43	0.46
1:0:200:GLU:OE1	1:0:204:ARG:NH1	2.49	0.46
22:3:34:PHE:HA	22:3:37:VAL:HG12	1.97	0.46
13:U:220:TRP:O	13:U:224:VAL:HG23	2.15	0.46
9:Q:200:CYS:SG	9:Q:224:LEU:HD13	2.56	0.46
15:W:414:ASP:N	28:G:148:ASP:OD1	2.40	0.46
22:3:28:ILE:HD11	22:3:250:ASN:HB2	1.98	0.46
17:Y:231:THR:OG1	17:Y:233:ILE:HG22	2.16	0.46
21:2:62:ASN:OD1	21:2:64:ASN:N	2.49	0.46
22:3:190:SER:N	22:3:193:GLU:OE1	2.42	0.46
17:Y:206:THR:OG1	17:Y:232:ASP:OD1	2.34	0.46
23:D:133:ASN:N	23:D:149:MET:O	2.41	0.46
30:I:87:ASP:O	30:I:91:LEU:HD23	2.17	0.46
1:0:167:VAL:HG12	1:0:277:GLN:OE1	2.16	0.45
16:X:58:HIS:O	16:X:61:THR:OG1	2.31	0.45
20:B:257:ARG:NH2	20:B:261:GLU:OE2	2.49	0.45
9:Q:126:ARG:O	9:Q:130:THR:HG23	2.15	0.45
1:0:128:VAL:HG13	1:0:201:MET:HE2	1.99	0.45
15:W:143:VAL:HG13	15:W:143:VAL:O	2.16	0.45
15:W:398:GLU:OE2	15:W:398:GLU:N	2.50	0.45
17:Y:291:ASP:OD1	17:Y:292:TYR:N	2.49	0.45
19:A:227:VAL:CG2	19:A:280:ILE:HD11	2.47	0.45
16:X:50:ASN:HD22	16:X:50:ASN:C	2.08	0.45
24:4:49:ASP:OD1	24:4:50:ALA:N	2.50	0.45
35:L:101:ASP:OD2	35:L:101:ASP:N	2.49	0.45
10:R:91:GLU:O	26:F:110:SER:OG	2.35	0.45
15:W:141:HIS:O	15:W:144:LYS:NZ	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:F:2:LEU:HD11	26:F:70:LEU:HG	1.97	0.45
28:G:113:THR:HG21	28:G:154:GLU:OE2	2.17	0.45
29:H:13:LEU:HD23	29:H:86:LEU:CD2	2.43	0.45
15:W:77:ALA:C	15:W:78:LEU:HD12	2.38	0.44
26:F:24:LEU:CD1	26:F:91:VAL:HG22	2.46	0.44
29:H:19:VAL:HG23	29:H:21:VAL:HG13	1.98	0.44
30:I:89:TYR:CZ	30:I:106:LEU:HD22	2.52	0.44
22:3:243:TYR:O	22:3:247:VAL:HG23	2.17	0.44
2:5:166:ILE:HG22	2:5:166:ILE:O	2.17	0.44
26:F:4:GLU:OE2	26:F:68:LEU:HD11	2.18	0.44
1:0:209:LEU:HD23	1:0:257:THR:HG21	1.99	0.44
1:0:506:GLY:HA2	1:0:526:ARG:HE	1.82	0.44
1:0:387:ASN:O	1:0:390:THR:OG1	2.32	0.44
23:D:149:MET:HE3	27:6:188:LEU:HD23	1.99	0.44
1:0:449:LEU:HD23	1:0:449:LEU:H	1.82	0.44
27:6:149:LEU:HD22	27:6:153:LEU:CD2	2.48	0.44
1:0:147:LEU:HD11	1:0:159:PHE:CZ	2.53	0.43
3:C:144:HIS:CE1	3:C:149:LEU:HD13	2.53	0.43
15:W:236:ASN:O	15:W:240:ALA:HB2	2.17	0.43
23:D:94:LEU:HD13	23:D:475:GLU:HG2	2.00	0.43
29:H:96:ASN:OD1	29:H:97:SER:N	2.51	0.43
32:J:63:LEU:HD11	32:J:76:PRO:HD3	2.00	0.43
1:0:96:HIS:NE2	1:0:129:ASP:OD2	2.51	0.43
1:0:279:LEU:HD21	1:0:281:ASP:O	2.17	0.43
2:5:73:ILE:HD12	2:5:73:ILE:H	1.83	0.43
3:C:99:ASN:O	3:C:102:LYS:NZ	2.47	0.43
1:0:195:ILE:HG21	1:0:201:MET:HG3	2.00	0.43
14:V:79:VAL:HG23	14:V:79:VAL:O	2.19	0.43
2:5:234:THR:HG21	2:5:284:LEU:HG	2.00	0.43
10:R:49:LEU:HD11	10:R:60:PHE:CZ	2.52	0.43
10:R:81:ASP:N	10:R:102:TYR:HH	2.16	0.43
13:U:138:LEU:HD11	13:U:179:LEU:HD13	2.01	0.43
17:Y:107:LEU:CD2	17:Y:115:ALA:HB2	2.49	0.43
14:V:210:ILE:HD11	14:V:219:LYS:HD3	1.99	0.43
17:Y:158:ALA:HA	17:Y:162:LEU:HD12	2.00	0.43
23:D:476:ARG:NH2	25:E:251:GLU:OE1	2.51	0.43
24:4:110:ARG:NH2	24:4:282:THR:O	2.51	0.43
1:0:196:LEU:HD11	1:0:277:GLN:OE1	2.18	0.43
26:F:124:VAL:HG22	26:F:124:VAL:O	2.18	0.43
1:0:408:ARG:NH1	1:0:444:ARG:O	2.52	0.43
24:4:121:ASP:OD2	24:4:124:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:K:151:MET:SD	33:K:155:ILE:HD11	2.59	0.42
20:B:324:ASN:OD1	20:B:324:ASN:N	2.53	0.42
28:G:184:ASN:OD1	28:G:187:GLN:NE2	2.48	0.42
15:W:442:LEU:O	15:W:446:VAL:HG22	2.19	0.42
16:X:70:ASP:O	16:X:70:ASP:OD2	2.38	0.42
25:E:135:VAL:HG11	25:E:140:ILE:HD11	2.01	0.42
21:2:57:ASP:OD1	21:2:58:THR:N	2.52	0.42
25:E:24:TYR:O	32:J:18:ARG:NH2	2.53	0.42
1:0:420:LEU:O	1:0:425:TRP:NE1	2.50	0.42
14:V:146:GLU:O	14:V:149:SER:OG	2.37	0.42
22:3:208:THR:O	22:3:208:THR:HG22	2.19	0.42
24:4:139:GLN:HG3	24:4:149:LEU:HD21	2.02	0.42
25:E:125:VAL:O	25:E:129:LEU:HD23	2.19	0.42
27:6:56:THR:HG22	27:6:59:ARG:NH2	2.35	0.42
28:G:156:SER:O	28:G:160:LEU:HD23	2.19	0.42
30:I:123:ASP:OD1	30:I:124:GLU:N	2.52	0.42
3:C:181:ASN:O	3:C:185:ASN:N	2.52	0.42
13:U:70:ASN:ND2	13:U:74:LEU:O	2.53	0.42
13:U:105:ARG:NE	13:U:147:GLU:OE1	2.40	0.42
32:J:116:THR:HG23	32:J:121:LEU:HD21	2.01	0.42
3:C:301:ASN:OD1	3:C:302:ILE:N	2.53	0.42
13:U:140:ILE:HG23	22:3:50:THR:HG21	2.02	0.42
15:W:432:LEU:HD21	30:I:197:MET:HE2	2.01	0.42
17:Y:312:VAL:HG23	17:Y:313:ASP:N	2.35	0.42
25:E:188:GLU:OE2	25:E:188:GLU:N	2.53	0.42
9:Q:59:ARG:NH1	9:Q:76:GLU:OE1	2.52	0.42
15:W:198:LEU:HD21	15:W:322:LYS:HD2	2.00	0.42
20:B:149:ARG:NH1	22:3:217:TRP:O	2.49	0.42
22:3:156:VAL:HG12	22:3:220:PRO:HA	2.01	0.42
28:G:113:THR:HG23	28:G:114:LEU:N	2.35	0.42
1:0:278:LEU:CD1	1:0:308:ILE:HG23	2.49	0.42
24:4:102:ARG:HE	24:4:295:ARG:HG2	1.85	0.42
25:E:43:ASP:OD1	25:E:43:ASP:N	2.52	0.42
3:C:313:ASN:OD1	3:C:314:ILE:N	2.53	0.42
23:D:106:ASP:OD1	23:D:107:PHE:N	2.53	0.42
23:D:397:LYS:O	23:D:401:LEU:HD23	2.20	0.42
9:Q:63:THR:HG22	9:Q:64:ARG:N	2.35	0.41
24:4:311:GLN:HG3	24:4:312:ARG:N	2.35	0.41
1:0:159:PHE:HE2	1:0:182:LEU:HD11	1.86	0.41
1:0:490:THR:OG1	1:0:492:ASN:OD1	2.37	0.41
5:M:39:LEU:HD11	5:M:57:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:161:LEU:HD13	27:6:212:LEU:HD11	2.02	0.41
9:Q:169:ILE:HD11	14:V:189:PHE:CE1	2.54	0.41
1:0:171:PRO:O	1:0:173:THR:N	2.53	0.41
2:5:224:ASN:OD1	2:5:225:THR:N	2.53	0.41
14:V:151:LEU:O	14:V:152:THR:HG22	2.21	0.41
