



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 01:55 PM UTC

PDB ID : 6HIW / pdb_00006hiw
EMDB ID : EMD-0230
Title : Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the complete small mitoribosomal subunit in complex with mt-IF-3
Authors : Ramrath, D.; Niemann, M.; Leibundgut, M.; Bieri, P.; Prange, C.; Horn, E.K.; Leitner, A.; Boehringer, D.; Schneider, A.; Ban, N.
Deposited on : 2018-08-31
Resolution : 3.37 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

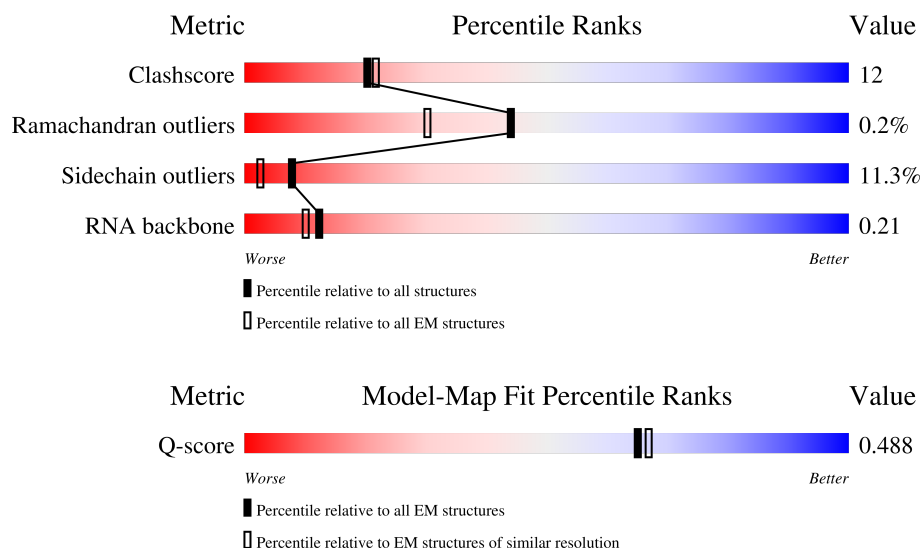
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



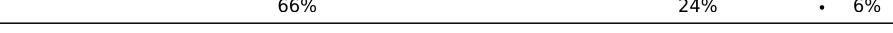
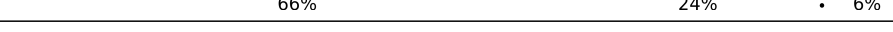
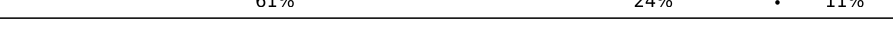
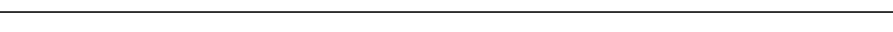
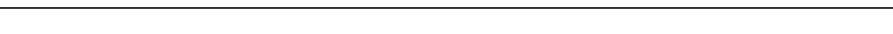
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14287 (2.87 - 3.87)

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	DA	1788	
2	DD	812	

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Mol	Chain	Length	Quality of chain
3	DI	407	
4	DL	307	
5	DM	294	
6	DN	293	
7	DO	282	
8	DP	274	
9	DQ	268	
10	DR	270	
11	DS	261	
12	DU	228	
13	DZ	94	
14	Da	64	
15	DB	1181	
16	DC	1165	
17	DE	747	
18	DF	666	
19	DG	631	
20	DH	581	
21	DJ	396	
22	DK	324	
23	DT	247	
24	DV	183	
25	DW	179	
26	DX	169	
27	DY	163	

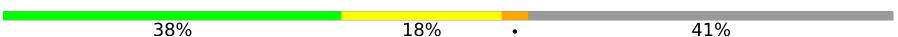
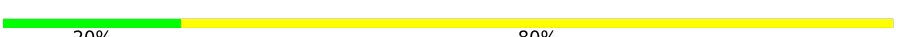
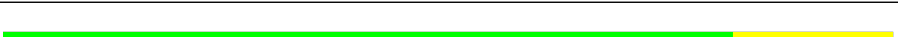
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Mol	Chain	Length	Quality of chain
28	CC	74	
29	CE	435	
30	CF	160	
31	CH	282	
32	CI	443	
33	CJ	817	
34	CK	326	
35	CL	87	
36	CN	166	
37	CO	429	
38	CP	188	
39	CQ	307	
40	CR	320	
41	CS	244	
42	CU	193	
43	CZ	360	
44	Ca	602	
45	Cb	325	
46	Cd	440	
47	Cg	498	
48	Ci	181	
49	Cj	257	
50	Ck	874	
51	Cm	215	
52	Cn	250	

