Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 09:55 am GMT

PDB ID	:	6YW5
EMDB ID	:	EMD-10958
Title	:	The structure of the small subunit of the mitoribosome from Neurospora crassa
Authors	:	Amunts, A.; Itoh, Y.; Naschberger, A.
Deposited on	:	2020-04-29
Resolution	:	2.85 Å(reported)

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

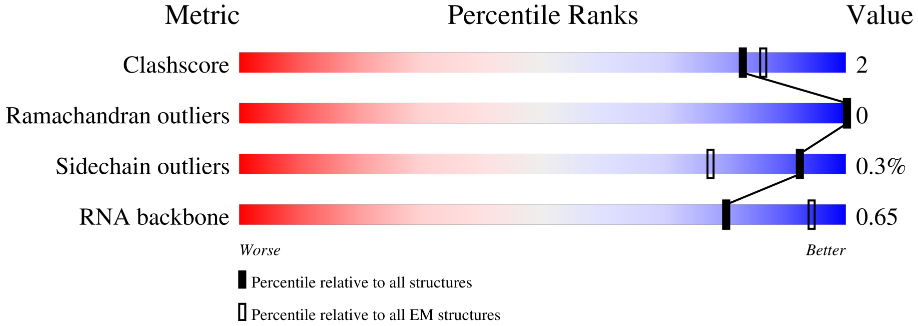
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

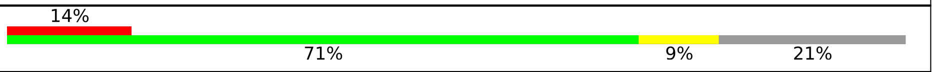
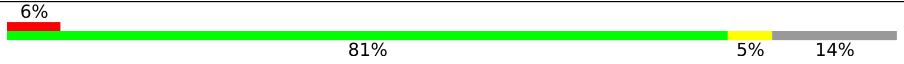
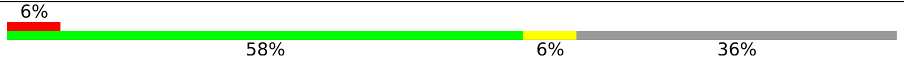
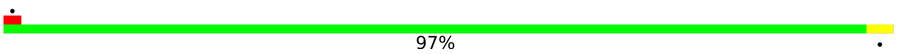
The reported resolution of this entry is 2.85 Å.

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 <=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	AA	470	
2	BB	428	
3	CC	508	
4	DD	453	
5	EE	477	
6	FF	117	
7	GG	309	

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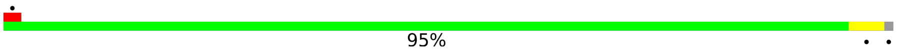
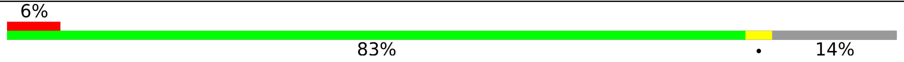
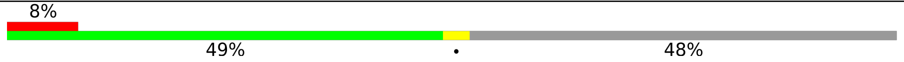
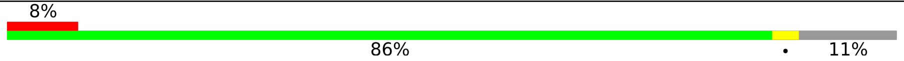
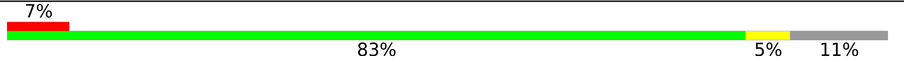
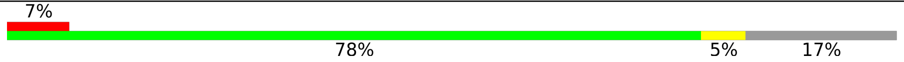
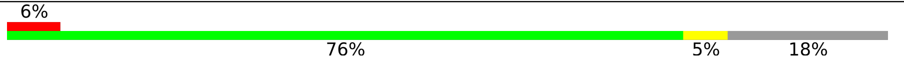
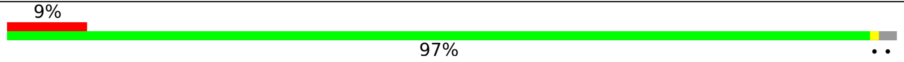
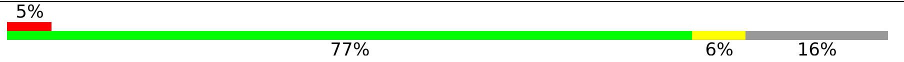
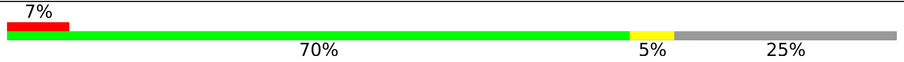
Mol	Chain	Length	Quality of chain
8	HH	161	
9	II	315	
10	JJ	268	
11	KK	376	
12	LL	174	
13	MM	119	
14	NN	113	
15	OO	320	
16	PP	107	
17	QQ	165	
18	RR	256	
19	SS	91	
20	TT	236	
21	UU	253	
22	VV	316	
23	WW	396	
24	XX	469	
25	YY	108	
26	ZZ	382	
27	11	90	
28	22	344	
29	33	236	
30	44	310	
30	55	310	
31	66	348	

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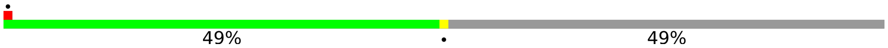
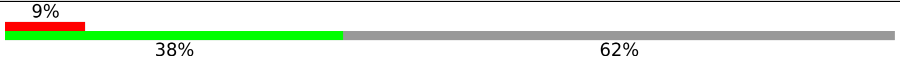
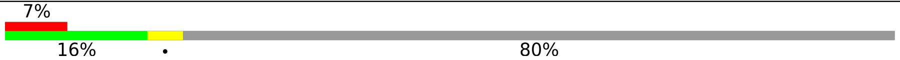
Mol	Chain	Length	Quality of chain
32	77	414	
33	88	508	
34	00	95	
34	99	95	
35	aa	1864	
36	V	219	

2 Entry composition ⓘ

There are 39 unique types of molecules in this entry. The entry contains 167560 atoms, of which 76668 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 uS2m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	AA	372	5790	1827	2907	507	543	6	0	0

- Molecule 2 is a protein called Mito ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	BB	290	4570	1426	2301	423	414	6	0	0

- Molecule 3 is a protein called Ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	CC	438	7539	2388	3897	636	613	5	0	0

- Molecule 4 is a protein called Mito ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	DD	290	4716	1501	2373	430	401	11	0	0

- Molecule 5 is a protein called 37S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	EE	367	5799	1799	2918	526	544	12	0	0

- Molecule 6 is a protein called Mito ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	FF	117	1902	591	966	176	166	3	0	0

- Molecule 7 is a protein called Ribosomal_S7 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	GG	223	3524	1098	1799	318	303	6	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	HH	160	2522	783	1286	226	221	6	0	0

- Molecule 9 is a protein called uS9m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	II	247	3995	1253	2026	366	345	5	0	0

- Molecule 10 is a protein called 37S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	JJ	188	3105	998	1554	273	272	8	0	0

- Molecule 11 is a protein called Mitochondrial ribosomal protein subunit S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	KK	124	2020	625	1025	195	170	5	0	0

- Molecule 12 is a protein called Mitochondrial 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	LL	128	1991	591	1032	198	165	5	0	0

- Molecule 13 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	MM	118	1925	586	987	186	162	4	0	0

- Molecule 14 is a protein called Mitochondrial 40S ribosomal protein MRP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	NN	112	Total	C	H	N	O	S	0	0
			1876	573	961	184	151	7		

- Molecule 15 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	OO	276	Total	C	H	N	O	S	0	0
			4429	1361	2230	431	402	5		

- Molecule 16 is a protein called Ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	PP	98	Total	C	H	N	O	0	0
			1612	510	826	141	135		

- Molecule 17 is a protein called Mitochondrial 37S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	QQ	158	Total	C	H	N	O	S	0	0
			2561	789	1314	234	219	5		

- Molecule 18 is a protein called Mito ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	RR	134	Total	C	H	N	O	S	0	0
			2169	679	1089	206	190	5		

- Molecule 19 is a protein called Mitochondrial ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	SS	81	Total	C	H	N	O	S	0	0
			1325	422	677	118	107	1		

- Molecule 20 is a protein called Mito ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	TT	88	Total	C	H	N	O	0	0
			1519	470	772	157	120		

- Molecule 21 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	UU	224	3686	1165	1842	342	330	7	0	0

- Molecule 22 is a protein called mS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	VV	261	4193	1300	2112	390	388	3	0	0

- Molecule 23 is a protein called mS27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	WW	353	5745	1804	2901	514	516	10	0	0

- Molecule 24 is a protein called Mitochondrial ribosomal protein DAP3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	XX	408	6447	2010	3271	562	588	16	0	0

- Molecule 25 is a protein called mS33.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	YY	99	1609	491	823	152	142	1	0	0

- Molecule 26 is a protein called 37S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	ZZ	312	5114	1631	2528	450	495	10	0	0

- Molecule 27 is a protein called 37S ribosomal protein mrp10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	11	88	1358	417	686	128	121	6	0	0

- Molecule 28 is a protein called DUF1713 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	22	33	661	187	359	70	44	1	0	0

- Molecule 29 is a protein called IGR domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	33	193	3161	989	1607	295	268	2	0	0

- Molecule 30 is a protein called Fe superoxide dismutase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	44	260	4045	1318	1983	355	378	11	0	0
			Total	C	H	N	O	S		
30	55	232	3651	1195	1793	316	337	10	0	0

- Molecule 31 is a protein called mS42.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	66	283	4629	1455	2330	425	415	4	0	0

- Molecule 32 is a protein called mS46.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	77	179	2796	893	1396	227	277	3	0	0

- Molecule 33 is a protein called 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	88	467	7327	2340	3650	634	691	12	0	0

- Molecule 34 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
34	00	48	823	252	417	77	77	0	0
			Total	C	H	N	O		
34	99	36	639	191	333	59	56	0	0

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
35	aa	1435	45984	13712	15376	5486	9975	1435	0	0

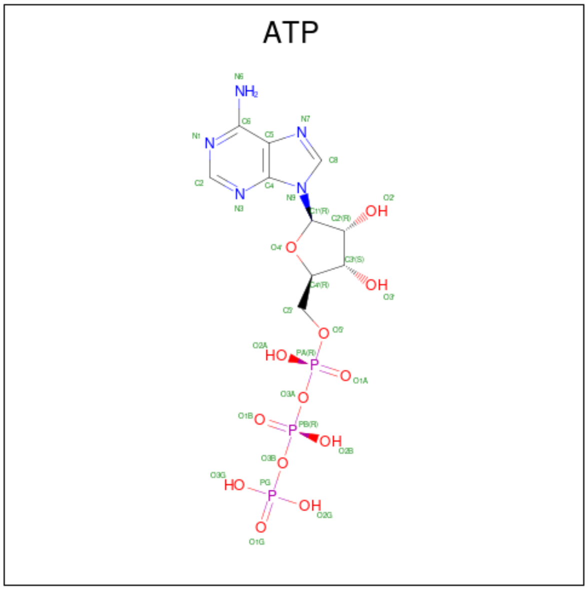
- Molecule 36 is a protein called IF1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	V	43	641	206	309	56	69	1	0	0

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
37	BB	1	1	1	0
37	KK	1	1	1	0
37	QQ	1	1	1	0
37	XX	1	1	1	0
37	YY	1	1	1	0
37	00	1	1	1	0
37	aa	91	91	91	0

- Molecule 38 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 39 is POTASSIUM ION (three-letter code: K) (formula: K).

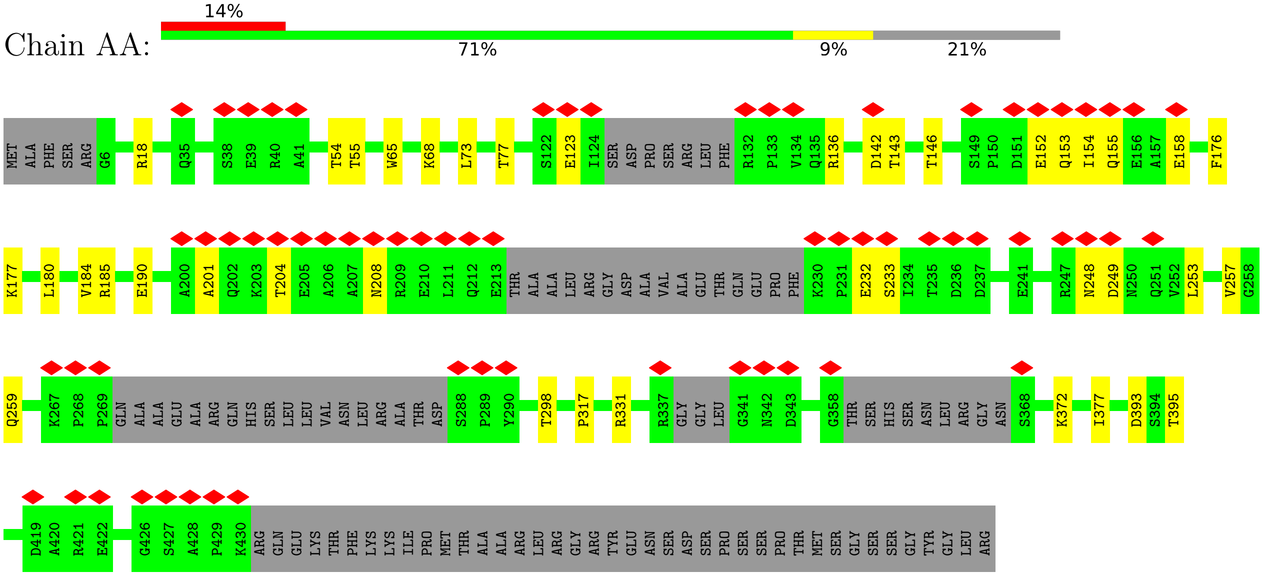
Mol	Chain	Residues	Atoms		AltConf
39	77	1	Total 1	K 1	0
39	88	1	Total 1	K 1	0
39	aa	20	Total 20	K 20	0

3 Residue-property plots ⓘ

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

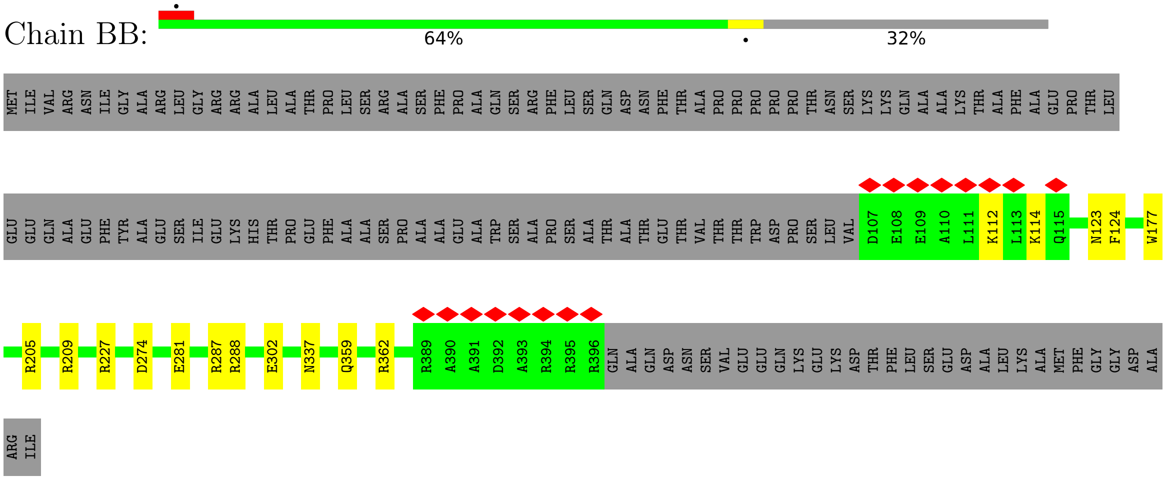
- Molecule 1: uS2m

Chain AA:



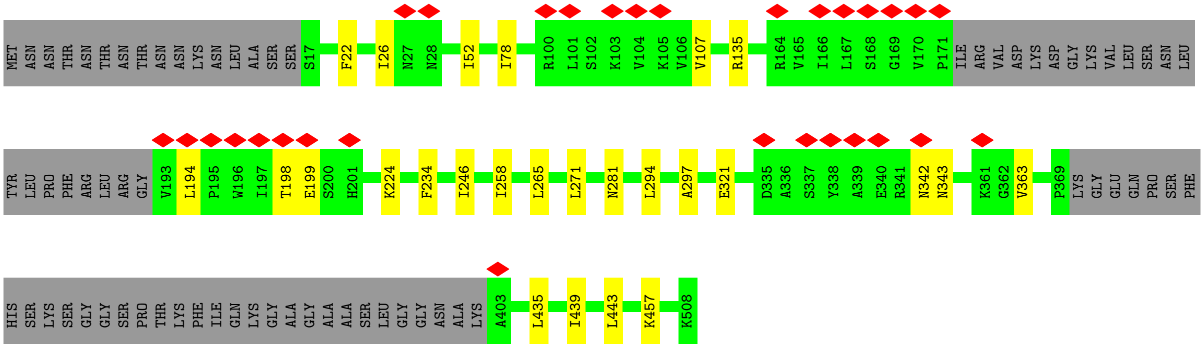
- Molecule 2: Mito ribosomal protein S2

Chain BB:



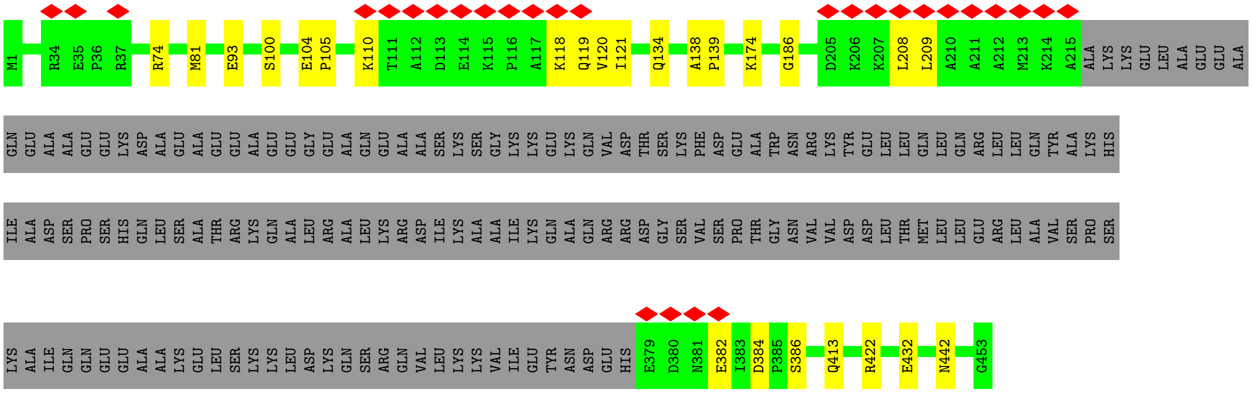
- Molecule 3: Ribosomal protein S5, mitochondrial

Chain CC:



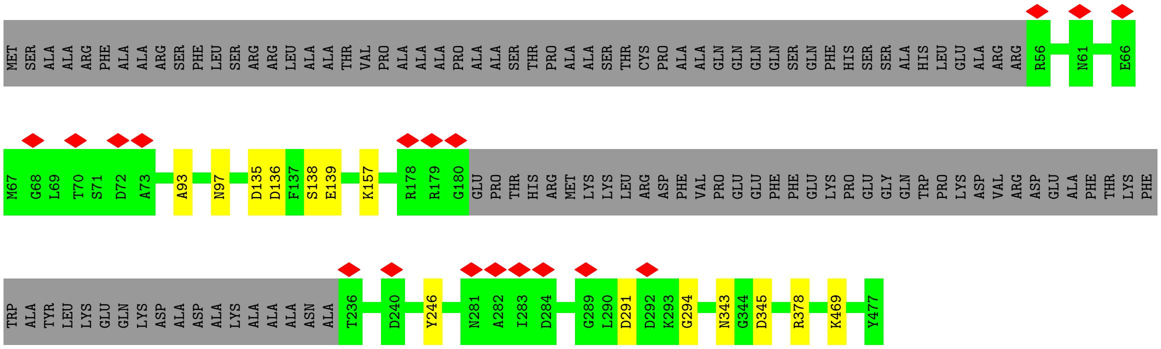
- Molecule 4: Mito ribosomal protein S4

Chain DD:



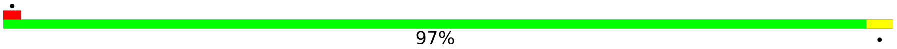
- Molecule 5: 37S ribosomal protein S5

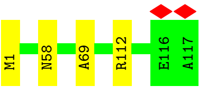
Chain EE:



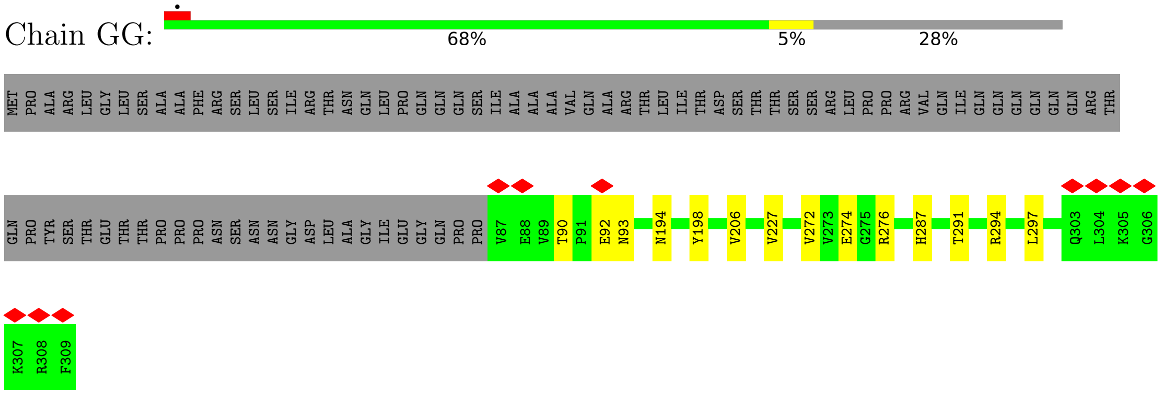
- Molecule 6: Mito ribosomal protein S6

Chain FF:

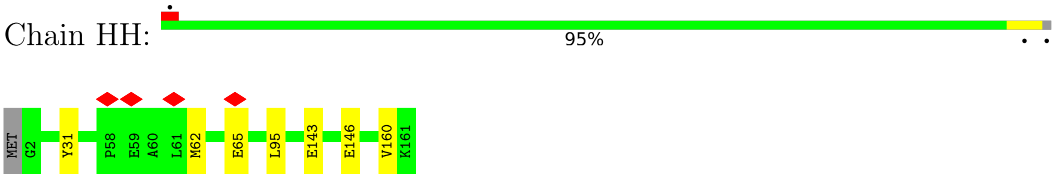




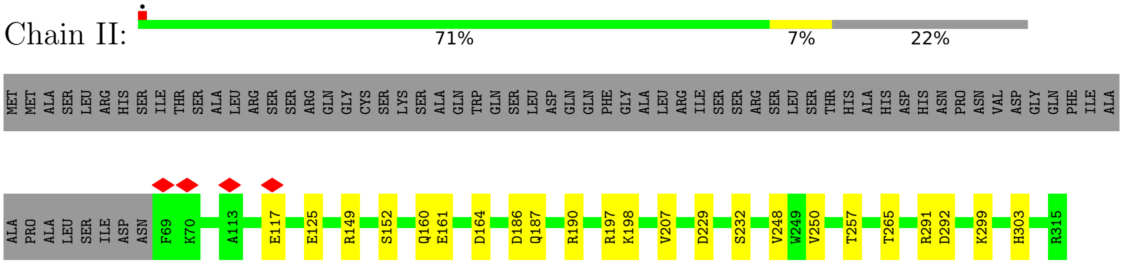
- Molecule 7: Ribosomal_S7 domain-containing protein



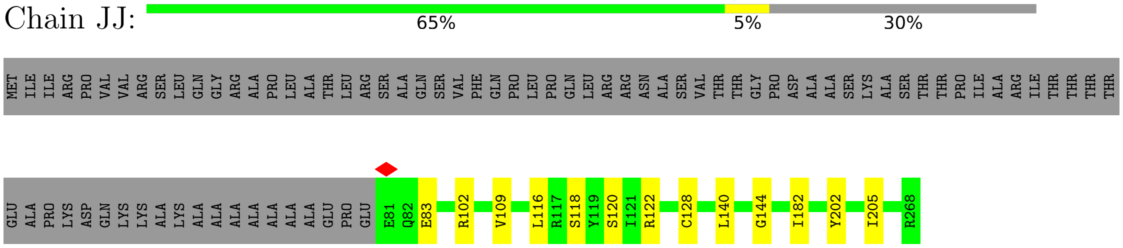
- Molecule 8: 40S ribosomal protein S8



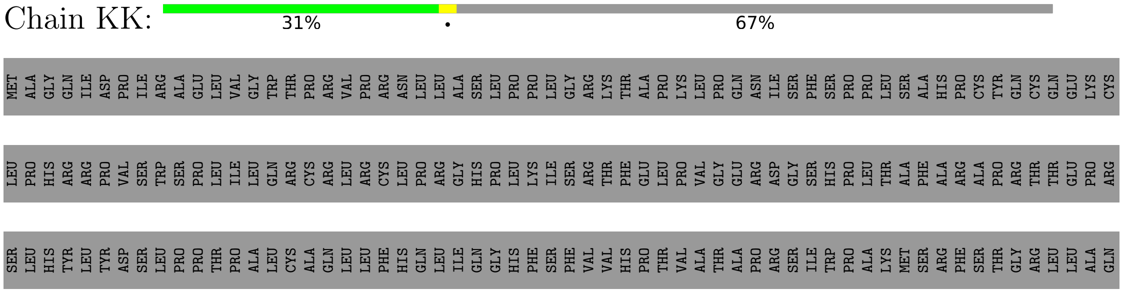
- Molecule 9: uS9m

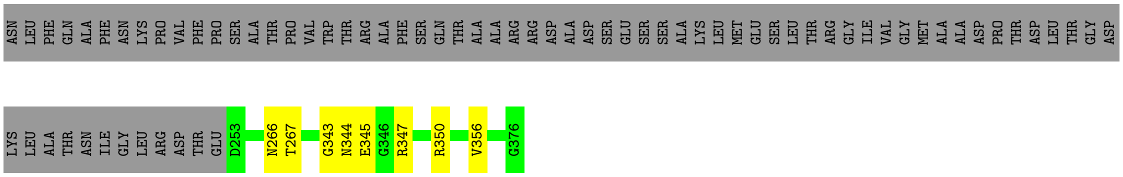


- Molecule 10: 37S ribosomal protein S10, mitochondrial



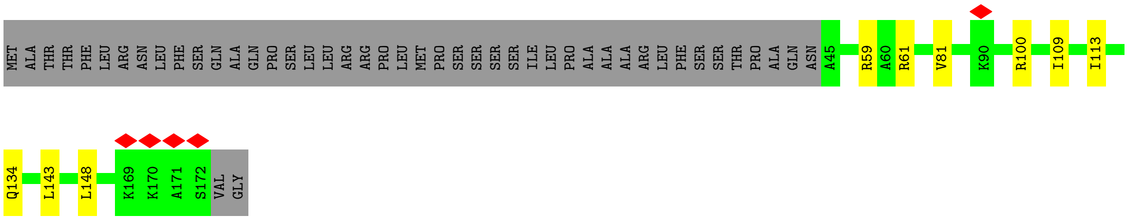
- Molecule 11: Mitochondrial ribosomal protein subunit S18





- Molecule 12: Mitochondrial 30S ribosomal protein S12

Chain LL:

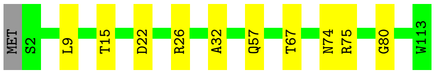


- Molecule 13: 40S ribosomal protein S13

Chain MM:

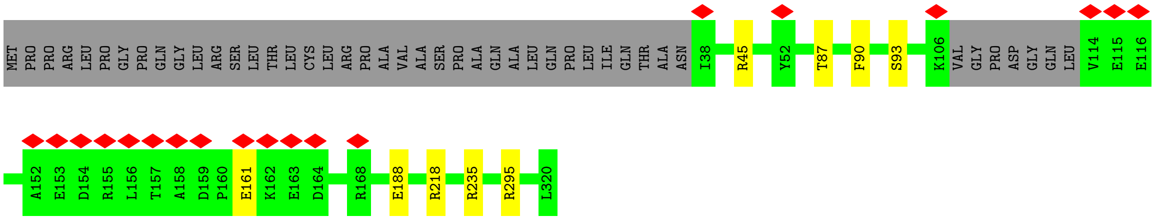
- Molecule 14: Mitochondrial 40S ribosomal protein MRP2

Chain NN:



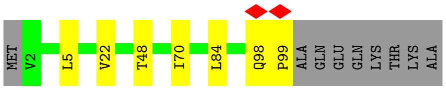
- Molecule 15: Ribosomal protein S15

Chain OO:



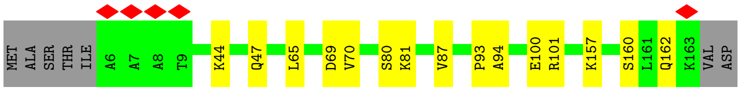
- Molecule 16: Ribosomal protein S16, mitochondrial

Chain PP:



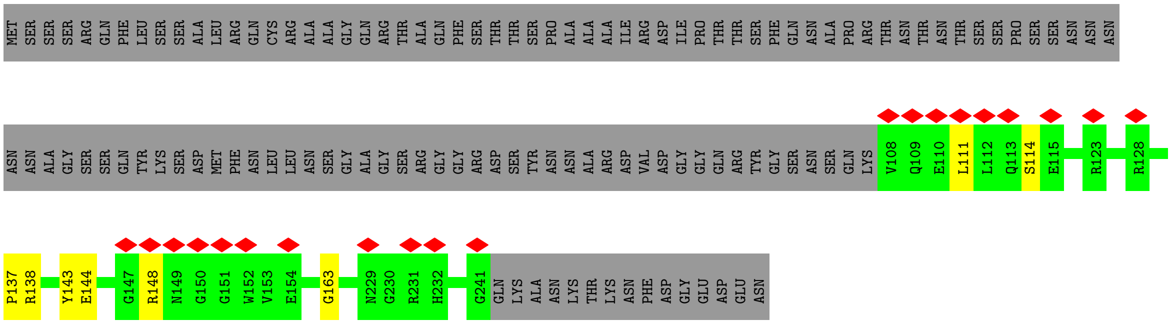
- Molecule 17: Mitochondrial 37S ribosomal protein S17

Chain QQ:



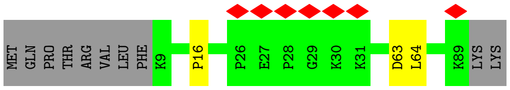
- Molecule 18: Mito ribosomal protein S18

Chain RR:



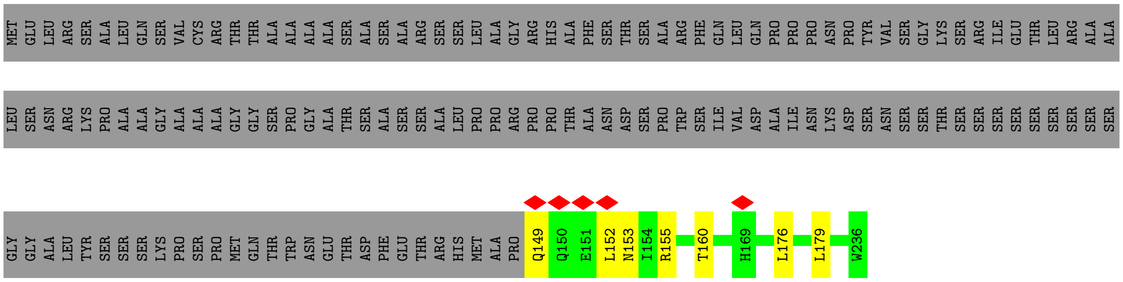
- Molecule 19: Mitochondrial ribosomal protein S19

Chain SS:



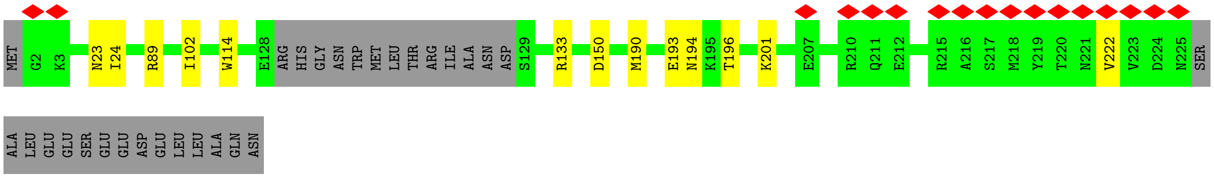
- Molecule 20: Mito ribosomal protein S21

Chain TT:

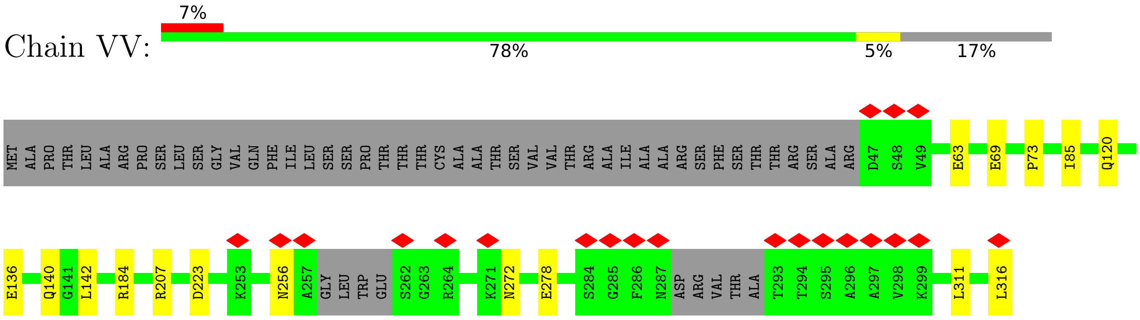


- Molecule 21: 37S ribosomal protein S25, mitochondrial

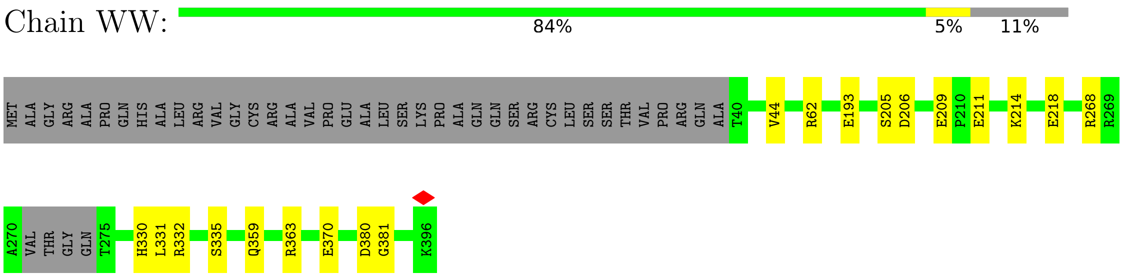
Chain UU:



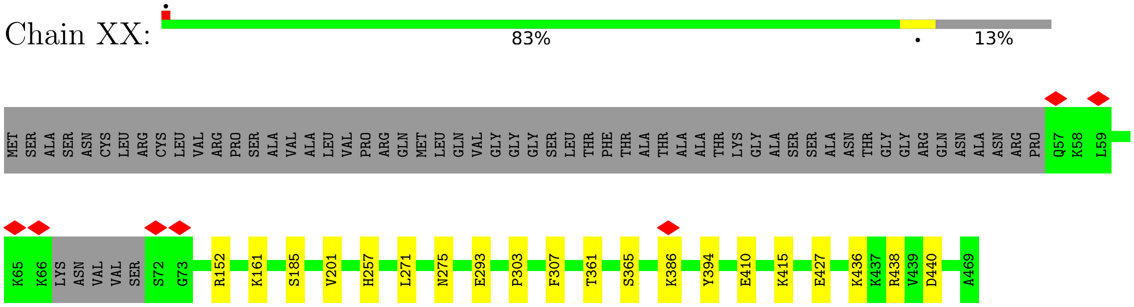
- Molecule 22: mS26



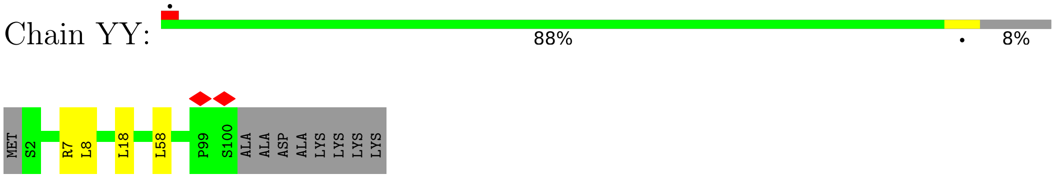
- Molecule 23: mS27



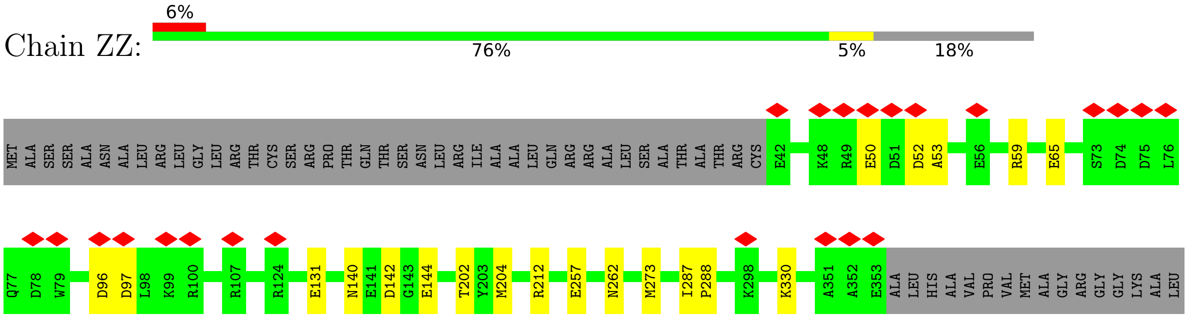
- Molecule 24: Mitochondrial ribosomal protein DAP3



- Molecule 25: mS33

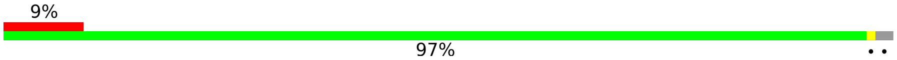


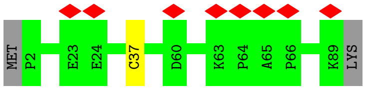
- Molecule 26: 37S ribosomal protein S24, mitochondrial



- Molecule 27: 37S ribosomal protein mrp10, mitochondrial

Chain 11:



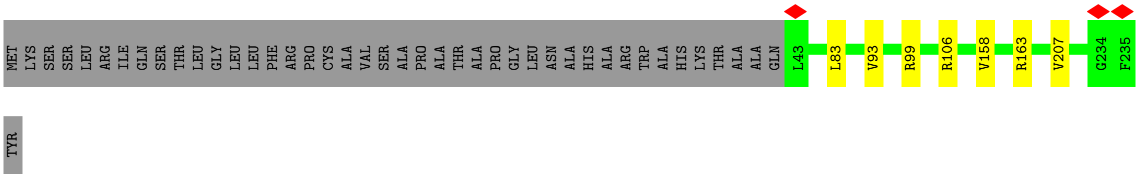


- Molecule 28: DUF1713 domain-containing protein

Chain 22:

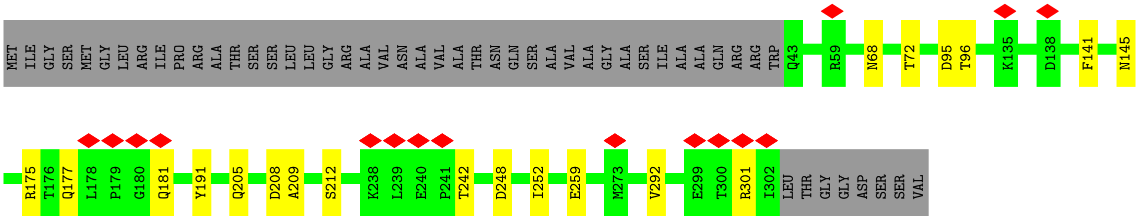
- Molecule 29: IGR domain-containing protein

Chain 33:

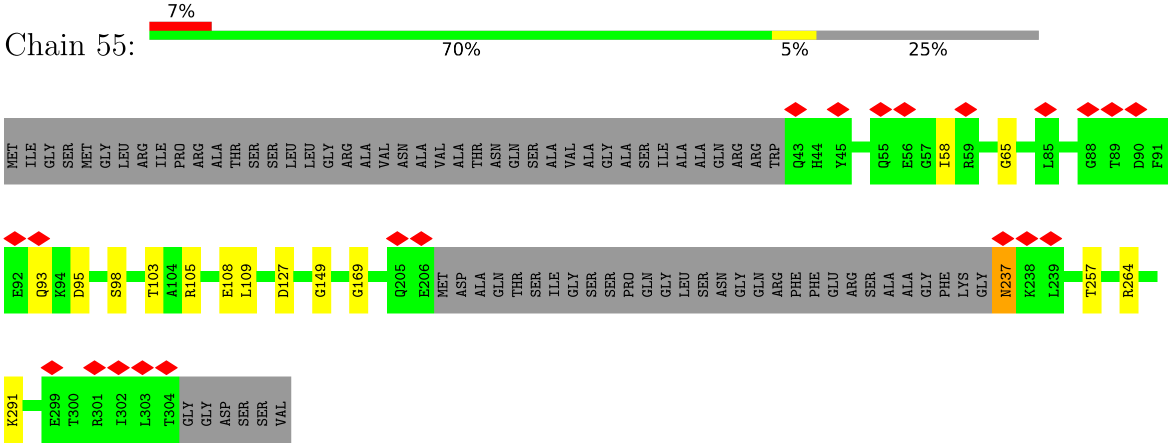


- Molecule 30: Fe superoxide dismutase

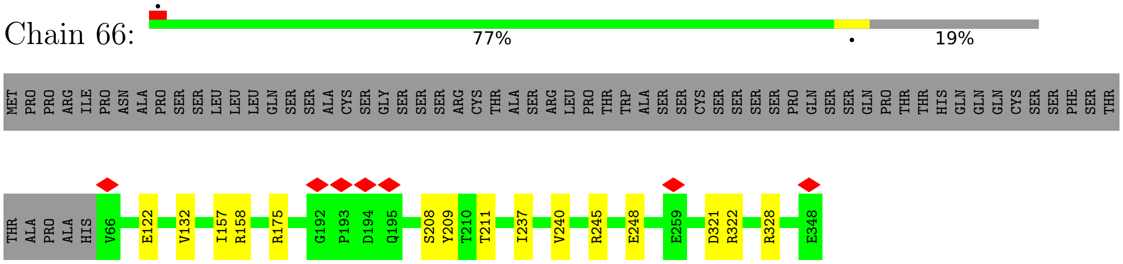
Chain 44:



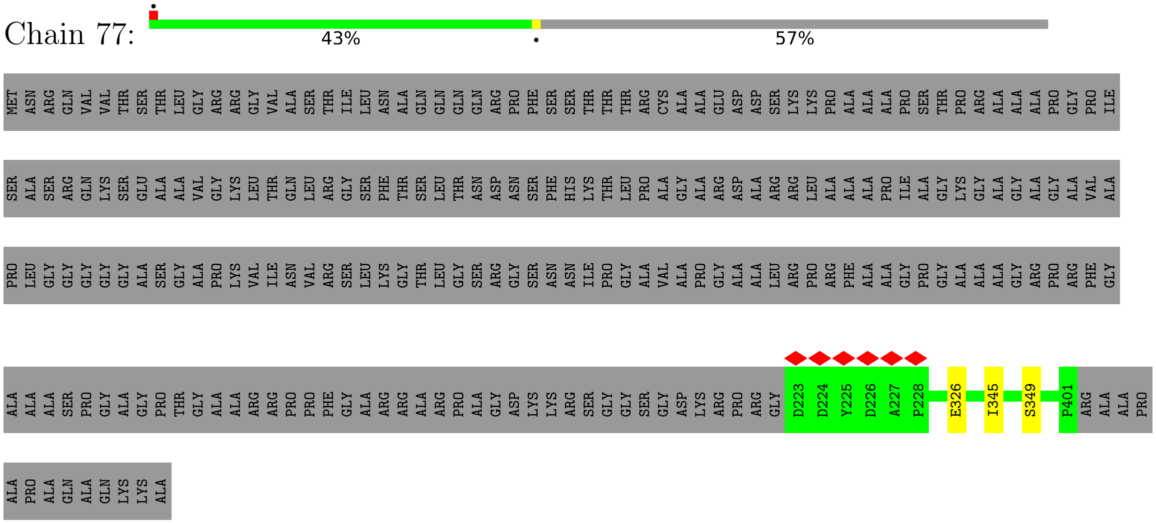
- Molecule 30: Fe superoxide dismutase



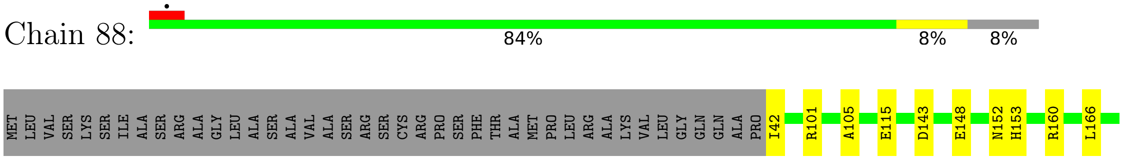
- Molecule 31: mS42

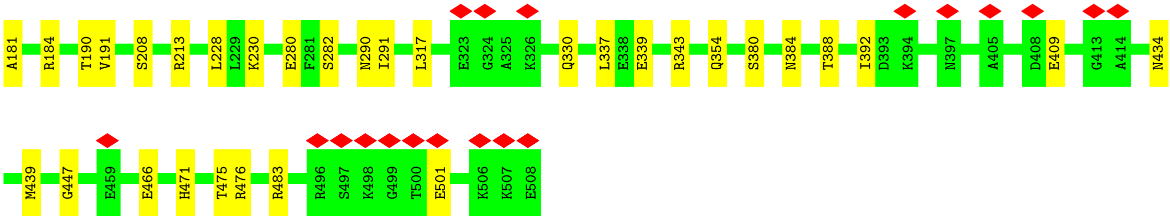


- Molecule 32: mS46



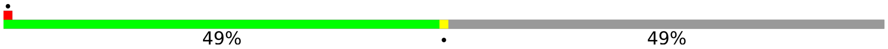
- Molecule 33: 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial

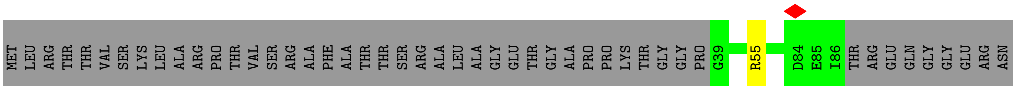




- Molecule 34: mS47

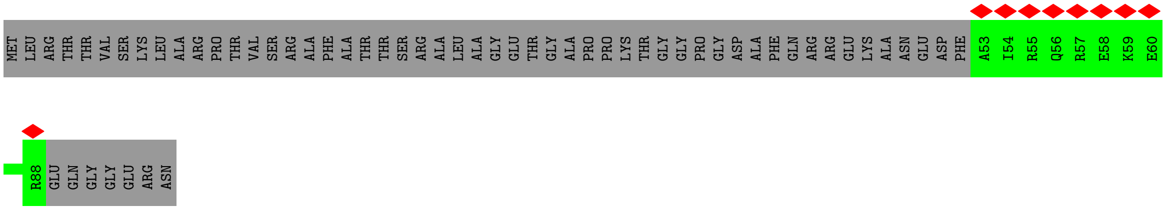
Chain 00:





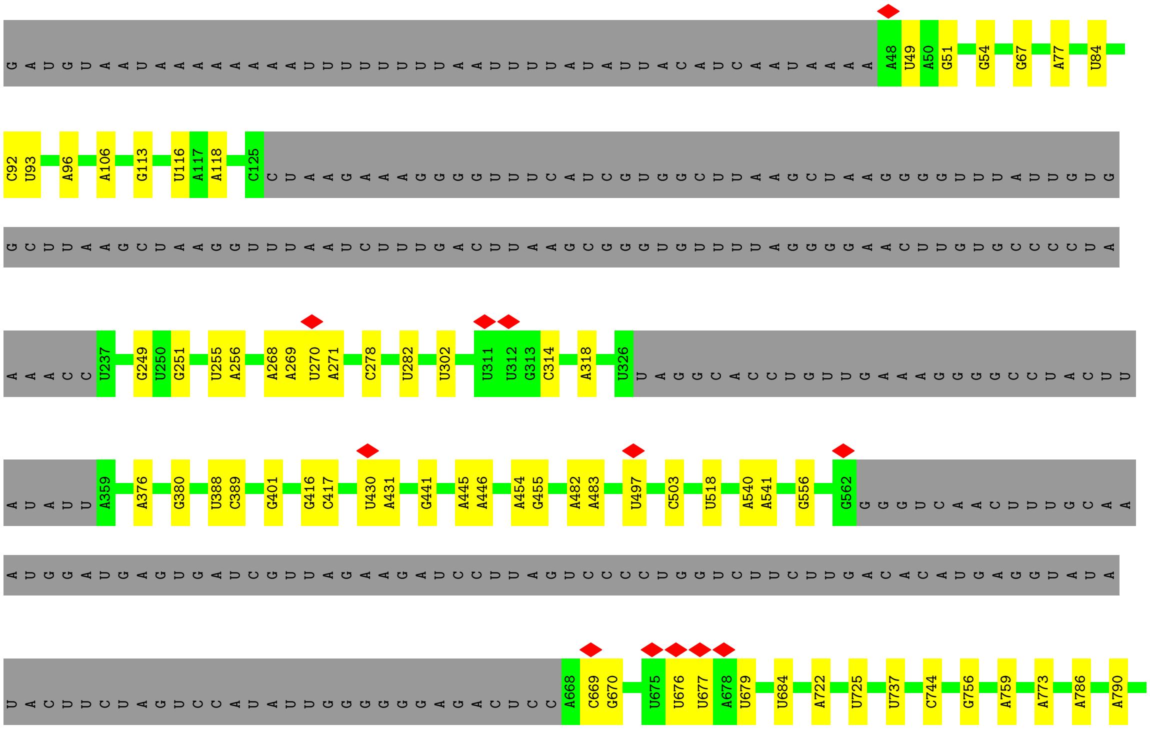
- Molecule 34: mS47

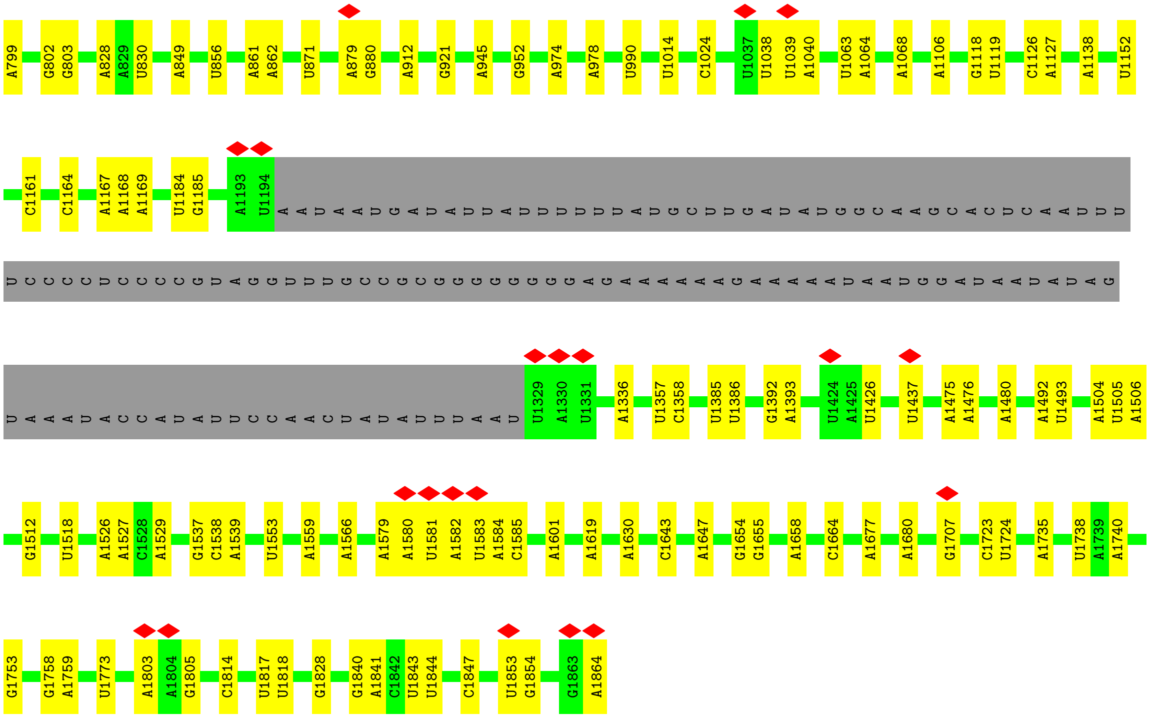
Chain 99:



- Molecule 35: 16S rRNA

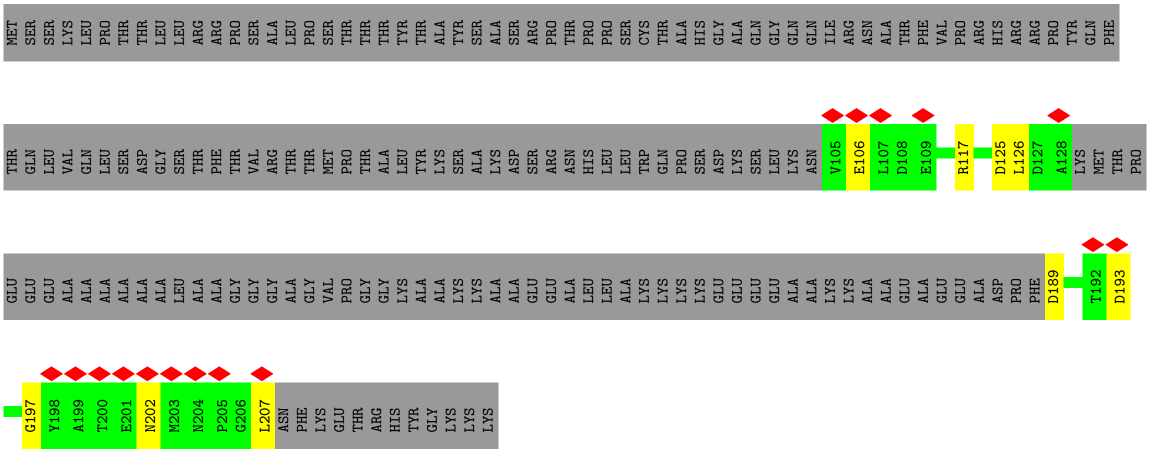
Chain aa:





- Molecule 36: IF1

Chain V:



4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131806	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 ($e^-/\text{Å}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	49.868	Depositor
Minimum map value	-22.282	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.102	Depositor
Recommended contour level	3.74	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, 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	AA	0.25	0/2948	0.40	0/3995
2	BB	0.24	0/2314	0.39	0/3142
3	CC	0.25	0/3713	0.39	0/4978
4	DD	0.25	0/2409	0.38	0/3255
5	EE	0.24	0/2929	0.40	0/3947
6	FF	0.24	0/953	0.41	0/1285
7	GG	0.24	0/1766	0.37	0/2392
8	HH	0.25	0/1260	0.41	0/1707
9	II	0.24	0/2013	0.39	0/2720
10	JJ	0.25	0/1590	0.38	0/2140
11	KK	0.24	0/1015	0.42	0/1357
12	LL	0.24	0/973	0.44	0/1305
13	MM	0.23	0/951	0.40	0/1274
14	NN	0.24	0/930	0.39	0/1243
15	OO	0.23	0/2243	0.37	0/3016
16	PP	0.24	0/806	0.42	0/1096
17	QQ	0.24	0/1268	0.39	0/1701
18	RR	0.24	0/1105	0.38	0/1491
19	SS	0.24	0/667	0.41	0/902
20	TT	0.23	0/762	0.36	0/1015
21	UU	0.24	0/1890	0.38	0/2554
22	VV	0.23	0/2121	0.37	0/2851
23	WW	0.24	0/2898	0.36	0/3911
24	XX	0.24	0/3235	0.40	0/4374
25	YY	0.24	0/797	0.40	0/1070
26	ZZ	0.24	0/2645	0.38	0/3566
27	11	0.24	0/686	0.40	0/929
28	22	0.22	0/302	0.39	0/388
29	33	0.24	0/1589	0.40	0/2140
30	44	0.24	0/2121	0.38	0/2879
30	55	0.24	0/1912	0.38	0/2600
31	66	0.24	0/2349	0.38	0/3163

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	77	0.25	0/1431	0.38	0/1934
33	88	0.24	0/3760	0.38	0/5085
34	00	0.22	0/409	0.34	0/540
34	99	0.21	0/307	0.32	0/405
35	aa	0.22	0/34270	0.66	0/53383
36	V	0.23	0/336	0.41	0/452
All	All	0.23	0/95673	0.51	0/136185

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2883	2907	2907	35	0
2	BB	2269	2301	2301	10	0
3	CC	3642	3897	3897	20	0
4	DD	2343	2373	2373	19	0
5	EE	2881	2918	2918	9	0
6	FF	936	966	966	4	0
7	GG	1725	1799	1799	9	0
8	HH	1236	1286	1286	5	0
9	II	1969	2026	2026	14	0
10	JJ	1551	1554	1554	8	0
11	KK	995	1025	1025	7	0
12	LL	959	1032	1032	6	0
13	MM	938	987	986	5	0
14	NN	915	961	961	7	0
15	OO	2199	2230	2230	7	0
16	PP	786	826	826	5	0
17	QQ	1247	1314	1314	10	0
18	RR	1080	1089	1089	6	0
19	SS	648	677	677	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	TT	747	772	772	6	0
21	UU	1844	1842	1842	12	0
22	VV	2081	2112	2112	14	0
23	WW	2844	2901	2900	10	0
24	XX	3176	3271	3271	11	0
25	YY	786	823	823	4	0
26	ZZ	2586	2528	2528	15	0
27	11	672	686	686	1	0
28	22	302	359	359	0	0
29	33	1554	1607	1607	4	0
30	44	2062	1983	1982	13	0
30	55	1858	1793	1793	12	0
31	66	2299	2330	2330	10	0
32	77	1400	1396	1396	2	0
33	88	3677	3650	3650	24	0
34	00	406	417	417	1	0
34	99	306	333	333	0	0
35	aa	30608	15376	15374	0	0
36	V	332	309	309	6	0
37	00	1	0	0	0	0
37	BB	1	0	0	0	0
37	KK	1	0	0	0	0
37	QQ	1	0	0	0	0
37	XX	1	0	0	0	0
37	YY	1	0	0	0	0
37	aa	91	0	0	0	0
38	XX	31	12	12	1	0
39	77	1	0	0	0	0
39	88	1	0	0	0	0
39	aa	20	0	0	0	0
All	All	90892	76668	76663	280	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 2.