23:D:403:ASN:OD1	23:D:403:ASN:O	2.39	0.41
23:D:416:ASP:H	23:D:423:THR:HG21	1.83	0.41
33:K:86:ASN:OD1	33:K:87:THR:N	2.50	0.41
2:5:235:LEU:O	2:5:239:ILE:HD12	2.20	0.41
9:Q:131:ILE:HD11	9:Q:147:ILE:CG2	2.50	0.41
15:W:107:LEU:O	15:W:176:ASN:ND2	2.48	0.41
17:Y:184:TYR:CE2	17:Y:202:LEU:HD12	2.55	0.41
24:4:161:LEU:HD12	24:4:289:LYS:HD3	2.01	0.41
3:C:182:ILE:HD13	16:X:66:ILE:HD13	2.02	0.41
13:U:178:ALA:HB2	24:4:123:ASN:OD1	2.21	0.41
19:A:281:LEU:N	19:A:294:HIS:O	2.54	0.41
20:B:193:VAL:HG22	20:B:368:SER:HB2	2.02	0.41
23:D:190:LYS:NZ	23:D:377:ALA:O	2.52	0.41
32:J:71:ILE:HD11	32:J:120:VAL:HG12	2.01	0.41
12:T:106:ILE:HG23	12:T:119:ARG:HH21	1.84	0.41
15:W:345:ILE:HG22	15:W:346:SER:N	2.36	0.41
15:W:446:VAL:HG23	15:W:447:LEU:HG	2.01	0.41
30:I:167:VAL:HG22	30:I:230:ALA:HB1	2.02	0.41
1:0:326:ILE:HD13	1:0:329:ARG:HH22	1.85	0.41
7:O:97:GLU:OE1	9:Q:167:LEU:HD22	2.21	0.41
9:Q:169:ILE:HD11	14:V:189:PHE:CD1	2.55	0.41
15:W:84:ASP:N	15:W:84:ASP:OD1	2.51	0.41
16:X:70:ASP:OD2	16:X:73:GLU:HB3	2.21	0.41
1:0:147:LEU:HD11	1:0:159:PHE:HZ	1.85	0.41
1:0:198:ASN:OD1	1:0:199:ALA:N	2.53	0.41
1:0:297:LEU:HD23	1:0:297:LEU:O	2.21	0.41
2:5:186:ASN:HB3	2:5:280:ILE:HD13	2.02	0.41
15:W:188:ASN:O	15:W:305:TYR:OH	2.36	0.41
15:W:197:LYS:O	15:W:198:LEU:HD12	2.21	0.41
30:I:227:ILE:HG22	30:I:231:ILE:HD12	2.02	0.41
33:K:200:ASP:OD1	33:K:202:THR:OG1	2.39	0.41
3:C:129:ASN:OD1	3:C:130:MET:N	2.52	0.41
17:Y:164:LEU:HD23	25:E:35:LEU:HD12	2.03	0.41
2:5:227:LEU:O	2:5:231:LEU:HD13	2.20	0.40
17:Y:54:PRO:HA	17:Y:57:TRP:CH2	2.56	0.40
15:W:198:LEU:HD23	15:W:319:GLN:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:279:LEU:HA	1:0:288:GLN:OE1	2.21	0.40
9:Q:23:ARG:NE	9:Q:42:ASP:OD2	2.55	0.40
23:D:442:GLU:HA	23:D:442:GLU:OE1	2.22	0.40
3:C:169:ASN:ND2	25:E:93:ASP:OD2	2.54	0.40
5:M:17:LYS:HG3	5:M:18:ILE:HD12	2.03	0.40
7:O:109:LYS:HG3	26:F:131:ILE:HG21	2.03	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	421/628 (67%)	405 (96%)	16 (4%)	0	100	100
2	5	264/339 (78%)	260 (98%)	4 (2%)	0	100	100
3	C	227/398 (57%)	224 (99%)	3 (1%)	0	100	100
4	d	652/864 (76%)	639 (98%)	13 (2%)	0	100	100
5	M	81/143 (57%)	81 (100%)	0	0	100	100
6	N	111/115 (96%)	111 (100%)	0	0	100	100
7	O	206/286 (72%)	205 (100%)	1 (0%)	0	100	100
8	P	112/121 (93%)	110 (98%)	2 (2%)	0	100	100
9	Q	195/237 (82%)	195 (100%)	0	0	100	100
10	R	87/138 (63%)	85 (98%)	2 (2%)	0	100	100
11	S	73/91 (80%)	72 (99%)	1 (1%)	0	100	100
12	T	90/177 (51%)	88 (98%)	2 (2%)	0	100	100
13	U	231/264 (88%)	229 (99%)	2 (1%)	0	100	100
14	V	231/318 (73%)	228 (99%)	3 (1%)	0	100	100
15	W	393/450 (87%)	386 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	X	94/110 (86%)	94 (100%)	0	0	100	100
17	Y	259/319 (81%)	252 (97%)	7 (3%)	0	100	100
18	Z	80/95 (84%)	79 (99%)	1 (1%)	0	100	100
19	A	191/344 (56%)	189 (99%)	2 (1%)	0	100	100
20	B	264/394 (67%)	260 (98%)	4 (2%)	0	100	100
21	2	97/130 (75%)	97 (100%)	0	0	100	100
22	3	240/266 (90%)	234 (98%)	6 (2%)	0	100	100
23	D	302/486 (62%)	298 (99%)	4 (1%)	0	100	100
24	4	265/321 (83%)	256 (97%)	9 (3%)	0	100	100
25	E	287/307 (94%)	279 (97%)	8 (3%)	0	100	100
26	F	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
27	6	247/345 (72%)	243 (98%)	4 (2%)	0	100	100
28	G	144/247 (58%)	143 (99%)	1 (1%)	0	100	100
29	H	153/155 (99%)	152 (99%)	1 (1%)	0	100	100
30	I	202/278 (73%)	200 (99%)	2 (1%)	0	100	100
32	J	138/203 (68%)	133 (96%)	5 (4%)	0	100	100
33	K	137/217 (63%)	135 (98%)	2 (2%)	0	100	100
35	L	119/153 (78%)	119 (100%)	0	0	100	100
All	All	6722/9070 (74%)	6605 (98%)	117 (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	382/564 (68%)	382 (100%)	0	100	100
2	5	239/303 (79%)	239 (100%)	0	100	100
3	C	237/385 (62%)	237 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	610/803 (76%)	609 (100%)	1 (0%)	93	97
5	M	69/121 (57%)	69 (100%)	0	100	100
6	N	101/103 (98%)	101 (100%)	0	100	100
7	O	183/250 (73%)	183 (100%)	0	100	100
8	P	101/106 (95%)	101 (100%)	0	100	100
9	Q	188/218 (86%)	188 (100%)	0	100	100
10	R	80/121 (66%)	80 (100%)	0	100	100
11	S	64/78 (82%)	64 (100%)	0	100	100
12	T	81/159 (51%)	80 (99%)	1 (1%)	71	87
13	U	208/236 (88%)	206 (99%)	2 (1%)	76	89
14	V	208/287 (72%)	208 (100%)	0	100	100
15	W	363/409 (89%)	362 (100%)	1 (0%)	92	97
16	X	84/92 (91%)	81 (96%)	3 (4%)	35	66
17	Y	242/289 (84%)	242 (100%)	0	100	100
18	Z	75/85 (88%)	75 (100%)	0	100	100
19	A	174/309 (56%)	174 (100%)	0	100	100
20	B	233/350 (67%)	233 (100%)	0	100	100
21	2	90/117 (77%)	90 (100%)	0	100	100
22	3	216/240 (90%)	216 (100%)	0	100	100
23	D	277/437 (63%)	277 (100%)	0	100	100
24	4	239/281 (85%)	238 (100%)	1 (0%)	91	96
25	E	250/266 (94%)	250 (100%)	0	100	100
26	F	120/120 (100%)	120 (100%)	0	100	100
27	6	230/312 (74%)	230 (100%)	0	100	100
28	G	128/211 (61%)	127 (99%)	1 (1%)	81	92
29	H	142/142 (100%)	142 (100%)	0	100	100
30	I	180/245 (74%)	179 (99%)	1 (1%)	86	94
32	J	130/183 (71%)	130 (100%)	0	100	100
33	K	121/192 (63%)	121 (100%)	0	100	100
35	L	100/131 (76%)	100 (100%)	0	100	100
All	All	6145/8145 (75%)	6134 (100%)	11 (0%)	93	97