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Mol	Chain	Length	Quality of chain
53	Cp	187	
54	Cq	263	
55	Cr	439	
56	Cv	1211	
57	CA	621	
58	UO	5	
59	UP	7	
60	UQ	32	
61	UR	8	
62	US	54	
63	UT	44	

2 Entry composition [i](#)

There are 70 unique types of molecules in this entry. The entry contains 177122 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 mS48.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DA	1557	Total	C	N	O	S	0	0
			12482	7881	2226	2337	38		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	894	HIS	ASN	conflict	UNP Q57UJ2
DA	1181	THR	ILE	conflict	UNP Q57UJ2
DA	1333	ALA	VAL	conflict	UNP Q57UJ2
DA	1700	ARG	HIS	conflict	UNP Q57UJ2
DA	1761	LYS	ARG	conflict	UNP Q57UJ2

- Molecule 2 is a protein called mS51.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DD	791	Total	C	N	O	S	0	0
			6523	4127	1184	1171	41		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DD	371	PRO	SER	conflict	UNP Q385L8
DD	599	ALA	VAL	conflict	UNP Q385L8

- Molecule 3 is a protein called mS56.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DI	390	Total	C	N	O	S	0	0
			3182	2020	554	594	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	92	GLU	GLY	conflict	UNP Q587C2
DI	116	ASP	GLU	conflict	UNP Q587C2

- Molecule 4 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	DL	283	Total	C	N	O	S	0	0
			2287	1451	423	401	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DL	274	THR	ALA	conflict	UNP Q38BS2

- Molecule 5 is a protein called mS60.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	DM	294	Total	C	N	O	S	0	0
			2430	1533	459	426	12		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DM	69	PHE	TYR	conflict	UNP Q57XL2
DM	97	ASN	SER	conflict	UNP Q57XL2
DM	138	SER	PRO	conflict	UNP Q57XL2
DM	173	ALA	THR	conflict	UNP Q57XL2
DM	206	ALA	THR	conflict	UNP Q57XL2

- Molecule 6 is a protein called mS61.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DN	257	Total	C	N	O	S	0	0
			2091	1331	379	371	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DN	51	GLY	SER	conflict	UNP Q38D60

- Molecule 7 is a protein called mS62.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	DO	222	Total	C	N	O	S	0	0
			1804	1127	327	340	10		

- Molecule 8 is a protein called mS63.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	DP	189	Total	C	N	O	S	0	0
			1613	1037	290	277	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DP	3	HIS	ARG	conflict	UNP Q38F25

- Molecule 9 is a protein called mS64.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	DQ	256	Total	C	N	O	S	0	0
			2061	1293	389	370	9		

- Molecule 10 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	DR	251	Total	C	N	O	S	0	0
			2025	1304	369	342	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DR	65	GLY	SER	conflict	UNP Q57UA2
DR	94	GLY	GLU	conflict	UNP Q57UA2
DR	128	PRO	SER	conflict	UNP Q57UA2
DR	229	ARG	GLN	conflict	UNP Q57UA2

- Molecule 11 is a protein called mS66.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	DS	238	Total	C	N	O	S	0	0
			1904	1185	356	348	15		

- Molecule 12 is a protein called mS68.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	DU	213	Total	C	N	O	S	0	0
			1754	1103	310	335	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DU	119	ILE	LEU	conflict	UNP Q582T9
DU	152	ILE	VAL	conflict	UNP Q582T9

- Molecule 13 is a protein called mS73.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	DZ	82	Total	C	N	O	S	0	0
			697	457	113	123	4		

- Molecule 14 is a protein called mS74.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Da	55	Total	C	N	O	S	0	0
			501	315	109	74	3		

- Molecule 15 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DB	1111	Total	C	N	O	S	0	0
			9148	5691	1717	1711	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	23	VAL	ALA	conflict	UNP Q586P5
DB	359	ILE	THR	conflict	UNP Q586P5
DB	384	GLN	HIS	conflict	UNP Q586P5
DB	402	THR	ILE	conflict	UNP Q586P5
DB	423	THR	ALA	conflict	UNP Q586P5
DB	586	ARG	HIS	conflict	UNP Q586P5
DB	593	ARG	LYS	conflict	UNP Q586P5
DB	647	SER	GLY	conflict	UNP Q586P5