All (280) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:359:GLN:OE1	2:BB:362:ARG:NH2	2.11	0.84
24:XX:152:ARG:NH1	24:XX:415:LYS:O	2.12	0.82
26:ZZ:212:ARG:NH1	26:ZZ:257:GLU:OE1	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:88:409:GLU:N	33:88:409:GLU:OE1	2.13	0.82
14:NN:22:ASP:OD2	14:NN:26:ARG:NH1	2.13	0.81
23:WW:44:VAL:O	23:WW:62:ARG:NH2	2.15	0.79
33:88:213:ARG:NH1	33:88:439:MET:O	2.16	0.78
5:EE:157:LYS:NZ	32:77:326:GLU:O	2.17	0.78
13:MM:23:TYR:OH	13:MM:119:GLY:OXT	2.01	0.78
29:33:158:VAL:O	29:33:163:ARG:NH2	2.17	0.78
17:QQ:94:ALA:O	17:QQ:101:ARG:NH2	2.18	0.77
30:44:208:ASP:O	30:44:212:SER:OG	2.02	0.77
4:DD:134:GLN:OE1	4:DD:442:ASN:ND2	2.19	0.76
33:88:166:LEU:O	33:88:190:THR:OG1	2.05	0.75
14:NN:75:ARG:NH1	14:NN:80:GLY:O	2.20	0.74
33:88:148:GLU:O	33:88:152:ASN:ND2	2.21	0.74
26:ZZ:140:ASN:ND2	26:ZZ:142:ASP:OD2	2.20	0.74
22:VV:136:GLU:OE2	22:VV:140:GLN:NE2	2.20	0.74
1:AA:204:THR:OG1	1:AA:208:ASN:OD1	2.07	0.73
11:KK:343:GLY:O	11:KK:350:ARG:NH2	2.22	0.72
33:88:42:ILE:O	33:88:101:ARG:NH2	2.22	0.71
1:AA:155:GLN:N	1:AA:155:GLN:OE1	2.23	0.71
24:XX:427:GLU:OE2	26:ZZ:330:LYS:NZ	2.23	0.71
13:MM:10:ASN:OD1	13:MM:11:GLU:N	2.24	0.70
24:XX:271:LEU:O	24:XX:275:ASN:ND2	2.23	0.70
1:AA:331:ARG:NH1	21:UU:190:MET:SD	2.65	0.70
18:RR:138:ARG:NH1	18:RR:144:GLU:OE2	2.26	0.69
4:DD:119:GLN:NE2	4:DD:120:VAL:O	2.25	0.69
23:WW:330:HIS:NE2	23:WW:370:GLU:OE2	2.25	0.69
18:RR:143:TYR:O	18:RR:148:ARG:NH1	2.26	0.68
15:OO:188:GLU:N	15:OO:188:GLU:OE1	2.27	0.68
1:AA:68:LYS:NZ	2:BB:337:ASN:OD1	2.27	0.68
11:KK:344:ASN:OD1	11:KK:347:ARG:NH2	2.27	0.68
9:II:117:GLU:N	9:II:117:GLU:OE1	2.27	0.67
15:OO:235:ARG:O	22:VV:207:ARG:NH2	2.28	0.67
23:WW:209:GLU:N	23:WW:209:GLU:OE1	2.27	0.67
1:AA:253:LEU:HD23	22:VV:316:LEU:HD22	1.77	0.66
10:JJ:83:GLU:OE1	10:JJ:83:GLU:N	2.28	0.66
1:AA:73:LEU:O	1:AA:77:THR:OG1	2.12	0.66
5:EE:138:SER:OG	5:EE:139:GLU:OE1	2.13	0.65
16:PP:70:ILE:HD11	16:PP:84:LEU:HD13	1.78	0.65
1:AA:146:THR:OG1	21:UU:150:ASP:OD1	2.13	0.65
2:BB:209:ARG:NH2	33:88:280:GLU:OE2	2.30	0.65
1:AA:377:ILE:O	21:UU:201:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FF:112:ARG:NH1	22:VV:278:GLU:OE1	2.30	0.65
30:55:127:ASP:OD2	30:55:291:LYS:NZ	2.20	0.64
25:YY:7:ARG:HG3	26:ZZ:287:ILE:HD11	1.79	0.64
3:CC:22:PHE:CE2	3:CC:26:ILE:HD11	2.32	0.64
26:ZZ:52:ASP:OD1	26:ZZ:53:ALA:N	2.31	0.64
9:II:232:SER:O	9:II:265:THR:OG1	2.14	0.64
20:TT:149:GLN:N	20:TT:152:LEU:O	2.30	0.64
30:44:141:PHE:O	30:44:145:ASN:ND2	2.31	0.64
7:GG:90:THR:OG1	7:GG:92:GLU:OE2	2.16	0.63
17:QQ:162:GLN:O	34:00:55:ARG:NH2	2.31	0.63
1:AA:142:ASP:OD1	1:AA:143:THR:HG23	1.98	0.63
30:44:181:GLN:N	30:44:181:GLN:OE1	2.31	0.63
1:AA:393:ASP:OD2	1:AA:395:THR:OG1	2.16	0.63
11:KK:345:GLU:N	11:KK:345:GLU:OE1	2.32	0.63
26:ZZ:50:GLU:OE1	26:ZZ:50:GLU:N	2.32	0.62
33:88:290:ASN:OD1	33:88:291:ILE:N	2.33	0.61
2:BB:205:ARG:NH2	33:88:282:SER:O	2.33	0.61
7:GG:194:ASN:OD1	24:XX:436:LYS:NZ	2.29	0.61
3:CC:439:ILE:HG22	3:CC:443:LEU:HD11	1.82	0.61
4:DD:186:GLY:O	31:66:158:ARG:NH1	2.33	0.61
30:44:175:ARG:HB2	30:44:252:ILE:HD11	1.83	0.61
30:55:95:ASP:OD1	30:55:98:SER:OG	2.11	0.61
4:DD:174:LYS:HD2	16:PP:48:THR:HG23	1.83	0.60
33:88:191:VAL:HG13	33:88:228:LEU:HD21	1.82	0.60
26:ZZ:212:ARG:O	26:ZZ:262:ASN:ND2	2.35	0.60
3:CC:135:ARG:NH2	26:ZZ:144:GLU:OE1	2.35	0.60
7:GG:92:GLU:N	7:GG:92:GLU:OE1	2.34	0.59
5:EE:291:ASP:OD1	5:EE:294:GLY:N	2.34	0.59
3:CC:224:LYS:NZ	5:EE:246:TYR:O	2.33	0.59
1:AA:190:GLU:N	1:AA:190:GLU:OE1	2.36	0.58
31:66:321:ASP:O	31:66:328:ARG:NH1	2.35	0.58
4:DD:384:ASP:OD1	4:DD:386:SER:OG	2.16	0.58
30:55:108:GLU:OE1	30:55:108:GLU:N	2.36	0.58
33:88:208:SER:OG	33:88:354:GLN:OE1	2.21	0.57
23:WW:214:LYS:NZ	23:WW:218:GLU:OE2	2.37	0.57
3:CC:199:GLU:N	3:CC:199:GLU:OE1	2.37	0.57
10:JJ:102:ARG:NH1	10:JJ:144:GLY:O	2.38	0.57
1:AA:317:PRO:O	30:55:105:ARG:NH1	2.37	0.57
30:44:95:ASP:OD1	30:44:96:THR:N	2.37	0.57
33:88:181:ALA:O	33:88:184:ARG:NH1	2.37	0.57
6:FF:1:MET:N	6:FF:69:ALA:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:88:339:GLU:OE1	33:88:343:ARG:NH2	2.37	0.57
7:GG:291:THR:O	7:GG:294:ARG:NH2	2.37	0.56
9:II:125:GLU:N	9:II:125:GLU:OE1	2.39	0.56
11:KK:356:VAL:HG12	20:TT:179:LEU:HD22	1.87	0.56
4:DD:105:PRO:O	4:DD:110:LYS:NZ	2.20	0.56
24:XX:361:THR:HG23	24:XX:365:SER:HB2	1.88	0.56
9:II:161:GLU:N	9:II:161:GLU:OE1	2.37	0.55
9:II:299:LYS:NZ	9:II:303:HIS:O	2.39	0.55
26:ZZ:59:ARG:NH1	26:ZZ:65:GLU:OE1	2.39	0.55
8:HH:65:GLU:OE1	8:HH:65:GLU:N	2.40	0.55
24:XX:257:HIS:NE2	24:XX:293:GLU:OE2	2.39	0.55
30:44:208:ASP:OD1	30:44:209:ALA:N	2.39	0.55
24:XX:394:TYR:OH	26:ZZ:288:PRO:O	2.21	0.55
31:66:208:SER:O	31:66:211:THR:OG1	2.25	0.55
1:AA:331:ARG:NH1	21:UU:193:GLU:OE1	2.40	0.55
4:DD:382:GLU:OE1	4:DD:382:GLU:N	2.40	0.54
5:EE:343:ASN:ND2	21:UU:24:ILE:O	2.40	0.54
13:MM:68:ASP:OD1	13:MM:71:ARG:NH2	2.40	0.54
6:FF:58:ASN:ND2	20:TT:153:ASN:OD1	2.40	0.54
23:WW:359:GLN:OE1	23:WW:363:ARG:NH1	2.40	0.54
31:66:248:GLU:N	31:66:248:GLU:OE1	2.37	0.54
14:NN:26:ARG:NH2	14:NN:74:ASN:OD1	2.40	0.54
3:CC:52:ILE:HD11	10:JJ:122:ARG:HB2	1.90	0.53
32:77:345:ILE:O	32:77:349:SER:OG	2.21	0.53
33:88:330:GLN:N	33:88:330:GLN:OE1	2.38	0.53
1:AA:123:GLU:N	1:AA:123:GLU:OE1	2.41	0.53
12:LL:113:ILE:HG12	12:LL:143:LEU:HD12	1.91	0.53
30:44:175:ARG:NH1	30:44:177:GLN:OE1	2.41	0.53
1:AA:153:GLN:N	1:AA:153:GLN:OE1	2.42	0.53
30:44:191:TYR:N	30:44:205:GLN:O	2.41	0.53
4:DD:104:GLU:OE1	4:DD:104:GLU:N	2.42	0.53
12:LL:134:GLN:OE1	12:LL:134:GLN:N	2.38	0.53
15:OO:161:GLU:OE1	15:OO:161:GLU:N	2.38	0.53
33:88:466:GLU:OE2	33:88:483:ARG:NH1	2.42	0.53
1:AA:298:THR:HG22	21:UU:89:ARG:O	2.09	0.52
2:BB:281:GLU:N	2:BB:281:GLU:OE1	2.40	0.52
8:HH:95:LEU:HD23	8:HH:160:VAL:HG22	1.91	0.52
23:WW:205:SER:OG	23:WW:211:GLU:OE1	2.21	0.52
18:RR:137:PRO:O	21:UU:196:THR:HG21	2.10	0.52
31:66:122:GLU:OE1	31:66:175:ARG:NH2	2.42	0.52
30:44:242:THR:OG1	30:44:248:ASP:OD2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:JJ:202:TYR:HB3	10:JJ:205:ILE:HD12	1.91	0.52
33:88:501:GLU:OE1	33:88:501:GLU:N	2.42	0.51
17:QQ:44:LYS:O	17:QQ:47:GLN:NE2	2.43	0.51
30:55:103:THR:HG22	30:55:109:LEU:HD13	1.93	0.51
1:AA:18:ARG:NH1	21:UU:102:ILE:O	2.42	0.51
3:CC:78:ILE:HD12	3:CC:246:ILE:HG23	1.93	0.51
25:YY:18:LEU:HD21	26:ZZ:273:MET:HG2	1.93	0.51
17:QQ:157:LYS:O	17:QQ:160:SER:OG	2.25	0.51
36:V:193:ASP:O	36:V:197:GLY:N	2.42	0.51
6:FF:112:ARG:NH2	22:VV:272:ASN:O	2.38	0.51
7:GG:274:GLU:OE1	7:GG:276:ARG:NE	2.38	0.50
11:KK:266:ASN:OD1	11:KK:267:THR:N	2.40	0.50
22:VV:63:GLU:OE1	31:66:245:ARG:NH2	2.42	0.50
5:EE:93:ALA:O	5:EE:97:ASN:ND2	2.43	0.50
30:55:169:GLY:O	30:55:257:THR:OG1	2.20	0.50
36:V:202:ASN:O	36:V:202:ASN:ND2	2.44	0.50
1:AA:158:GLU:OE1	1:AA:158:GLU:N	2.43	0.50
30:55:237:ASN:N	30:55:237:ASN:HD22	2.08	0.50
5:EE:135:ASP:OD1	5:EE:136:ASP:N	2.45	0.50
7:GG:90:THR:OG1	7:GG:93:ASN:OD1	2.28	0.50
1:AA:331:ARG:NH2	21:UU:194:ASN:OD1	2.38	0.50
4:DD:74:ARG:NH1	22:VV:69:GLU:OE1	2.42	0.50
1:AA:136:ARG:NH1	1:AA:142:ASP:OD2	2.44	0.49
3:CC:294:LEU:HD11	3:CC:457:LYS:HB3	1.94	0.49
36:V:106:GLU:OE2	36:V:117:ARG:NH2	2.43	0.49
18:RR:111:LEU:O	18:RR:114:SER:OG	2.26	0.49
22:VV:85:ILE:HD12	22:VV:142:LEU:HD13	1.94	0.49
5:EE:345:ASP:OD1	5:EE:378:ARG:NH1	2.46	0.49
3:CC:234:PHE:CD1	3:CC:258:ILE:HG21	2.48	0.48
4:DD:208:LEU:HD23	4:DD:208:LEU:O	2.13	0.48
15:OO:90:PHE:O	15:OO:93:SER:OG	2.29	0.48
19:SS:63:ASP:OD1	19:SS:64:LEU:N	2.46	0.48
33:88:447:GLY:O	33:88:476:ARG:NH1	2.46	0.48
1:AA:372:LYS:NZ	18:RR:114:SER:OG	2.42	0.48
36:V:117:ARG:NH2	36:V:125:ASP:OD2	2.46	0.48
3:CC:22:PHE:CE1	10:JJ:109:VAL:HG21	2.47	0.48
3:CC:342:ASN:OD1	3:CC:343:ASN:N	2.45	0.48
23:WW:380:ASP:OD1	23:WW:381:GLY:N	2.47	0.48
25:YY:8:LEU:HD23	26:ZZ:287:ILE:HD12	1.96	0.48
10:JJ:118:SER:OG	10:JJ:120:SER:O	2.31	0.47
12:LL:148:LEU:HD12	12:LL:148:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:WW:206:ASP:O	23:WW:268:ARG:NH1	2.47	0.47
1:AA:154:ILE:HD12	1:AA:154:ILE:N	2.30	0.47
2:BB:302:GLU:N	2:BB:302:GLU:OE1	2.48	0.47
30:44:209:ALA:O	30:55:105:ARG:NH2	2.47	0.47
1:AA:180:LEU:HA	1:AA:184:VAL:HG22	1.97	0.47
26:ZZ:96:ASP:OD1	26:ZZ:97:ASP:N	2.47	0.47
30:44:259:GLU:N	30:44:259:GLU:OE1	2.47	0.47
3:CC:198:THR:OG1	3:CC:199:GLU:OE1	2.31	0.47
26:ZZ:202:THR:HG22	26:ZZ:204:MET:H	1.79	0.47
3:CC:281:ASN:ND2	26:ZZ:131:GLU:OE2	2.47	0.47
4:DD:100:SER:O	5:EE:469:LYS:NZ	2.48	0.47
3:CC:294:LEU:HD23	3:CC:435:LEU:HD23	1.97	0.47
14:NN:67:THR:O	14:NN:67:THR:HG22	2.15	0.47
20:TT:155:ARG:O	20:TT:160:THR:OG1	2.30	0.47
33:88:471:HIS:O	33:88:475:THR:OG1	2.24	0.46
3:CC:321:GLU:OE1	3:CC:321:GLU:N	2.44	0.46
24:XX:161:LYS:NZ	24:XX:410:GLU:OE2	2.48	0.46
12:LL:59:ARG:O	12:LL:61:ARG:NH2	2.48	0.46
13:MM:26:GLY:O	13:MM:30:SER:OG	2.20	0.46
14:NN:32:ALA:HB3	14:NN:67:THR:HG23	1.98	0.46
30:55:58:ILE:HD12	30:55:58:ILE:H	1.80	0.46
33:88:380:SER:O	33:88:384:ASN:ND2	2.49	0.46
9:II:186:ASP:OD1	9:II:187:GLN:N	2.45	0.46
1:AA:185:ARG:NH1	22:VV:223:ASP:OD2	2.49	0.46
9:II:291:ARG:NH2	9:II:292:ASP:O	2.48	0.46
24:XX:201:VAL:HG23	24:XX:303:PRO:HG2	1.97	0.46
4:DD:422:ARG:NH2	4:DD:432:GLU:OE2	2.48	0.46
30:55:58:ILE:HD12	30:55:58:ILE:N	2.31	0.46
10:JJ:116:LEU:HD12	10:JJ:128:CYS:SG	2.56	0.45
17:QQ:69:ASP:OD1	17:QQ:70:VAL:N	2.49	0.45
3:CC:234:PHE:HD1	3:CC:258:ILE:HG21	1.82	0.45
1:AA:54:THR:HG22	1:AA:55:THR:N	2.30	0.45
8:HH:62:MET:O	22:VV:184:ARG:NE	2.42	0.45
11:KK:356:VAL:HG11	20:TT:176:LEU:HD23	1.98	0.45
22:VV:73:PRO:O	31:66:322:ARG:NH1	2.50	0.45
25:YY:58:LEU:HD13	25:YY:58:LEU:O	2.17	0.45
1:AA:152:GLU:O	1:AA:259:GLN:NE2	2.49	0.44
1:AA:136:ARG:NH2	30:55:149:GLY:O	2.51	0.44
2:BB:123:ASN:OD1	2:BB:124:PHE:N	2.50	0.44
17:QQ:65:LEU:HD11	17:QQ:87:VAL:HG21	1.99	0.44
24:XX:438:ARG:NH2	24:XX:440:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:II:197:ARG:HG3	9:II:198:LYS:H	1.81	0.44
9:II:248:VAL:HG12	9:II:250:VAL:HG23	1.98	0.44
14:NN:57:GLN:NE2	19:SS:16:PRO:O	2.50	0.44
21:UU:23:ASN:OD1	21:UU:24:ILE:N	2.51	0.44
21:UU:222:VAL:HG23	27:11:37:CYS:SG	2.58	0.44
29:33:83:LEU:O	29:33:106:ARG:NH2	2.40	0.44
15:OO:295:ARG:NH2	17:QQ:93:PRO:O	2.48	0.43
17:QQ:69:ASP:OD2	17:QQ:101:ARG:NH1	2.49	0.43
1:AA:201:ALA:HA	1:AA:204:THR:HG22	2.00	0.43
2:BB:227:ARG:NH2	2:BB:302:GLU:OE2	2.48	0.43
4:DD:93:GLU:OE1	4:DD:93:GLU:N	2.45	0.43
7:GG:206:VAL:CG1	7:GG:272:VAL:HG13	2.48	0.43
22:VV:256:ASN:O	22:VV:256:ASN:ND2	2.51	0.43
23:WW:193:GLU:OE2	23:WW:332:ARG:NH2	2.50	0.43
3:CC:271:LEU:CD2	3:CC:435:LEU:HD11	2.48	0.43
30:44:68:ASN:O	30:44:72:THR:OG1	2.30	0.43
30:55:65:GLY:O	30:55:264:ARG:NH1	2.51	0.43
1:AA:176:PHE:CE2	1:AA:180:LEU:HD11	2.54	0.43
21:UU:114:TRP:O	21:UU:133:ARG:NH2	2.49	0.43
1:AA:177:LYS:NZ	18:RR:163:GLY:O	2.46	0.43
23:WW:331:LEU:O	23:WW:335:SER:OG	2.29	0.43
31:66:132:VAL:HG11	31:66:157:ILE:CD1	2.49	0.43
2:BB:274:ASP:OD1	2:BB:362:ARG:NH1	2.52	0.42
2:BB:287:ARG:NH2	2:BB:288:ARG:O	2.52	0.42
33:88:317:LEU:HB2	33:88:337:LEU:HD21	2.01	0.42
9:II:160:GLN:NE2	9:II:164:ASP:OD1	2.52	0.42
30:44:252:ILE:HG22	30:44:292:VAL:HG13	2.01	0.42
24:XX:185:SER:OG	38:XX:501:ATP:O2B	2.37	0.42
29:33:93:VAL:O	29:33:99:ARG:NH1	2.51	0.42
36:V:189:ASP:N	36:V:189:ASP:OD1	2.52	0.42
36:V:207:LEU:N	36:V:207:LEU:HD12	2.35	0.42
8:HH:95:LEU:CD2	8:HH:160:VAL:HG22	2.50	0.42
12:LL:81:VAL:N	12:LL:100:ARG:O	2.45	0.42
16:PP:5:LEU:CD2	16:PP:22:VAL:HG22	2.50	0.42
33:88:388:THR:HG22	33:88:392:ILE:HD12	2.02	0.42
4:DD:413:GLN:OE1	4:DD:413:GLN:N	2.51	0.42
15:OO:218:ARG:NH2	17:QQ:100:GLU:OE2	2.46	0.42
33:88:115:GLU:N	33:88:115:GLU:OE1	2.53	0.41
3:CC:194:LEU:N	3:CC:194:LEU:HD22	2.35	0.41
31:66:209:TYR:CB	31:66:237:ILE:HD11	2.49	0.41
3:CC:107:VAL:O	3:CC:107:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:265:LEU:HD13	3:CC:297:ALA:HA	2.02	0.41
4:DD:209:LEU:O	4:DD:209:LEU:HD23	2.19	0.41
8:HH:143:GLU:O	8:HH:146:GLU:N	2.54	0.41
13:MM:95:LEU:O	13:MM:113:ASN:ND2	2.49	0.41
33:88:105:ALA:O	33:88:160:ARG:NE	2.51	0.41
17:QQ:80:SER:OG	17:QQ:81:LYS:N	2.53	0.41
9:II:190:ARG:CB	9:II:207:VAL:HG22	2.50	0.41
10:JJ:140:LEU:HD13	10:JJ:182:ILE:HD13	2.03	0.41
1:AA:232:GLU:O	1:AA:233:SER:OG	2.33	0.41
4:DD:138:ALA:N	4:DD:139:PRO:CD	2.83	0.41
7:GG:206:VAL:HG11	7:GG:272:VAL:HG13	2.03	0.41
9:II:149:ARG:O	9:II:152:SER:OG	2.31	0.41
4:DD:81:MET:HE2	31:66:240:VAL:HG21	2.02	0.41
9:II:229:ASP:OD2	9:II:257:THR:HG22	2.21	0.41
15:OO:87:THR:HG23	15:OO:87:THR:O	2.21	0.41
29:33:207:VAL:HG23	29:33:207:VAL:O	2.20	0.41
1:AA:55:THR:HG21	1:AA:65:TRP:HA	2.02	0.40
1:AA:55:THR:CG2	1:AA:65:TRP:HA	2.51	0.40
4:DD:174:LYS:CD	16:PP:48:THR:HG23	2.51	0.40
11:KK:356:VAL:HG12	20:TT:179:LEU:CD2	2.51	0.40
14:NN:9:LEU:HD21	14:NN:15:THR:HG21	2.03	0.40
16:PP:98:GLN:N	16:PP:99:PRO:CD	2.84	0.40
22:VV:120:GLN:OE1	22:VV:120:GLN:N	2.51	0.40
33:88:153:HIS:NE2	33:88:434:ASN:OD1	2.52	0.40
33:88:228:LEU:HD22	33:88:230:LYS:HE3	2.03	0.40
7:GG:227:VAL:CG1	7:GG:297:LEU:HD23	2.51	0.40
9:II:190:ARG:HB3	9:II:207:VAL:HG22	2.03	0.40
1:AA:257:VAL:HG13	22:VV:311:LEU:HD23	2.04	0.40
4:DD:121:ILE:N	4:DD:121:ILE:HD12	2.36	0.40
12:LL:109:ILE:C	12:LL:109:ILE:HD12	2.42	0.40
1:AA:248:ASN:OD1	1:AA:249:ASP:N	2.54	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	AA	360/470 (77%)	355 (99%)	5 (1%)	0	100	100
2	BB	288/428 (67%)	285 (99%)	3 (1%)	0	100	100
3	CC	432/508 (85%)	425 (98%)	7 (2%)	0	100	100
4	DD	286/453 (63%)	282 (99%)	4 (1%)	0	100	100
5	EE	363/477 (76%)	358 (99%)	5 (1%)	0	100	100
6	FF	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
7	GG	221/309 (72%)	218 (99%)	3 (1%)	0	100	100
8	HH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
9	II	245/315 (78%)	242 (99%)	3 (1%)	0	100	100
10	JJ	186/268 (69%)	181 (97%)	5 (3%)	0	100	100
11	KK	122/376 (32%)	118 (97%)	4 (3%)	0	100	100
12	LL	126/174 (72%)	119 (94%)	7 (6%)	0	100	100
13	MM	116/119 (98%)	112 (97%)	4 (3%)	0	100	100
14	NN	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
15	OO	272/320 (85%)	266 (98%)	6 (2%)	0	100	100
16	PP	96/107 (90%)	94 (98%)	2 (2%)	0	100	100
17	QQ	156/165 (94%)	155 (99%)	1 (1%)	0	100	100
18	RR	132/256 (52%)	130 (98%)	2 (2%)	0	100	100
19	SS	79/91 (87%)	78 (99%)	1 (1%)	0	100	100
20	TT	86/236 (36%)	85 (99%)	1 (1%)	0	100	100
21	UU	222/253 (88%)	219 (99%)	3 (1%)	0	100	100
22	VV	255/316 (81%)	253 (99%)	2 (1%)	0	100	100
23	WW	349/396 (88%)	345 (99%)	4 (1%)	0	100	100
24	XX	404/469 (86%)	399 (99%)	5 (1%)	0	100	100
25	YY	97/108 (90%)	95 (98%)	2 (2%)	0	100	100
26	ZZ	310/382 (81%)	309 (100%)	1 (0%)	0	100	100
27	11	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
28	22	31/344 (9%)	31 (100%)	0	0	100	100
29	33	191/236 (81%)	189 (99%)	2 (1%)	0	100	100
30	44	258/310 (83%)	253 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	55	228/310 (74%)	222 (97%)	6 (3%)	0	100	100
31	66	281/348 (81%)	279 (99%)	2 (1%)	0	100	100
32	77	177/414 (43%)	176 (99%)	1 (1%)	0	100	100
33	88	465/508 (92%)	452 (97%)	13 (3%)	0	100	100
34	00	46/95 (48%)	46 (100%)	0	0	100	100
34	99	34/95 (36%)	34 (100%)	0	0	100	100
36	V	39/219 (18%)	36 (92%)	3 (8%)	0	100	100
All	All	7422/10356 (72%)	7303 (98%)	119 (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	AA	314/393 (80%)	314 (100%)	0	100	100
2	BB	237/347 (68%)	234 (99%)	3 (1%)	69	88
3	CC	405/461 (88%)	404 (100%)	1 (0%)	93	98
4	DD	242/377 (64%)	241 (100%)	1 (0%)	91	96
5	EE	308/392 (79%)	308 (100%)	0	100	100
6	FF	99/99 (100%)	99 (100%)	0	100	100
7	GG	186/260 (72%)	184 (99%)	2 (1%)	73	90
8	HH	134/135 (99%)	133 (99%)	1 (1%)	84	94
9	II	206/263 (78%)	206 (100%)	0	100	100
10	JJ	166/227 (73%)	166 (100%)	0	100	100
11	KK	108/324 (33%)	108 (100%)	0	100	100
12	LL	103/142 (72%)	103 (100%)	0	100	100
13	MM	98/99 (99%)	97 (99%)	1 (1%)	76	91
14	NN	96/97 (99%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	OO	230/265 (87%)	229 (100%)	1 (0%)	91	96
16	PP	85/92 (92%)	85 (100%)	0	100	100
17	QQ	132/138 (96%)	132 (100%)	0	100	100
18	RR	118/218 (54%)	118 (100%)	0	100	100
19	SS	70/80 (88%)	70 (100%)	0	100	100
20	TT	75/191 (39%)	75 (100%)	0	100	100
21	UU	193/218 (88%)	193 (100%)	0	100	100
22	VV	224/268 (84%)	224 (100%)	0	100	100
23	WW	300/333 (90%)	300 (100%)	0	100	100
24	XX	345/391 (88%)	343 (99%)	2 (1%)	86	95
25	YY	83/89 (93%)	83 (100%)	0	100	100
26	ZZ	278/328 (85%)	278 (100%)	0	100	100
27	11	73/75 (97%)	73 (100%)	0	100	100
28	22	33/293 (11%)	33 (100%)	0	100	100
29	33	163/195 (84%)	163 (100%)	0	100	100
30	44	215/250 (86%)	214 (100%)	1 (0%)	88	96
30	55	195/250 (78%)	193 (99%)	2 (1%)	76	91
31	66	245/303 (81%)	245 (100%)	0	100	100
32	77	153/304 (50%)	153 (100%)	0	100	100
33	88	388/419 (93%)	387 (100%)	1 (0%)	92	97
34	00	43/78 (55%)	43 (100%)	0	100	100
34	99	34/78 (44%)	34 (100%)	0	100	100
36	V	33/170 (19%)	32 (97%)	1 (3%)	41	72
All	All	6410/8642 (74%)	6393 (100%)	17 (0%)	92	97