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	268	ARG
12	T	99	ARG
13	U	90	ARG
13	U	103	ARG
15	W	273	LYS
16	X	22	ASN
16	X	50	ASN
16	X	92	LYS
24	4	16	ARG
28	G	167	LYS
30	I	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	5	168	HIS
2	5	196	ASN
3	C	128	ASN
7	O	54	GLN
14	V	120	HIS
14	V	192	HIS
14	V	204	HIS
15	W	188	ASN
17	Y	113	GLN
17	Y	148	HIS
19	A	33	HIS
21	2	92	HIS
24	4	21	HIS
25	E	198	HIS
29	H	67	ASN
30	I	114	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1524/1713 (88%)	365 (23%)	0

All (365) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	a	-7	A
31	a	-5	G
31	a	-4	G
31	a	-3	A
31	a	-2	A
31	a	-1	A
31	a	11	U
31	a	14	A
31	a	16	G
31	a	20	A
31	a	29	G
31	a	39	A
31	a	46	A
31	a	54	C
31	a	55	A
31	a	58	A
31	a	73	A
31	a	76	U
31	a	78	U
31	a	84	U
31	a	85	G
31	a	90	G
31	a	97	A
31	a	98	A
31	a	101	U
31	a	102	G
31	a	108	U
31	a	109	A
31	a	120	A
31	a	121	U
31	a	122	U
31	a	128	A
31	a	129	G
31	a	132	A
31	a	136	A
31	a	139	A
31	a	141	C
31	a	145	A
31	a	146	G
31	a	151	A
31	a	154	U
31	a	155	A
31	a	156	A

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Mol	Chain	Res	Type
31	a	159	A
31	a	161	U
31	a	175	U
31	a	178	A
31	a	180	A
31	a	184	A
31	a	185	A
31	a	191	A
31	a	192	U
31	a	194	A
31	a	195	U
31	a	196	A
31	a	197	A
31	a	202	G
31	a	204	U
31	a	205	A
31	a	208	U
31	a	209	A
31	a	210	U
31	a	216	A
31	a	218	A
31	a	222	U
31	a	224	A
31	a	234	A
31	a	235	A
31	a	250	A
31	a	251	G
31	a	254	A
31	a	255	G
31	a	261	U
31	a	263	A
31	a	270	G
31	a	271	U
31	a	286	G
31	a	294	A
31	a	331	A
31	a	334	U
31	a	336	U
31	a	346	C
31	a	347	U
31	a	348	A
31	a	350	A

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Mol	Chain	Res	Type
31	a	351	A
31	a	352	G
31	a	356	C
31	a	360	A
31	a	370	A
31	a	371	U
31	a	372	U
31	a	373	G
31	a	376	C
31	a	401	A
31	a	405	A
31	a	409	G
31	a	414	A
31	a	416	A
31	a	417	U
31	a	480	U
31	a	481	A
31	a	485	A
31	a	486	U
31	a	488	A
31	a	495	U
31	a	496	A
31	a	498	A
31	a	501	U
31	a	503	A
31	a	514	U
31	a	516	A
31	a	517	U
31	a	527	G
31	a	528	A
31	a	537	A
31	a	538	C
31	a	540	A
31	a	542	A
31	a	551	U
31	a	552	A
31	a	560	A
31	a	601	U
31	a	604	A
31	a	606	U
31	a	611	U
31	a	612	A

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Mol	Chain	Res	Type
31	a	625	A
31	a	635	G
31	a	641	G
31	a	645	U
31	a	646	A
31	a	661	A
31	a	668	A
31	a	673	A
31	a	674	A
31	a	676	G
31	a	677	G
31	a	681	A
31	a	682	A
31	a	685	G
31	a	686	A
31	a	694	A
31	a	698	A
31	a	704	A
31	a	709	A
31	a	710	U
31	a	713	U
31	a	716	A
31	a	728	A
31	a	729	U
31	a	741	A
31	a	749	A
31	a	752	A
31	a	753	A
31	a	764	A
31	a	780	G
31	a	789	A
31	a	799	A
31	a	820	A
31	a	839	A
31	a	843	G
31	a	858	U
31	a	859	A
31	a	865	G
31	a	870	U
31	a	880	A
31	a	882	C
31	a	894	U

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Mol	Chain	Res	Type
31	a	897	U
31	a	898	U
31	a	905	A
31	a	912	A
31	a	913	U
31	a	914	A
31	a	915	U
31	a	916	A
31	a	920	A
31	a	924	U
31	a	931	A
31	a	933	A
31	a	936	A
31	a	938	A
31	a	939	G
31	a	956	U
31	a	991	G
31	a	998	A
31	a	999	C
31	a	1002	A
31	a	1007	G
31	a	1010	G
31	a	1023	A
31	a	1025	U
31	a	1030	U
31	a	1032	A
31	a	1036	A
31	a	1037	C
31	a	1038	G
31	a	1041	U
31	a	1047	U
31	a	1057	U
31	a	1058	G
31	a	1059	A
31	a	1064	U
31	a	1066	U
31	a	1067	A
31	a	1070	A
31	a	1072	U
31	a	1073	U
31	a	1079	A
31	a	1080	A

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Mol	Chain	Res	Type
31	a	1082	U
31	a	1083	A
31	a	1089	U
31	a	1090	U
31	a	1092	C
31	a	1097	G
31	a	1100	A
31	a	1101	C
31	a	1102	A
31	a	1103	U
31	a	1106	U
31	a	1108	G
31	a	1113	U
31	a	1114	A
31	a	1115	G
31	a	1120	U
31	a	1131	U
31	a	1133	U
31	a	1135	G
31	a	1140	A
31	a	1141	G
31	a	1143	U
31	a	1144	C
31	a	1148	A
31	a	1149	A
31	a	1154	C
31	a	1157	A
31	a	1166	U
31	a	1173	U
31	a	1174	U
31	a	1177	A
31	a	1178	A
31	a	1188	A
31	a	1189	U
31	a	1192	U
31	a	1193	A
31	a	1200	U
31	a	1201	U
31	a	1202	A
31	a	1204	U
31	a	1205	A
31	a	1207	U

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Mol	Chain	Res	Type
31	a	1213	G
31	a	1217	G
31	a	1229	A
31	a	1230	A
31	a	1231	U
31	a	1232	C
31	a	1233	A
31	a	1235	A
31	a	1244	U
31	a	1245	A
31	a	1246	U
31	a	1260	G
31	a	1263	G
31	a	1265	G
31	a	1268	A
31	a	1270	A
31	a	1271	A
31	a	1272	U
31	a	1273	A
31	a	1279	A
31	a	1280	U
31	a	1281	A
31	a	1282	A
31	a	1292	A
31	a	1294	A
31	a	1301	A
31	a	1303	U
31	a	1304	U
31	a	1305	A
31	a	1315	A
31	a	1316	A
31	a	1318	U
31	a	1320	A
31	a	1326	U
31	a	1347	A
31	a	1351	U
31	a	1352	U
31	a	1360	A
31	a	1369	U
31	a	1373	A
31	a	1390	C
31	a	1403	A

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Mol	Chain	Res	Type
31	a	1404	A
31	a	1405	A
31	a	1409	U
31	a	1412	C
31	a	1413	U
31	a	1414	A
31	a	1420	A
31	a	1422	G
31	a	1428	U
31	a	1439	G
31	a	1443	A
31	a	1447	U
31	a	1448	U
31	a	1449	C
31	a	1457	U
31	a	1463	C
31	a	1465	A
31	a	1466	A
31	a	1478	G
31	a	1480	G
31	a	1484	A
31	a	1485	A
31	a	1486	A
31	a	1505	U
31	a	1508	A
31	a	1509	U
31	a	1510	A
31	a	1511	U
31	a	1512	A
31	a	1513	A
31	a	1516	U
31	a	1520	U
31	a	1522	A
31	a	1523	A
31	a	1525	A
31	a	1526	A
31	a	1527	A
31	a	1528	U
31	a	1537	U
31	a	1538	U
31	a	1539	A
31	a	1541	U

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Mol	Chain	Res	Type
31	a	1544	U
31	a	1548	U
31	a	1549	A
31	a	1550	U
31	a	1551	U
31	a	1552	U
31	a	1555	U
31	a	1564	A
31	a	1571	A
31	a	1575	A
31	a	1584	A
31	a	1586	G
31	a	1595	C
31	a	1597	G
31	a	1598	U
31	a	1609	G
31	a	1621	G
31	a	1622	G
31	a	1624	U
31	a	1625	U
31	a	1627	U
31	a	1628	A
31	a	1629	A
31	a	1633	U
31	a	1637	A
31	a	1638	A
31	a	1646	U
31	a	1648	C

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 72 are monoatomic - leaving 2 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
38	ATP	W	501	37	26,33,33	0.61	0	31,52,52	1.08	3 (9%)
36	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
38	ATP	W	501	37	-	2/18/38/38	0/3/3/3
36	SF4	0	701	1	-	-	0/6/5/5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	W	501	ATP	C5-C6-N6	2.29	123.83	120.35
38	W	501	ATP	O3'-C3'-C4'	-2.06	105.10	111.05
38	W	501	ATP	PB-O3B-PG	2.04	139.83	132.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