- Molecule 16 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	DC	1095	Total	C	N	O	S	0	0
			8748	5519	1544	1654	31		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	53	ALA	THR	conflict	UNP Q57YB5
DC	365	LYS	GLU	conflict	UNP Q57YB5
DC	385	THR	ALA	conflict	UNP Q57YB5
DC	405	ILE	VAL	conflict	UNP Q57YB5
DC	641	SER	PRO	conflict	UNP Q57YB5
DC	651	LYS	GLU	conflict	UNP Q57YB5
DC	731	GLU	ASP	conflict	UNP Q57YB5
DC	814	GLN	HIS	conflict	UNP Q57YB5
DC	1097	ALA	VAL	conflict	UNP Q57YB5
DC	1113	THR	ILE	conflict	UNP Q57YB5

- Molecule 17 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	DE	590	Total	C	N	O	S	0	0
			4831	3075	874	863	19		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DE	514	THR	SER	conflict	UNP Q386Q7

- Molecule 18 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	DF	590	Total	C	N	O	S	0	0
			4747	2979	896	847	25		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DF	18	THR	ALA	conflict	UNP Q38ET1
DF	258	ASP	ASN	conflict	UNP Q38ET1
DF	372	ASN	ASP	conflict	UNP Q38ET1
DF	406	ASN	SER	conflict	UNP Q38ET1
DF	510	ASP	GLY	conflict	UNP Q38ET1

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Chain	Residue	Modelled	Actual	Comment	Reference
DF	577	ALA	VAL	conflict	UNP Q38ET1
DF	636	UNK	GLY	conflict	UNP Q38ET1
DF	638	LYS	ARG	conflict	UNP Q38ET1

- Molecule 19 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DG	566	Total	C	N	O	S	0	0
			4575	2875	835	834	31		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DG	428	ASN	SER	conflict	UNP Q57ZP8
DG	429	GLY	SER	conflict	UNP Q57ZP8

- Molecule 20 is a protein called mS55.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DH	564	Total	C	N	O	S	0	0
			4578	2872	850	834	22		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DH	191	HIS	GLN	conflict	UNP Q580V1
DH	194	PRO	ARG	conflict	UNP Q580V1
DH	488	GLY	SER	conflict	UNP Q580V1

- Molecule 21 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	DJ	315	Total	C	N	O	S	0	0
			2572	1646	452	460	14		

- Molecule 22 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DK	255	Total	C	N	O	S	0	0
			2007	1260	365	377	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DK	61	SER	PRO	conflict	UNP Q38BP1
DK	257	GLY	SER	conflict	UNP Q38BP1

- Molecule 23 is a protein called mS67.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	DT	239	Total	C	N	O	S	0	0
			2058	1321	364	362	11		

- Molecule 24 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	DV	160	Total	C	N	O	S	0	0
			1346	855	252	235	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DV	163	ALA	THR	conflict	UNP Q57UZ6

- Molecule 25 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	DW	161	Total	C	N	O	S	0	0
			1359	866	260	228	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DW	74	THR	MET	conflict	UNP Q383N9

- Molecule 26 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	DX	141	Total	C	N	O	S	0	0
			1196	762	226	201	7		

- Molecule 27 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	DY	154	Total	C	N	O	S	0	0
			1293	827	245	216	5		

- Molecule 28 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CC	74	Total	C	N	O	S	0	0
			646	451	96	98	1		

- Molecule 29 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CE	417	Total	C	N	O	S	0	0
			3399	2151	632	600	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	341	ARG	LYS	conflict	UNP Q38AX6

- Molecule 30 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CF	159	Total	C	N	O	S	0	0
			1292	821	228	237	6		

- Molecule 31 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CH	273	Total	C	N	O	S	0	0
			2228	1387	432	398	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CH	74	ASN	SER	conflict	UNP Q388R7

- Molecule 32 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CI	424	Total	C	N	O	S	0	0
			3386	2136	611	622	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	370	ALA	VAL	conflict	UNP Q57W62

- Molecule 33 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CJ	800	Total	C	N	O	S	0	0
			6516	4119	1151	1216	30		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	311	LEU	TYR	conflict	UNP Q57Z45
CJ	484	HIS	ARG	conflict	UNP Q57Z45
CJ	488	SER	ASN	conflict	UNP Q57Z45
CJ	594	GLU	VAL	conflict	UNP Q57Z45
CJ	629	ARG	LYS	conflict	UNP Q57Z45

- Molecule 34 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	CK	293	Total	C	N	O	S	0	0
			2418	1506	458	437	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	conflict	UNP Q389T7
CK	138	UNK	ILE	conflict	UNP Q389T7