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BB	112	LYS
2	BB	114	LYS
2	BB	177	TRP
3	CC	363	VAL
4	DD	118	LYS
7	GG	198	TYR

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Mol	Chain	Res	Type
7	GG	287	HIS
8	HH	31	TYR
13	MM	66	GLU
15	OO	45	ARG
24	XX	307	PHE
24	XX	386	LYS
30	44	301	ARG
30	55	93	GLN
30	55	237	ASN
33	88	143	ASP
36	V	126	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	BB	303	ASN
4	DD	123	ASN
13	MM	8	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	aa	1430/1864 (76%)	174 (12%)	0

All (174) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	aa	49	U
35	aa	51	G
35	aa	54	G
35	aa	67	G
35	aa	77	A
35	aa	84	U
35	aa	92	C
35	aa	93	U
35	aa	96	A
35	aa	106	A
35	aa	113	G
35	aa	116	U
35	aa	118	A

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Mol	Chain	Res	Type
35	aa	249	G
35	aa	251	G
35	aa	255	U
35	aa	256	A
35	aa	268	A
35	aa	269	A
35	aa	270	U
35	aa	271	A
35	aa	278	C
35	aa	282	U
35	aa	302	U
35	aa	314	C
35	aa	318	A
35	aa	376	A
35	aa	380	G
35	aa	388	U
35	aa	389	C
35	aa	401	G
35	aa	416	G
35	aa	417	C
35	aa	430	U
35	aa	431	A
35	aa	441	G
35	aa	445	A
35	aa	446	A
35	aa	454	A
35	aa	455	G
35	aa	482	A
35	aa	483	A
35	aa	497	U
35	aa	503	C
35	aa	518	U
35	aa	540	A
35	aa	541	A
35	aa	556	G
35	aa	669	C
35	aa	670	G
35	aa	676	U
35	aa	677	U
35	aa	679	U
35	aa	684	U
35	aa	722	A

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Mol	Chain	Res	Type
35	aa	725	U
35	aa	737	U
35	aa	744	C
35	aa	756	G
35	aa	759	A
35	aa	773	A
35	aa	786	A
35	aa	790	A
35	aa	799	A
35	aa	802	G
35	aa	803	G
35	aa	828	A
35	aa	830	U
35	aa	849	A
35	aa	856	U
35	aa	861	A
35	aa	862	A
35	aa	871	U
35	aa	879	A
35	aa	880	G
35	aa	912	A
35	aa	921	G
35	aa	945	A
35	aa	952	G
35	aa	974	A
35	aa	978	A
35	aa	990	U
35	aa	1014	U
35	aa	1024	C
35	aa	1038	U
35	aa	1039	U
35	aa	1040	A
35	aa	1063	U
35	aa	1064	A
35	aa	1068	A
35	aa	1106	A
35	aa	1118	G
35	aa	1119	U
35	aa	1126	C
35	aa	1127	A
35	aa	1138	A
35	aa	1152	U

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Mol	Chain	Res	Type
35	aa	1161	C
35	aa	1164	C
35	aa	1167	A
35	aa	1168	A
35	aa	1169	A
35	aa	1184	U
35	aa	1185	G
35	aa	1336	A
35	aa	1357	U
35	aa	1358	C
35	aa	1385	U
35	aa	1386	U
35	aa	1392	G
35	aa	1393	A
35	aa	1426	U
35	aa	1437	U
35	aa	1475	A
35	aa	1476	A
35	aa	1480	A
35	aa	1492	A
35	aa	1493	U
35	aa	1504	A
35	aa	1505	U
35	aa	1506	A
35	aa	1512	G
35	aa	1518	U
35	aa	1526	A
35	aa	1527	A
35	aa	1529	A
35	aa	1537	G
35	aa	1538	C
35	aa	1539	A
35	aa	1553	U
35	aa	1559	A
35	aa	1566	A
35	aa	1579	A
35	aa	1580	A
35	aa	1581	U
35	aa	1582	A
35	aa	1583	U
35	aa	1584	A
35	aa	1585	C

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Mol	Chain	Res	Type
35	aa	1601	A
35	aa	1619	A
35	aa	1630	A
35	aa	1643	C
35	aa	1647	A
35	aa	1654	G
35	aa	1655	G
35	aa	1658	A
35	aa	1664	C
35	aa	1677	A
35	aa	1680	A
35	aa	1707	G
35	aa	1723	C
35	aa	1724	U
35	aa	1735	A
35	aa	1738	U
35	aa	1740	A
35	aa	1753	G
35	aa	1758	G
35	aa	1759	A
35	aa	1773	U
35	aa	1803	A
35	aa	1805	G
35	aa	1814	C
35	aa	1817	U
35	aa	1818	U
35	aa	1828	G
35	aa	1840	G
35	aa	1841	A
35	aa	1843	U
35	aa	1844	U
35	aa	1847	C
35	aa	1853	U
35	aa	1854	G
35	aa	1864	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 120 ligands modelled in this entry, 119 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	$\#\|Z\| > 2$
38	ATP	XX	501	37	26,33,33	3.42	1 (3%)	31,52,52	0.96	1 (3%)

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	XX	501	37	-	1/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	XX	501	ATP	C2'-C1'	-16.80	1.28	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	XX	501	ATP	C3'-C2'-C1'	3.67	106.50	100.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	XX	501	ATP	PA-O3A-PB-O2B

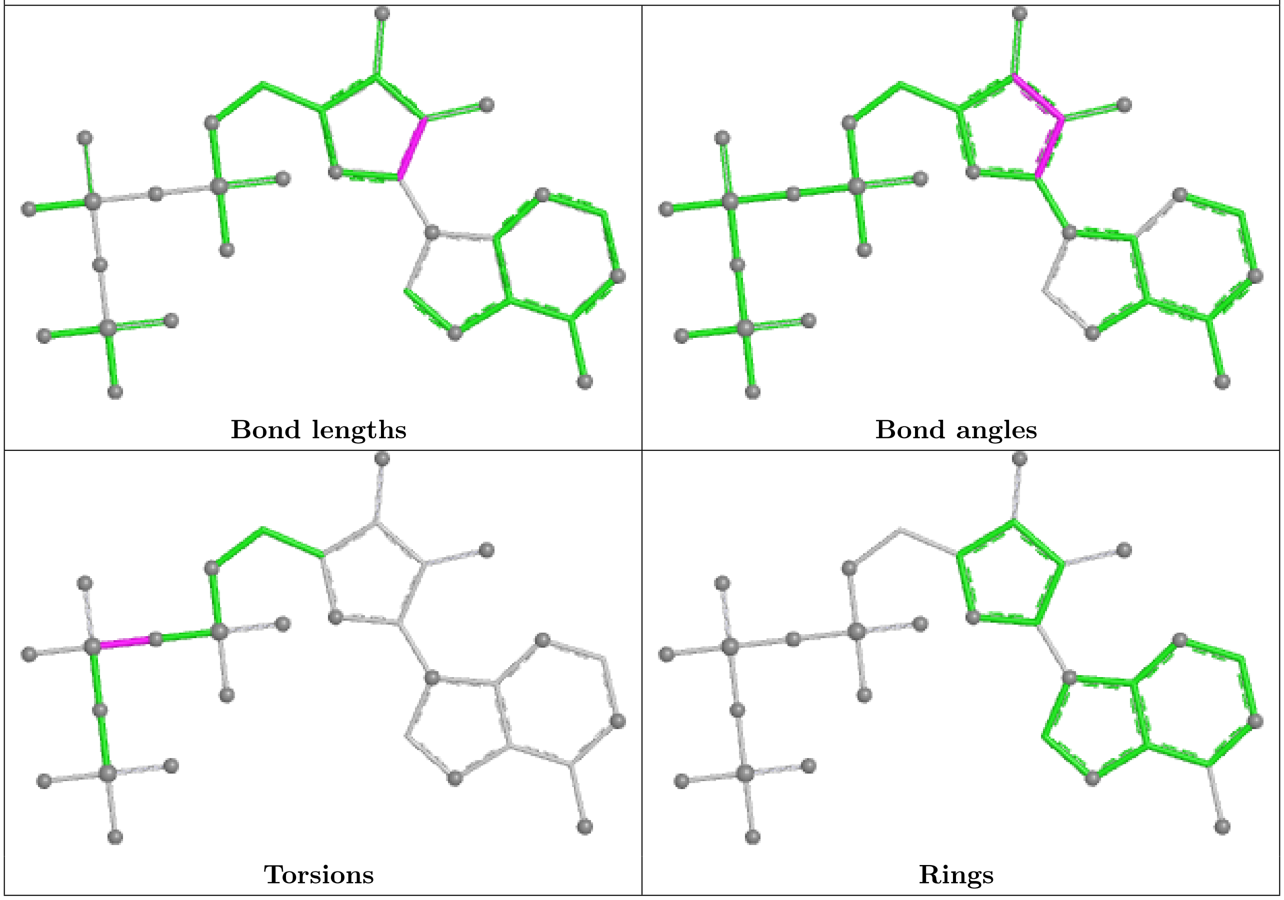
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	XX	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP XX 501



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

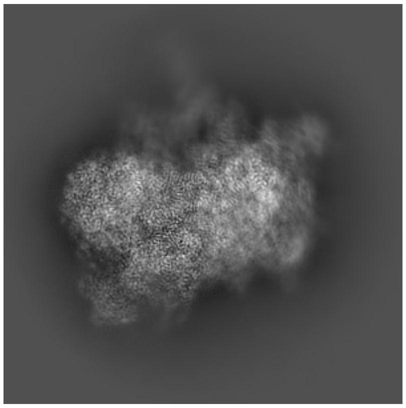
6 Map visualisation

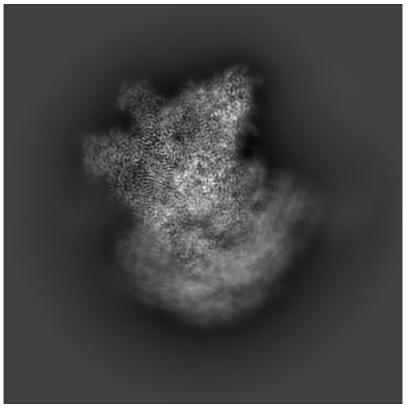
This section contains visualisations of the EMDB entry EMD-10958. These allow visual inspection of the internal detail of the map and identification of artifacts.

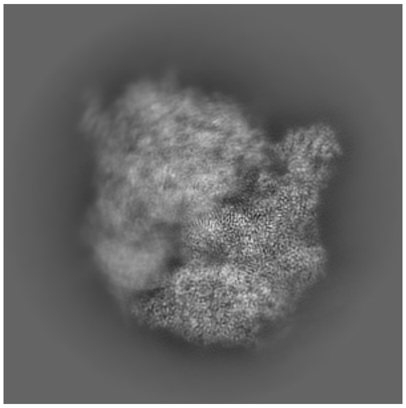
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

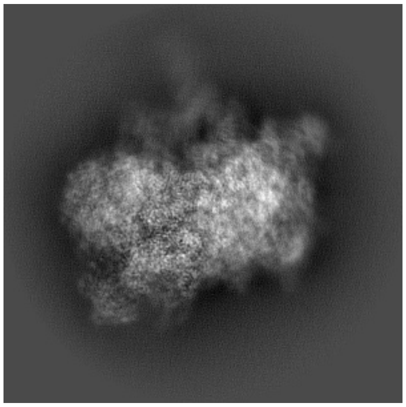
6.1.1 Primary map

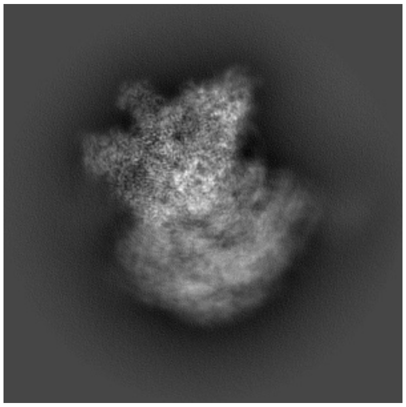

X

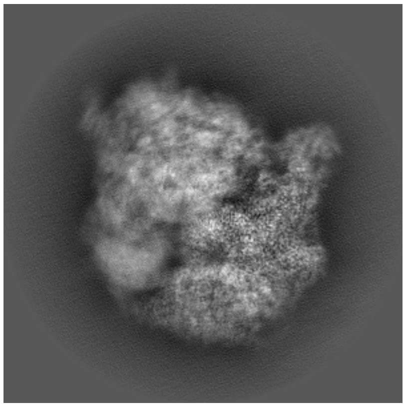

Y


Z

6.1.2 Raw map


X

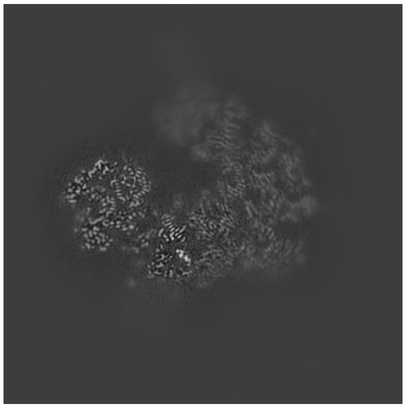

Y


Z

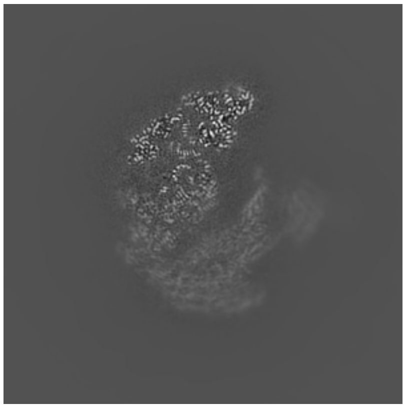
The images above show the map projected in three orthogonal directions.