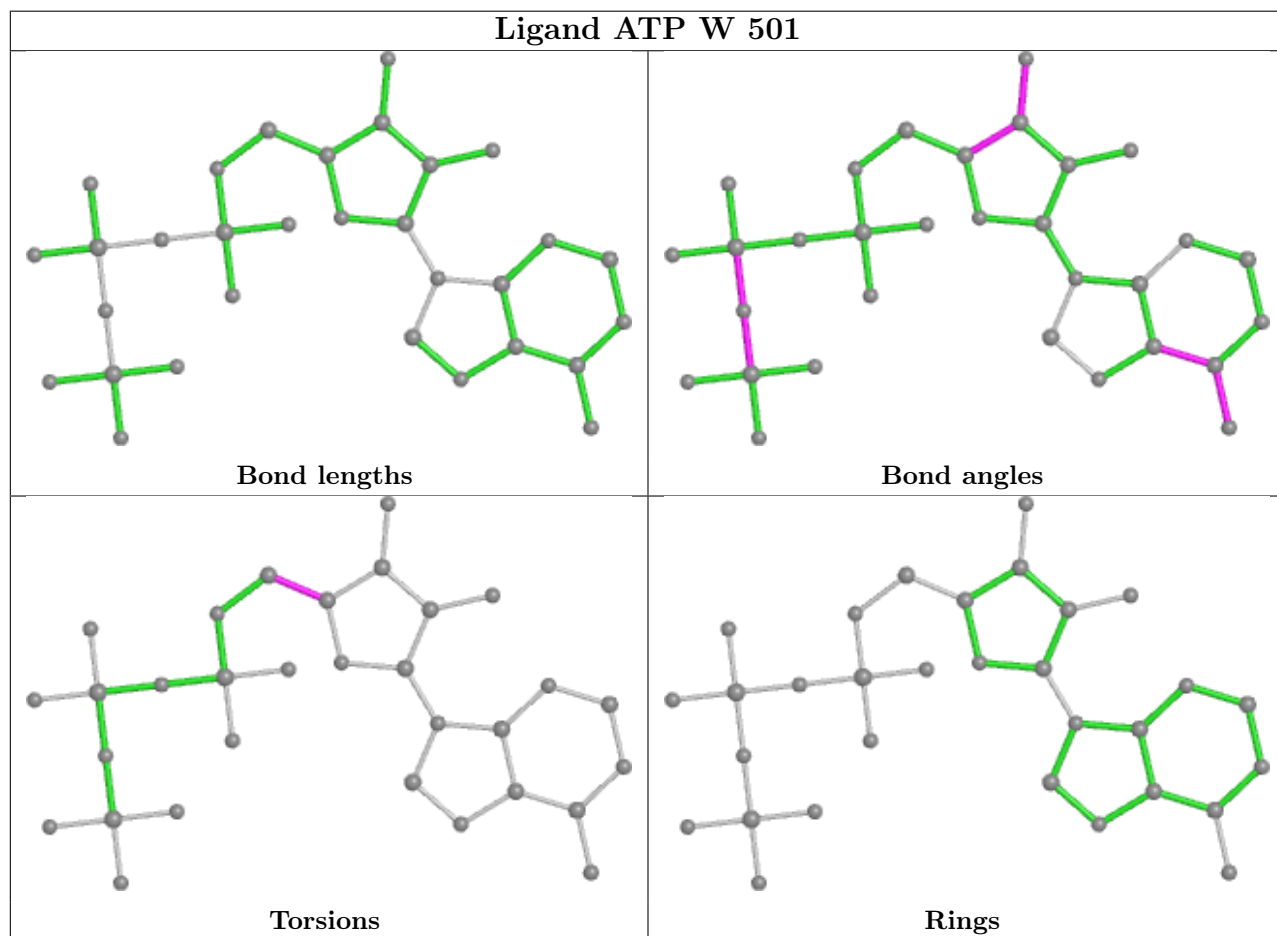
Mol	Chain	Res	Type	Atoms
38	W	501	ATP	O4'-C4'-C5'-O5'
38	W	501	ATP	C3'-C4'-C5'-O5'

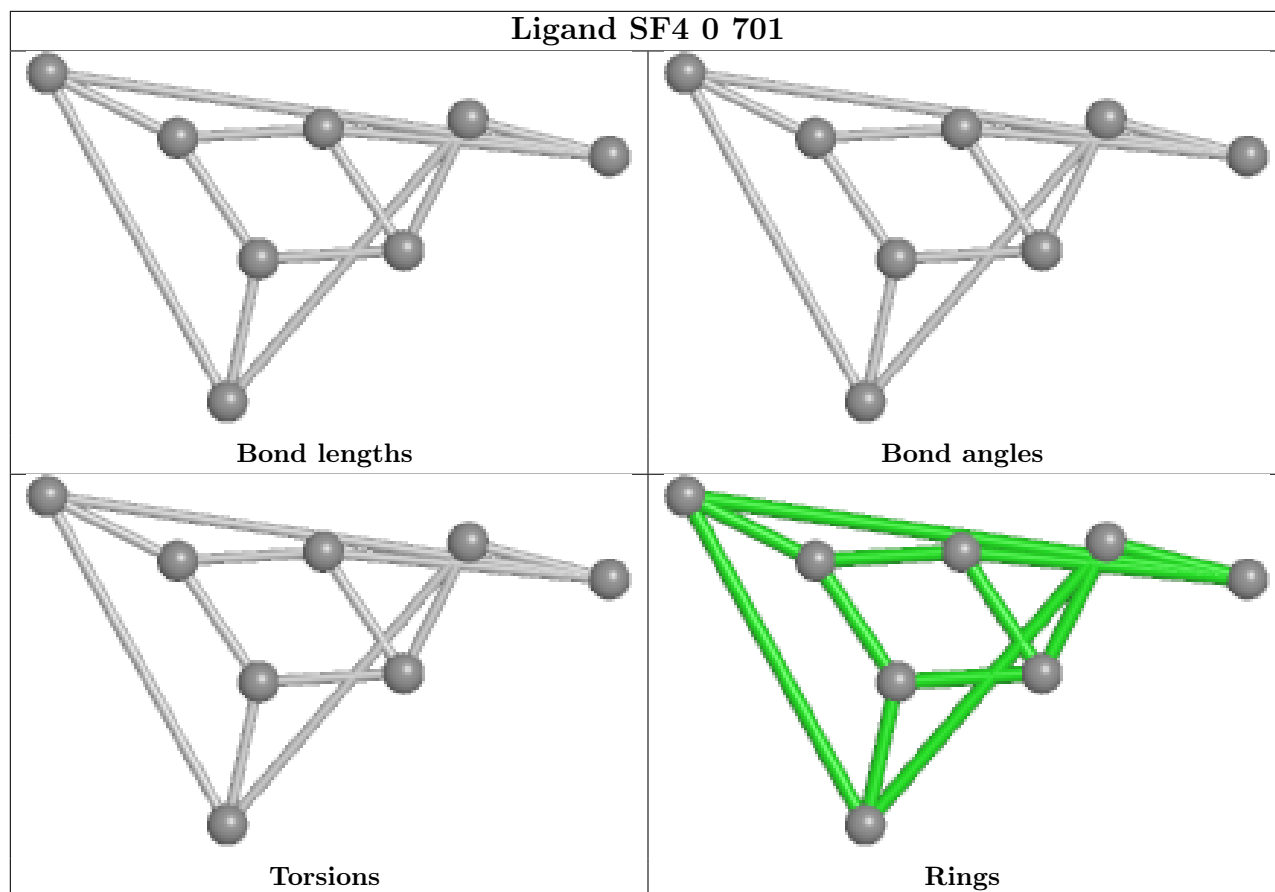
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	W	501	ATP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	c	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	59:UNK	C	76:UNK	N	23.27
1	c	93:UNK	C	105:UNK	N	20.76
1	c	37:UNK	C	40:UNK	N	10.25

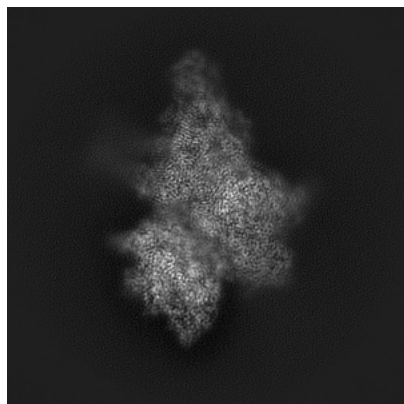
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27250. These allow visual inspection of the internal detail of the map and identification of artifacts.