6.2 Central slices

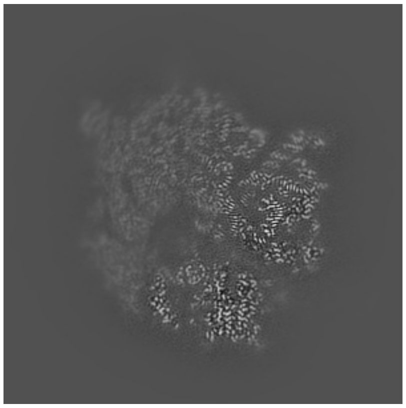
6.2.1 Primary map



X Index: 200

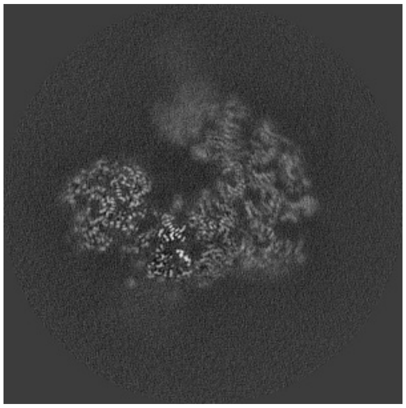


Y Index: 200

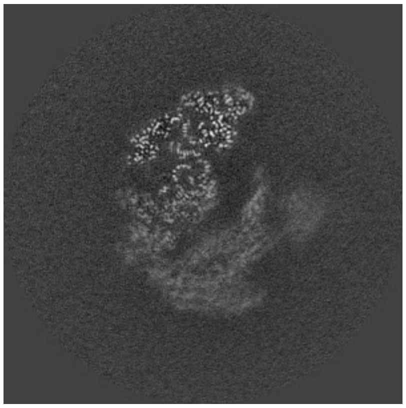


Z Index: 200

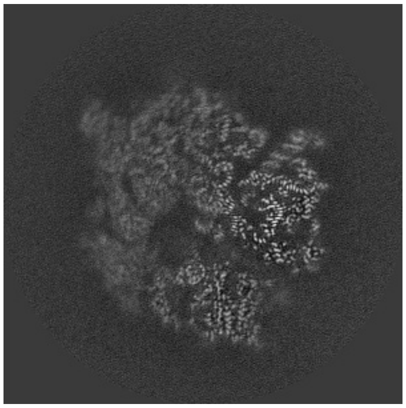
6.2.2 Raw map



X Index: 200



Y Index: 200

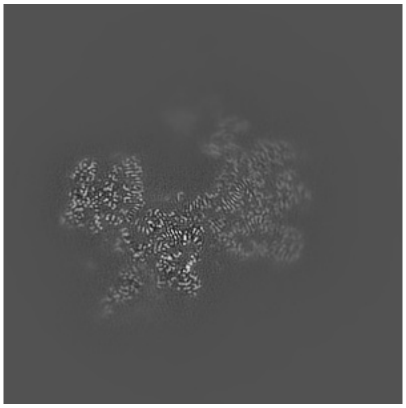


Z Index: 200

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

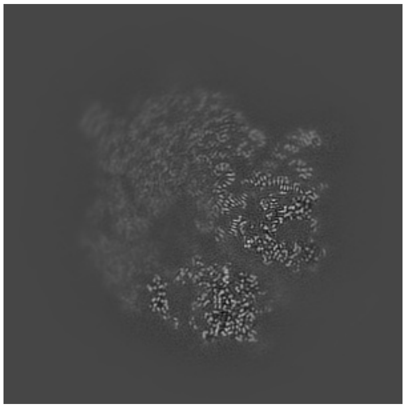
6.3 Largest variance slices ⓘ

6.3.1 Primary map



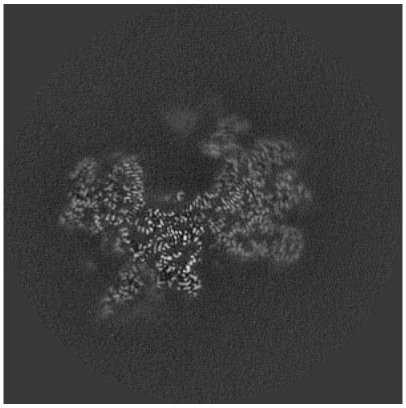
X Index: 225

Y Index: 181

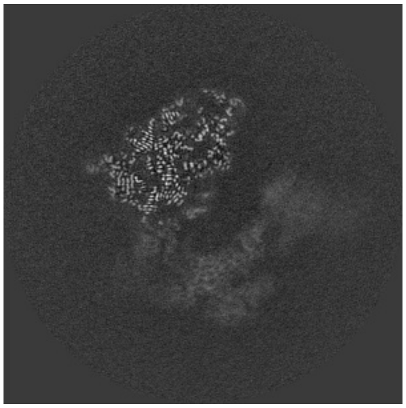


Z Index: 202

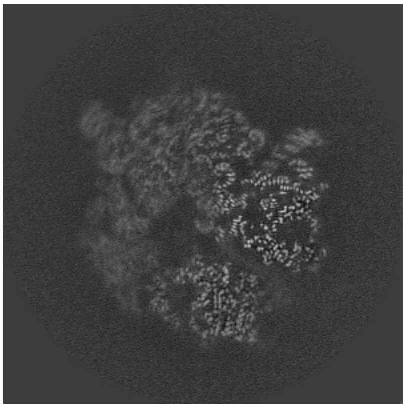
6.3.2 Raw map



X Index: 225



Y Index: 181



Z Index: 202

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X

Y

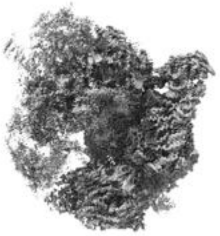
Z

The images above show the 3D surface view of the map at the recommended contour level 3.74. 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.

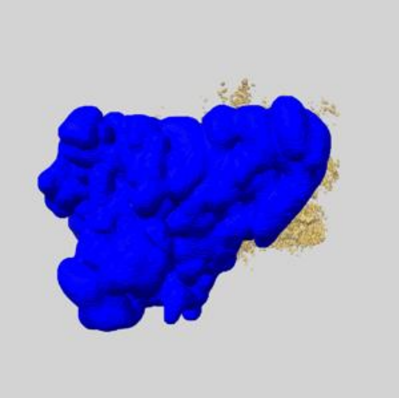
6.5 Mask visualisation ⓘ

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

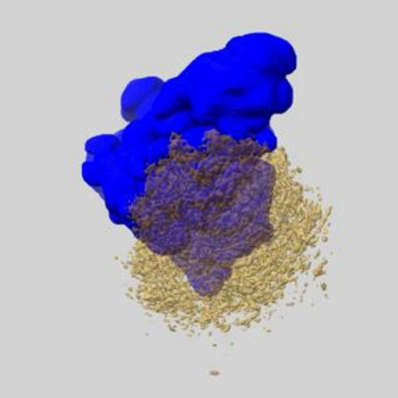
A mask typically either:

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

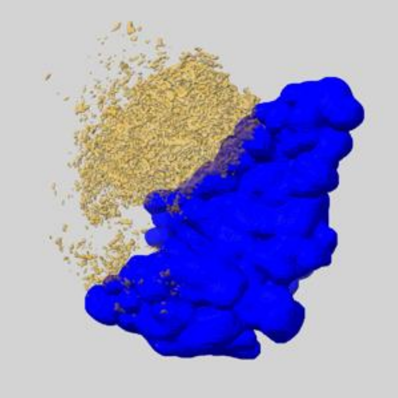
6.5.1 emd_10958_msk_1.map ⓘ



X



Y

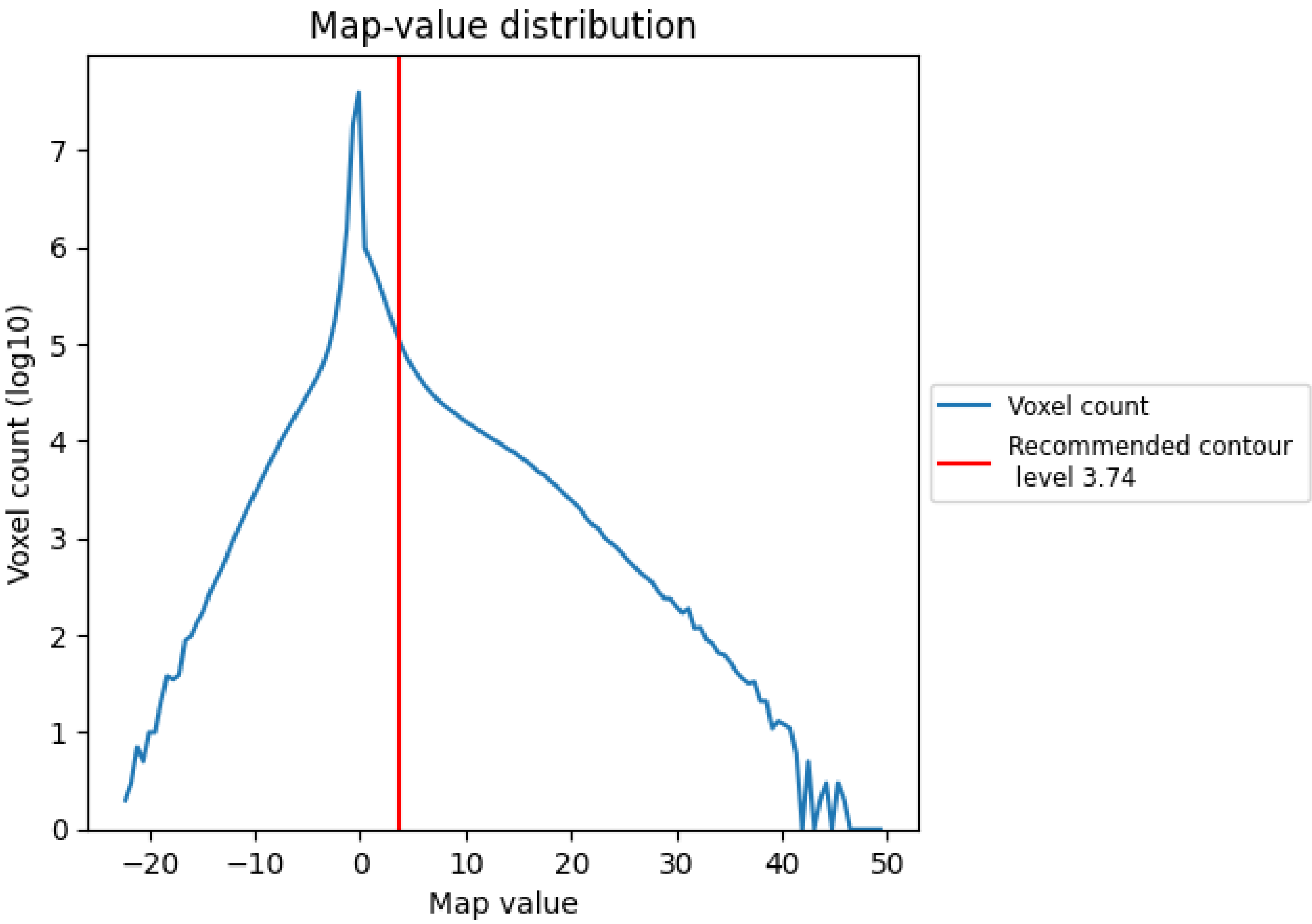


Z

7 Map analysis ⓘ

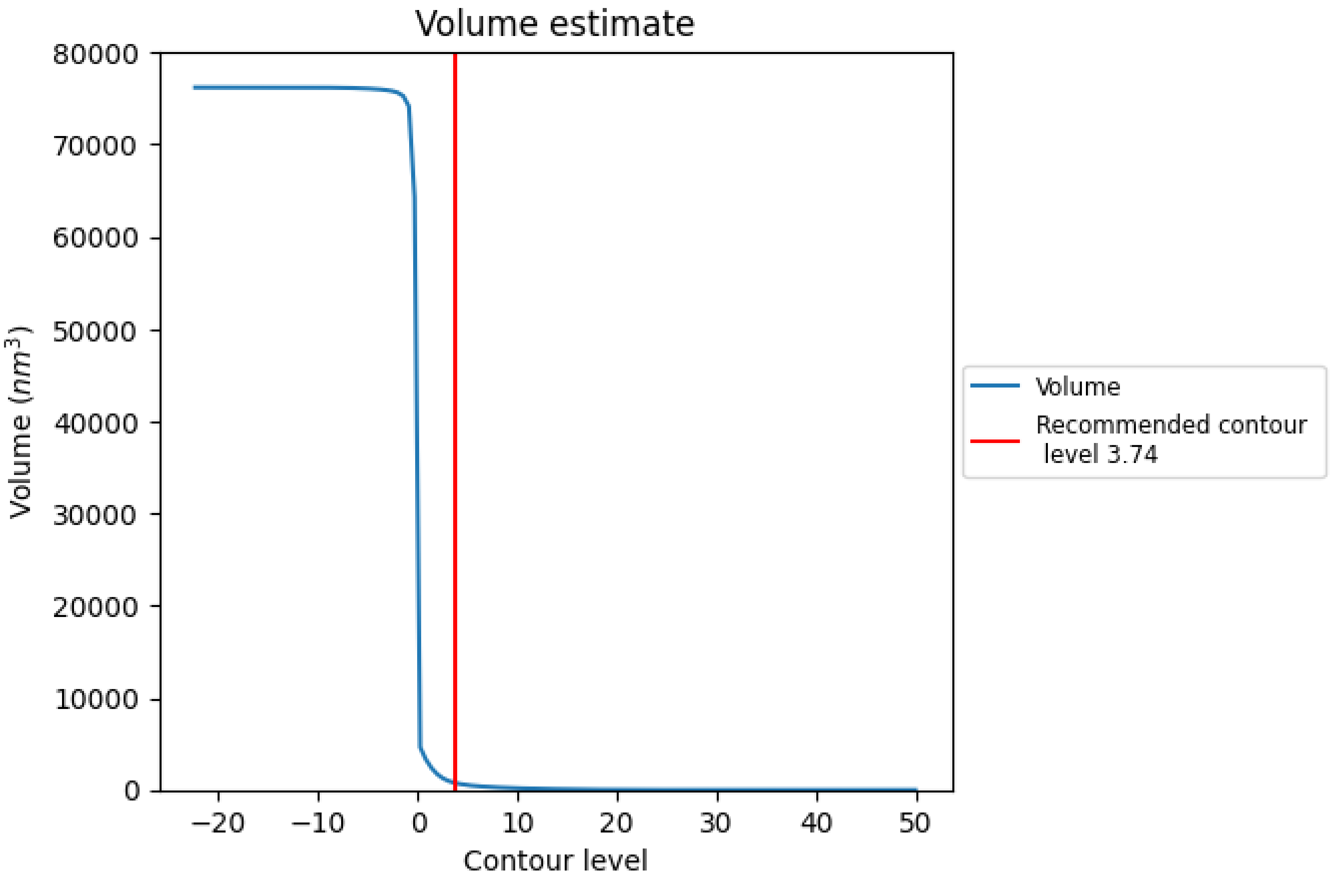
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