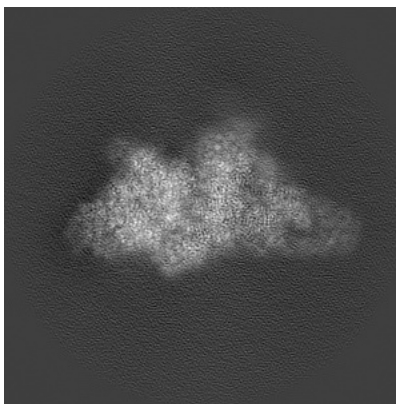
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

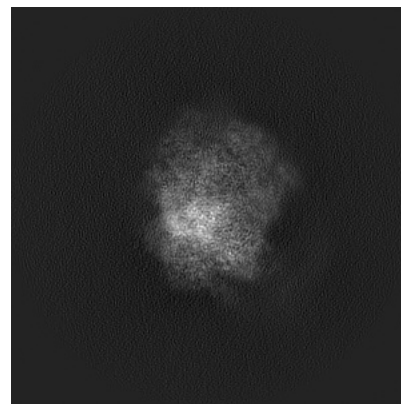
6.1.1 Primary map



X

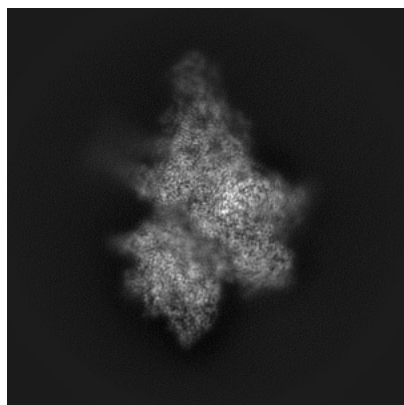


Y

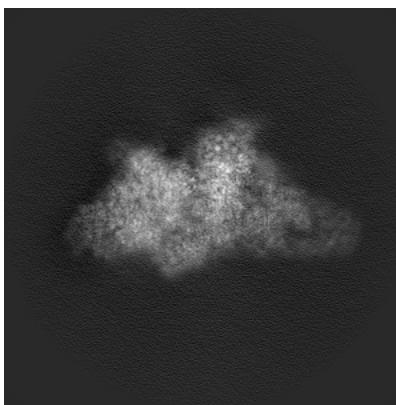


Z

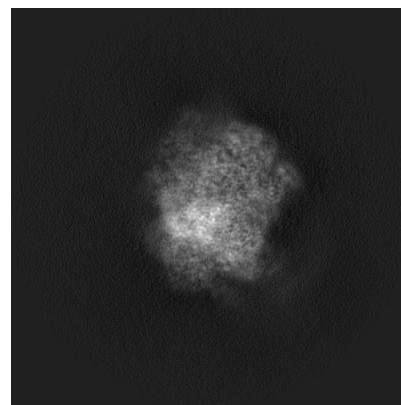
6.1.2 Raw map



X



Y

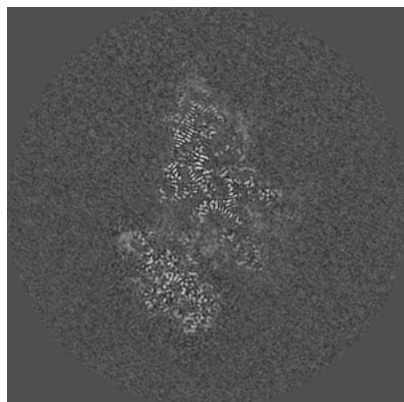


Z

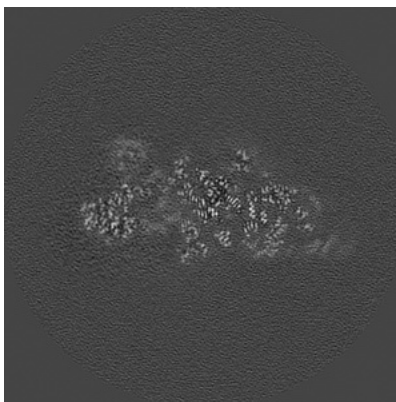
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

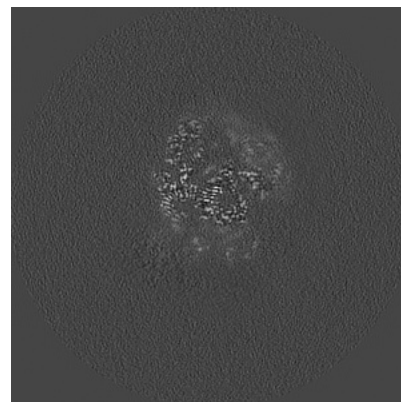
6.2.1 Primary map



X Index: 200

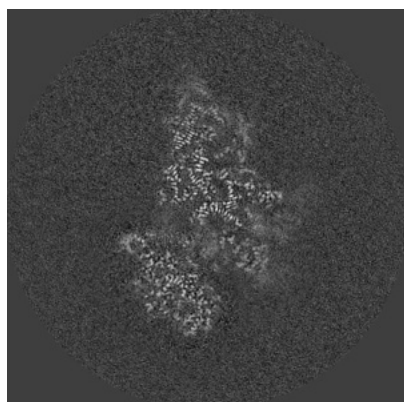


Y Index: 200

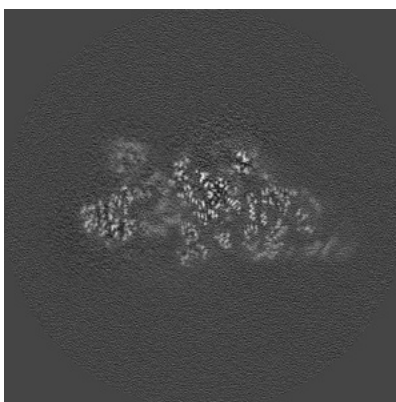


Z Index: 200

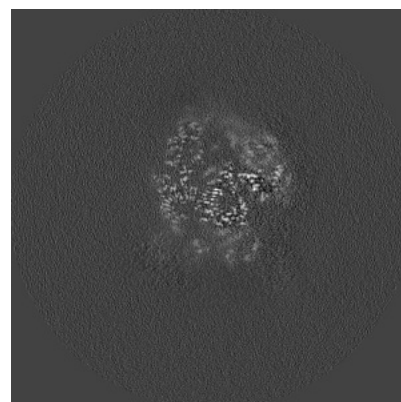
6.2.2 Raw map



X Index: 200



Y Index: 200

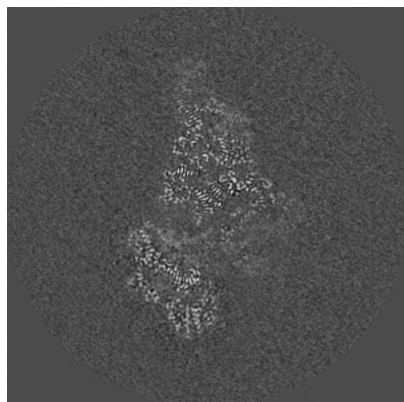


Z Index: 200

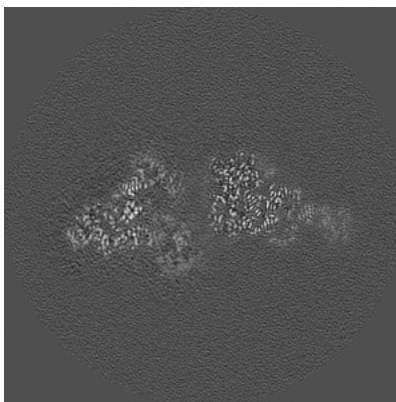
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

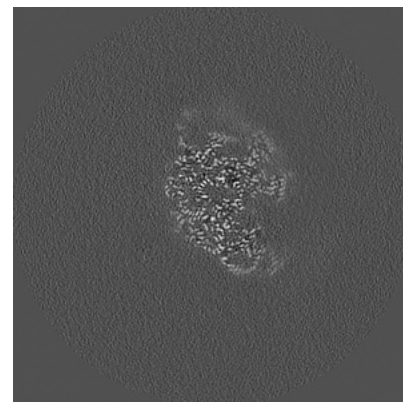
6.3.1 Primary map



X Index: 191

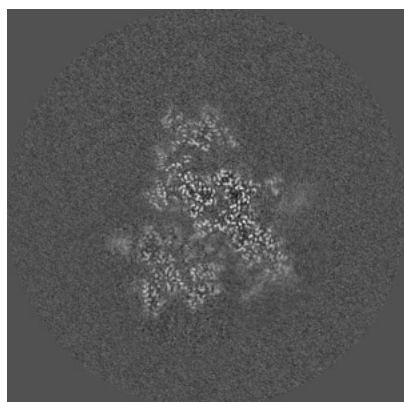


Y Index: 173

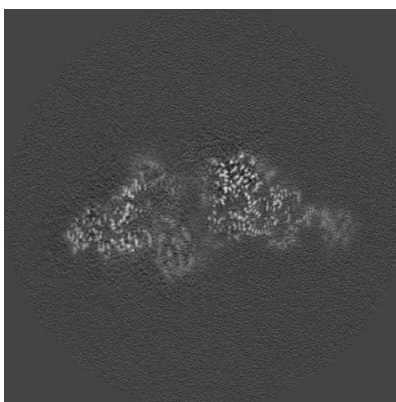


Z Index: 215

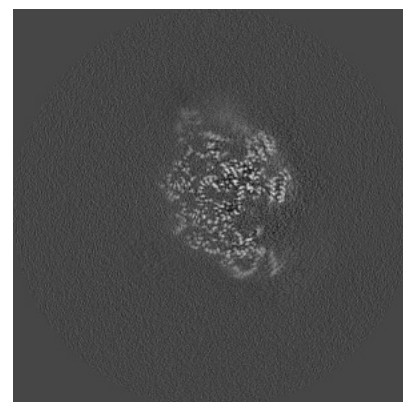
6.3.2 Raw map



X Index: 216



Y Index: 174

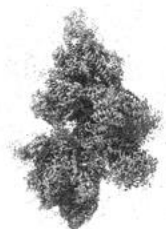


Z Index: 213

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

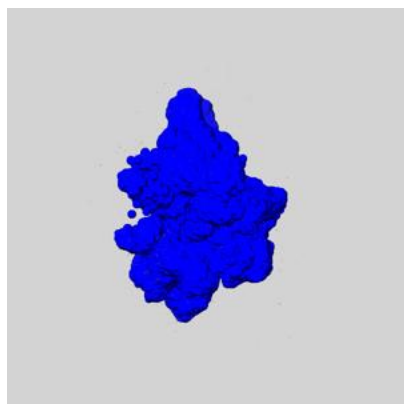
6.5 Mask visualisation [i](#)

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

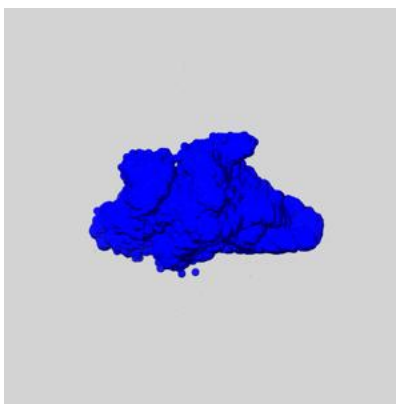
A mask typically either:

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

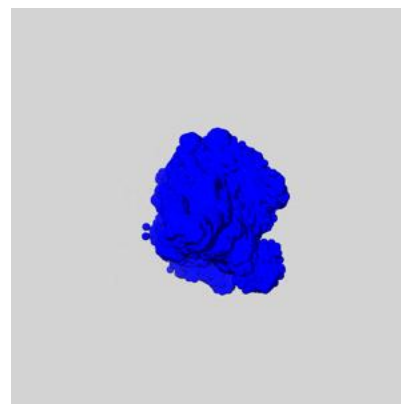
6.5.1 emd_27250_msk_1.map [i](#)



X



Y

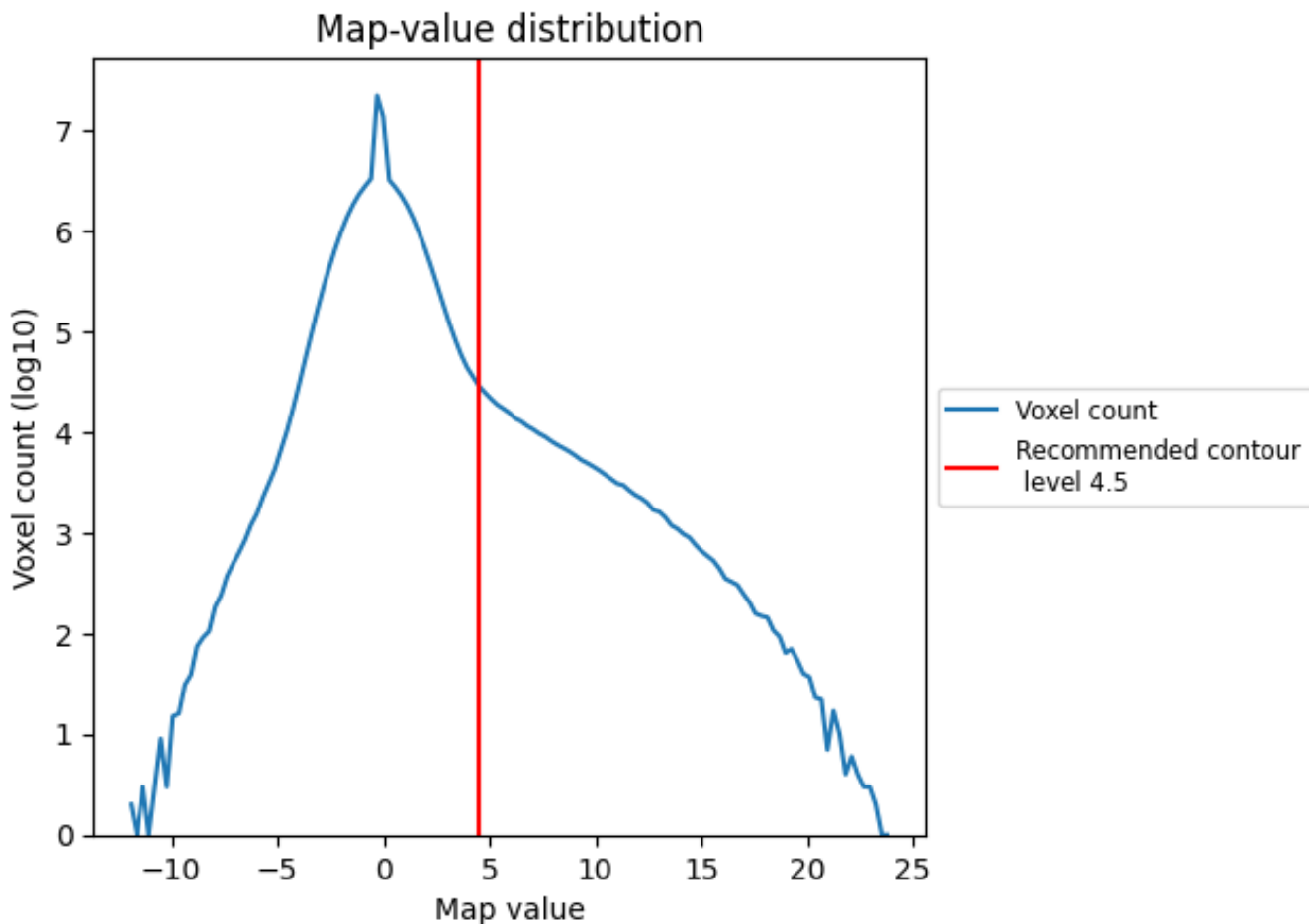


Z

7 Map analysis [i](#)

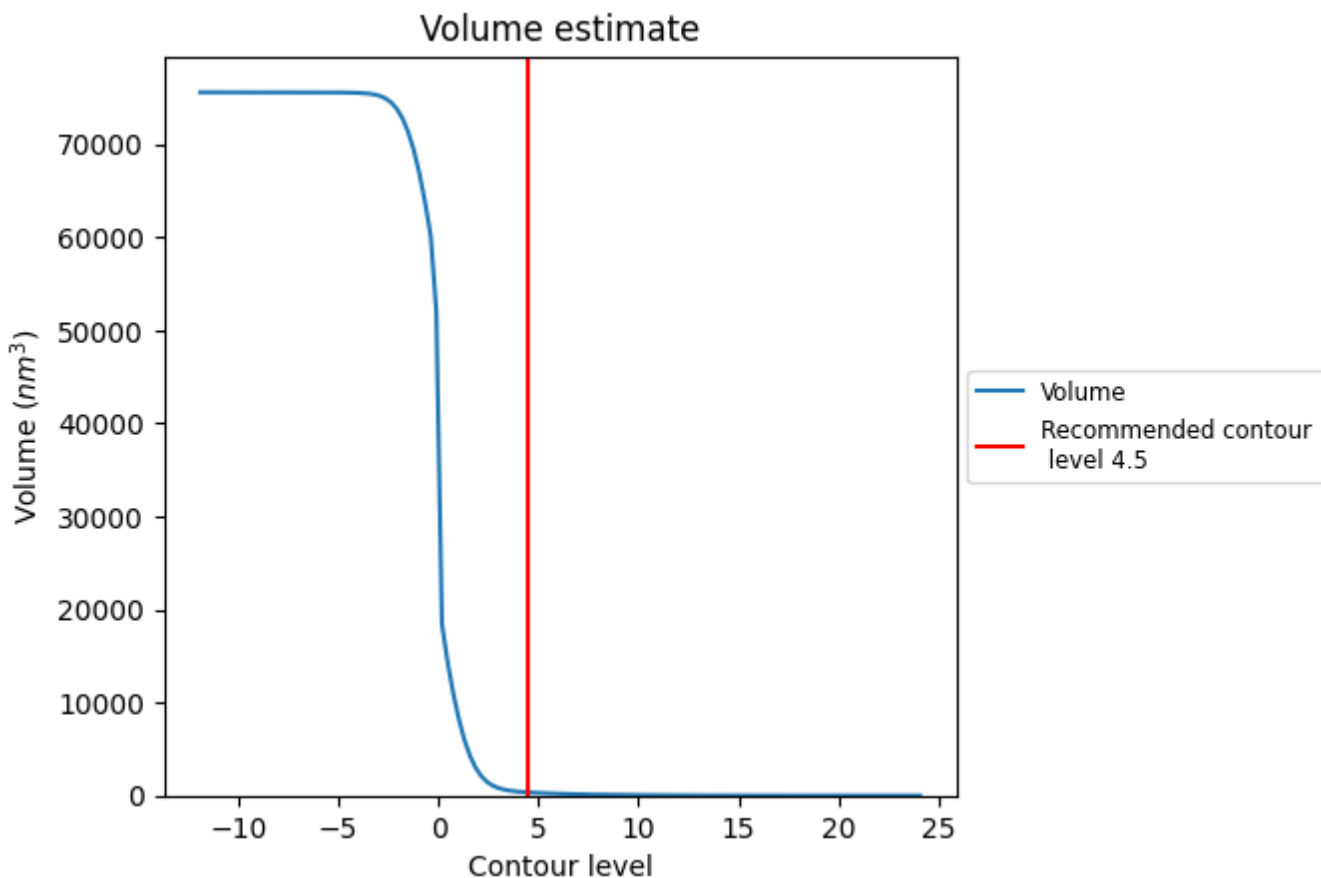
This section contains the results of statistical analysis of the map.

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.