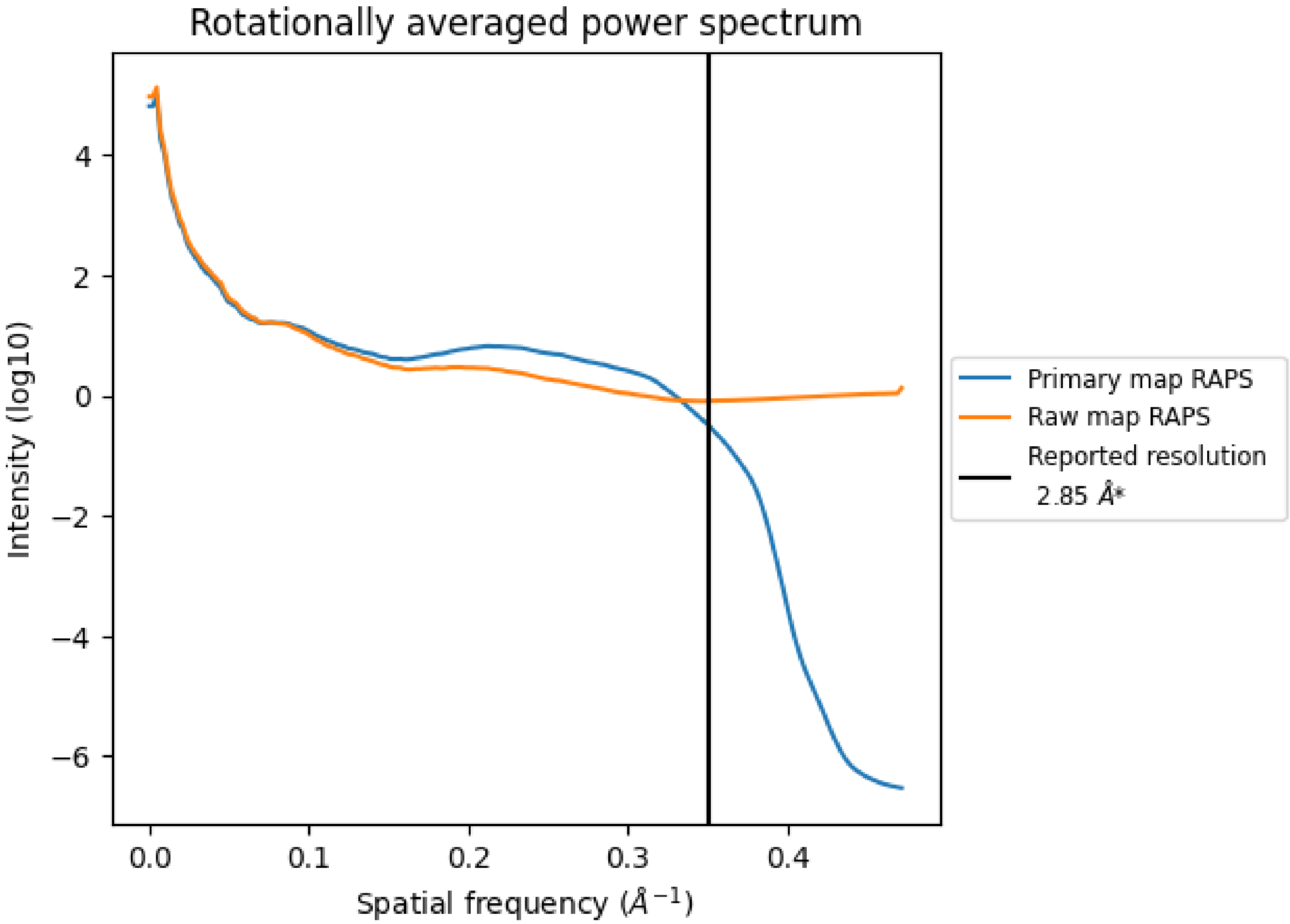
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 765 nm^3; this corresponds to an approximate mass of 691 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 ⓘ

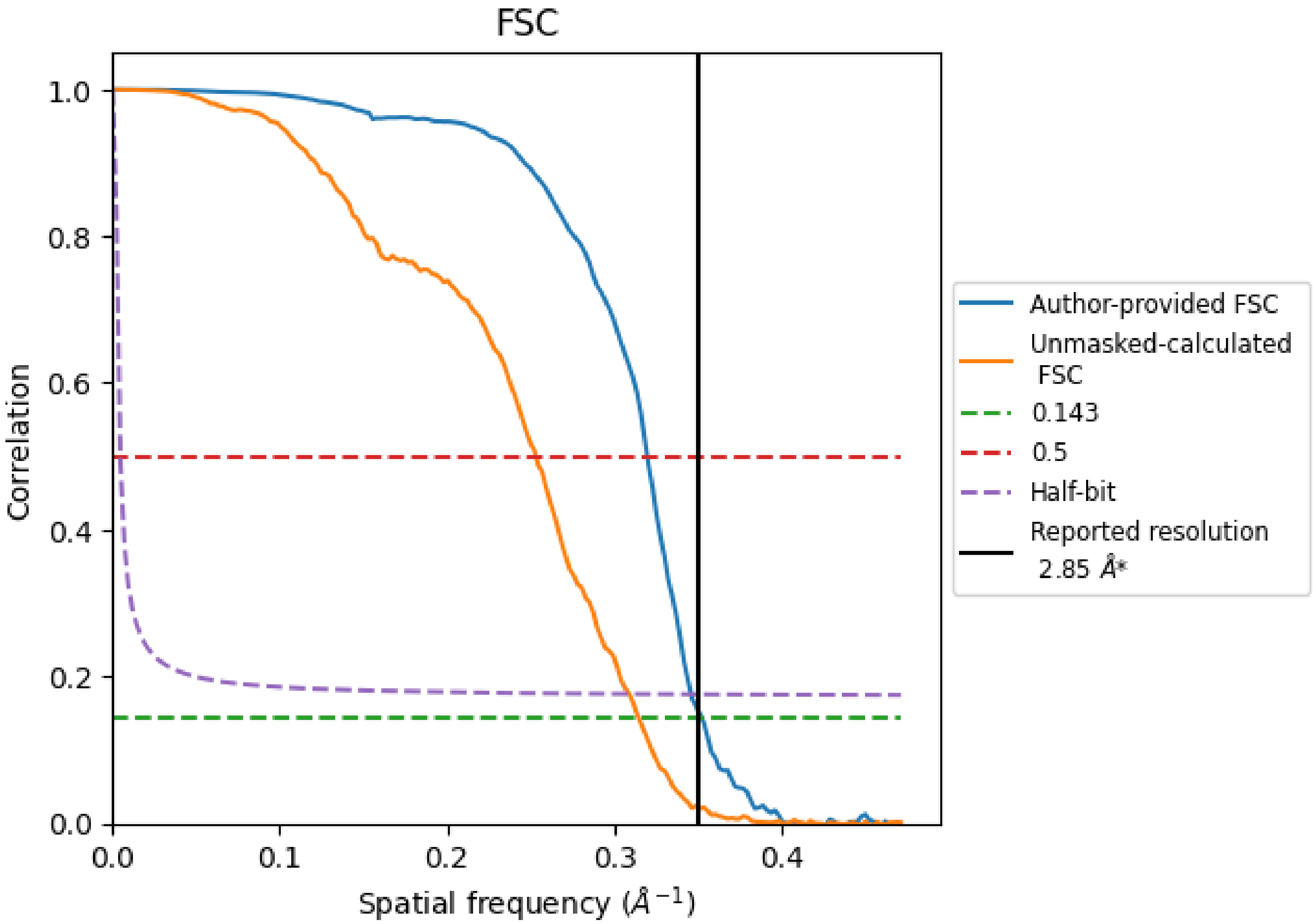


*Reported resolution corresponds to spatial frequency of 0.351 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.351 $Å^{-1}$

8.2 Resolution estimates ⓘ

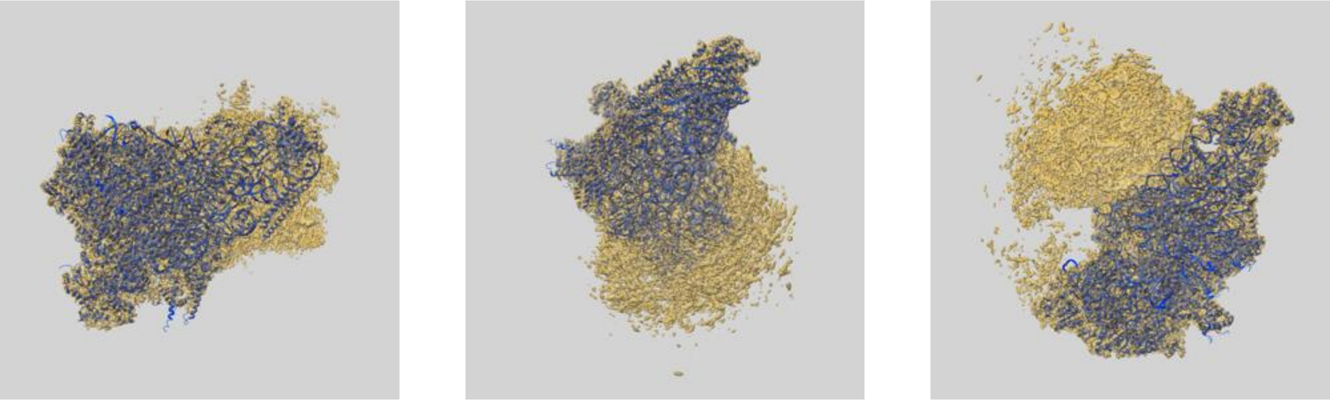
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.84	3.13	2.89
Unmasked-calculated*	3.18	3.95	3.24

*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 3.18 differs from the reported value 2.85 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10958 and PDB model 6YW5. Per-residue inclusion information can be found in section 3 on page 12.

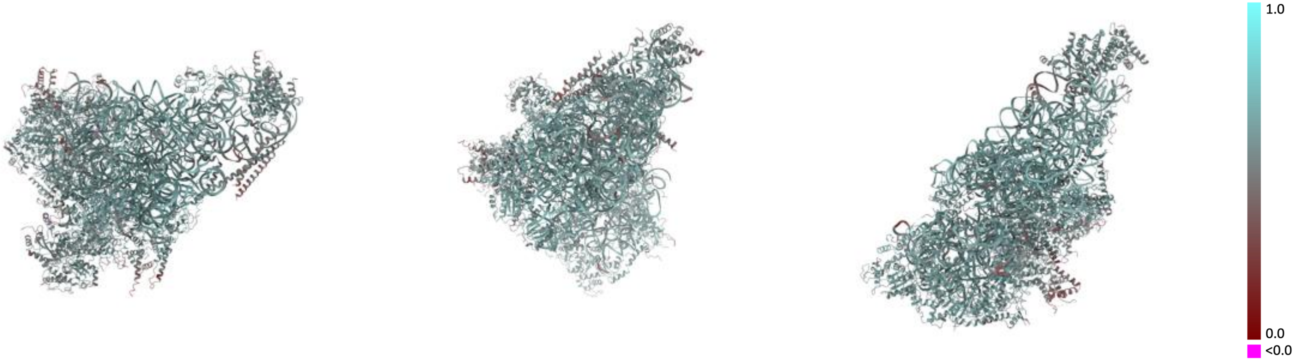
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.74 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.

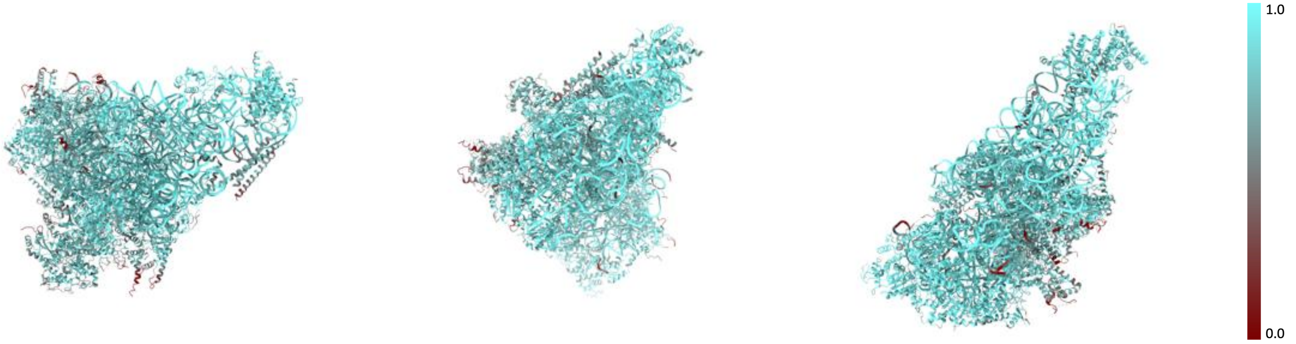
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

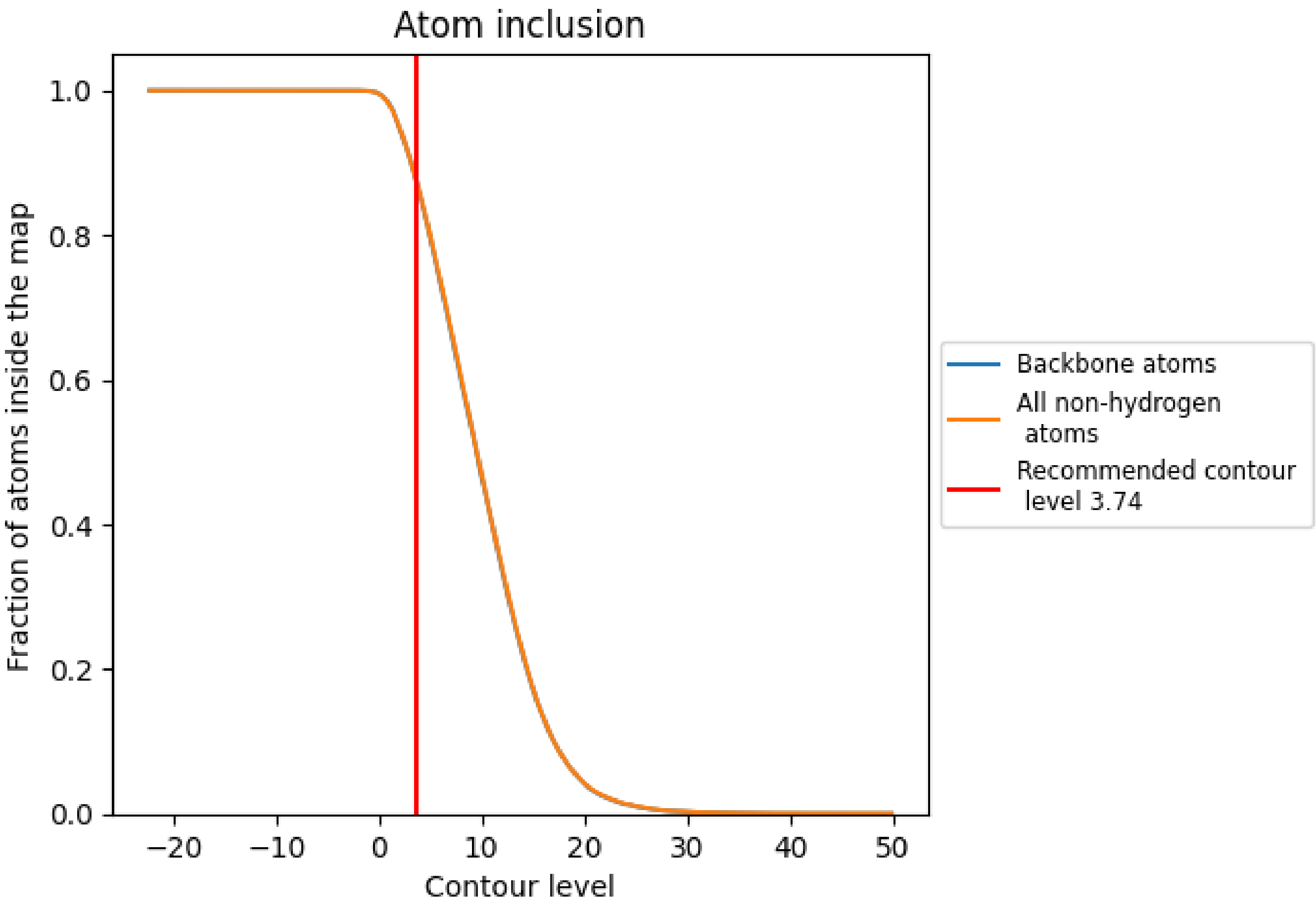
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.74).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 87% 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 (3.74) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8715	0.5920
00	0.6667	0.4860
11	0.8021	0.5780
22	0.8947	0.6220
33	0.8837	0.5730
44	0.7455	0.5390
55	0.7077	0.5290
66	0.8396	0.5910
77	0.8654	0.5860
88	0.8104	0.5720
99	0.5300	0.4110
AA	0.7004	0.5410
BB	0.8563	0.6010
CC	0.8362	0.5770
DD	0.8605	0.6040
EE	0.8609	0.5970
FF	0.9096	0.6270
GG	0.8410	0.5760
HH	0.9262	0.6370
II	0.8614	0.5820
JJ	0.9297	0.6160
KK	0.9092	0.6190
LL	0.9009	0.6170
MM	0.9142	0.6030
NN	0.9613	0.6370
OO	0.8320	0.5920
PP	0.9163	0.6250
QQ	0.8339	0.5910
RR	0.7727	0.5670
SS	0.8630	0.5930
TT	0.8869	0.6300
UU	0.8316	0.5920
V	0.5759	0.5110
VV	0.7702	0.5670
WW	0.8879	0.5500

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Chain	Atom inclusion	Q-score
XX	0.8999	0.5870
YY	0.8765	0.5980
ZZ	0.7972	0.5470
aa	0.9502	0.6150