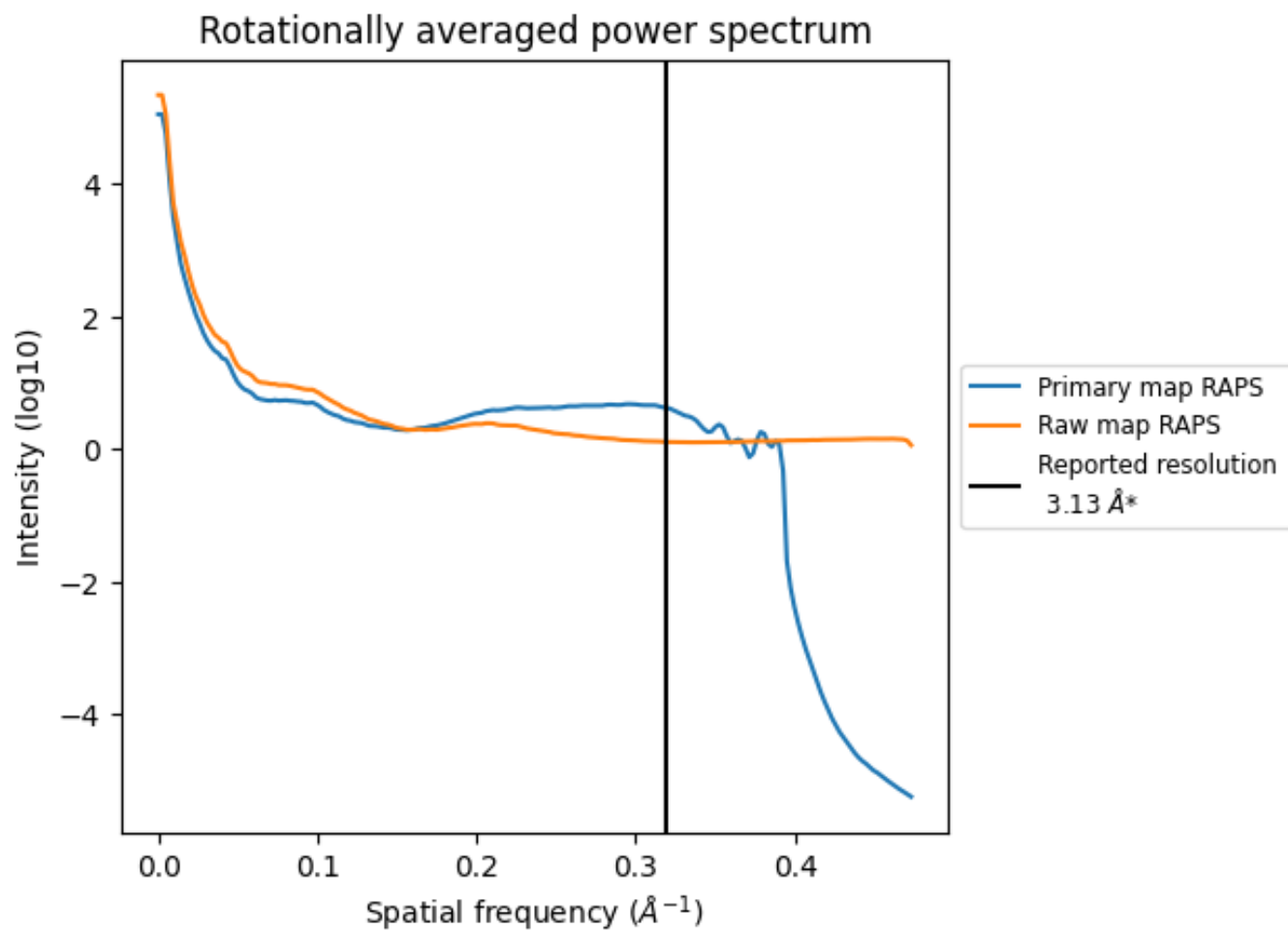
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 337 nm^3 ; this corresponds to an approximate mass of 305 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

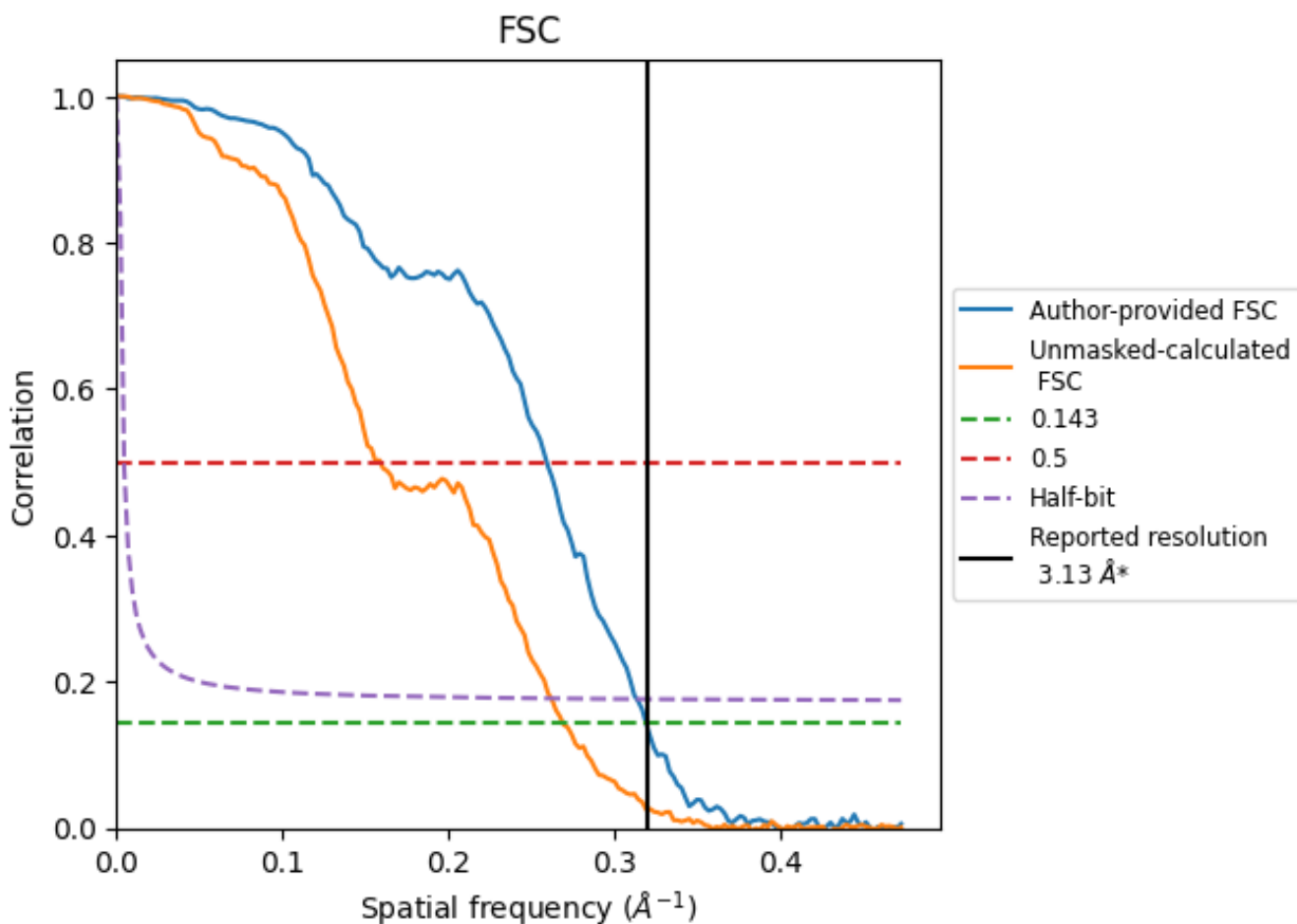


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

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 0.319 Å⁻¹

8.2 Resolution estimates [i](#)

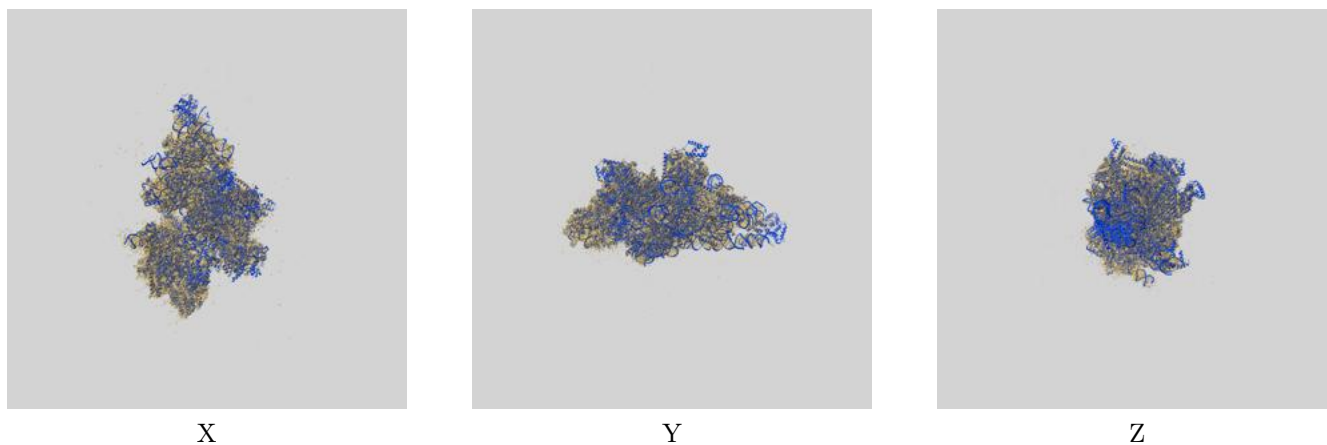
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.86	3.19
Unmasked-calculated*	3.71	6.29	3.81

*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 3.71 differs from the reported value 3.13 by more than 10 %

9 Map-model fit [i](#)

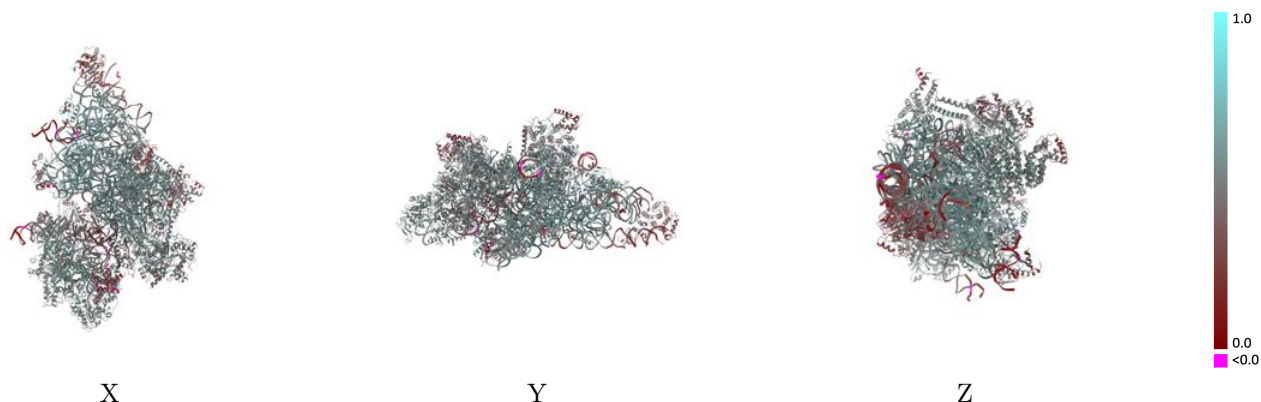
This section contains information regarding the fit between EMDB map EMD-27250 and PDB model 8D8K. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



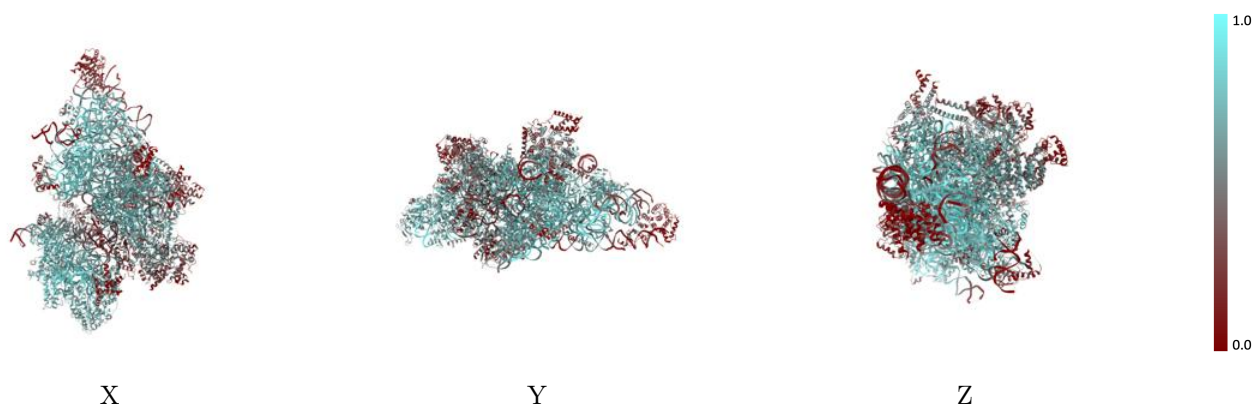
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



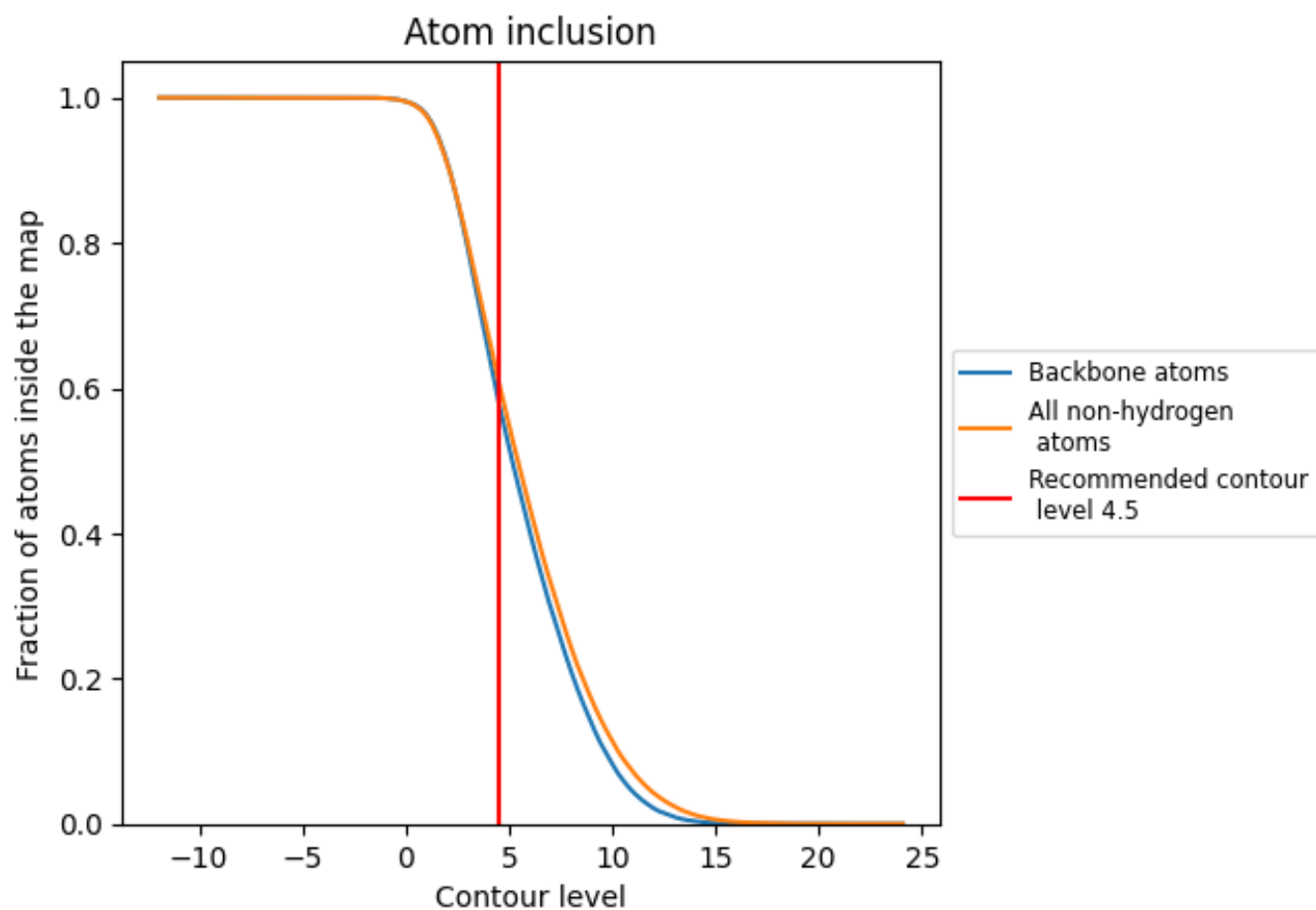
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 61% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6095	 0.5080
0	 0.3566	 0.3560
2	 0.5735	 0.5350
3	 0.5143	 0.5260
4	 0.3279	 0.4690
5	 0.1046	 0.3390
6	 0.7174	 0.5790
A	 0.5473	 0.5460
B	 0.6884	 0.5710
C	 0.6317	 0.4980
D	 0.6826	 0.5500
E	 0.6960	 0.5620
F	 0.5660	 0.5390
G	 0.6232	 0.4990
H	 0.8142	 0.6110
I	 0.6025	 0.5200
J	 0.7732	 0.5460
K	 0.4726	 0.5230
L	 0.6730	 0.5730
M	 0.6242	 0.4930
N	 0.7779	 0.5440
O	 0.6524	 0.5670
P	 0.6921	 0.5750
Q	 0.4579	 0.4940
R	 0.6096	 0.5700
S	 0.6833	 0.4950
T	 0.5122	 0.4950
U	 0.6275	 0.5560
V	 0.5518	 0.5290
W	 0.7056	 0.5360
X	 0.6799	 0.5080
Y	 0.6518	 0.4930
Z	 0.3426	 0.5010
a	 0.7000	 0.5060
c	 0.2043	 0.2480
d	 0.4440	 0.4920