- Molecule 35 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	CL	87	Total	C	N	O	S	0	0
			733	503	113	107	10		

- Molecule 36 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	CN	157	Total	C	N	O	S	0	0
			1322	843	251	220	8		

- Molecule 37 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	CO	361	Total	C	N	O	S	0	0
			3003	1907	560	520	16		

- Molecule 38 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	CP	180	Total	C	N	O	S	0	0
			1489	956	274	250	9		

- Molecule 39 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	CQ	190	Total	C	N	O	S	0	0
			1584	1015	302	259	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CQ	138	ALA	VAL	conflict	UNP Q38DP8

- Molecule 40 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	CR	314	Total	C	N	O	S	0	0
			2567	1623	471	465	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CR	8	ILE	VAL	conflict	UNP Q38AS2

- Molecule 41 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	CS	142	Total	C	N	O	S	0	0
			1175	761	210	198	6		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CS	-71	MET	-	initiating methionine	UNP Q584T8
CS	-70	ALA	-	expression tag	UNP Q584T8
CS	-69	PHE	-	expression tag	UNP Q584T8
CS	-68	ARG	-	expression tag	UNP Q584T8
CS	-67	ASN	-	expression tag	UNP Q584T8
CS	-66	THR	-	expression tag	UNP Q584T8
CS	-65	PHE	-	expression tag	UNP Q584T8
CS	-64	THR	-	expression tag	UNP Q584T8
CS	-63	THR	-	expression tag	UNP Q584T8
CS	-62	PRO	-	expression tag	UNP Q584T8
CS	-61	GLY	-	expression tag	UNP Q584T8
CS	-60	LYS	-	expression tag	UNP Q584T8
CS	-59	PHE	-	expression tag	UNP Q584T8
CS	-58	SER	-	expression tag	UNP Q584T8
CS	-57	THR	-	expression tag	UNP Q584T8
CS	-56	VAL	-	expression tag	UNP Q584T8
CS	-55	SER	-	expression tag	UNP Q584T8
CS	-54	LYS	-	expression tag	UNP Q584T8
CS	-53	ASN	-	expression tag	UNP Q584T8
CS	-52	ILE	-	expression tag	UNP Q584T8
CS	-51	VAL	-	expression tag	UNP Q584T8
CS	-50	LEU	-	expression tag	UNP Q584T8
CS	-49	LEU	-	expression tag	UNP Q584T8
CS	-48	LEU	-	expression tag	UNP Q584T8
CS	-47	ILE	-	expression tag	UNP Q584T8
CS	-46	TRP	-	expression tag	UNP Q584T8
CS	-45	ARG	-	expression tag	UNP Q584T8
CS	-44	VAL	-	expression tag	UNP Q584T8
CS	-43	LYS	-	expression tag	UNP Q584T8
CS	-42	VAL	-	expression tag	UNP Q584T8
CS	-41	PHE	-	expression tag	UNP Q584T8
CS	-40	LEU	-	expression tag	UNP Q584T8
CS	-39	ARG	-	expression tag	UNP Q584T8
CS	-38	ALA	-	expression tag	UNP Q584T8
CS	-37	GLU	-	expression tag	UNP Q584T8
CS	-36	GLY	-	expression tag	UNP Q584T8
CS	-35	PHE	-	expression tag	UNP Q584T8
CS	-34	ALA	-	expression tag	UNP Q584T8
CS	-33	HIS	-	expression tag	UNP Q584T8
CS	-32	SER	-	expression tag	UNP Q584T8
CS	-31	LEU	-	expression tag	UNP Q584T8
CS	-30	VAL	-	expression tag	UNP Q584T8
CS	-29	MET	-	expression tag	UNP Q584T8

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Chain	Residue	Modelled	Actual	Comment	Reference
CS	-28	LEU	-	expression tag	UNP Q584T8
CS	-27	PRO	-	expression tag	UNP Q584T8
CS	-26	VAL	-	expression tag	UNP Q584T8
CS	-25	SER	-	expression tag	UNP Q584T8
CS	-24	LEU	-	expression tag	UNP Q584T8
CS	-23	TYR	-	expression tag	UNP Q584T8
CS	-22	SER	-	expression tag	UNP Q584T8
CS	-21	LYS	-	expression tag	UNP Q584T8
CS	-20	ILE	-	expression tag	UNP Q584T8
CS	-19	LEU	-	expression tag	UNP Q584T8
CS	-18	LEU	-	expression tag	UNP Q584T8
CS	-17	CYS	-	expression tag	UNP Q584T8
CS	-16	ASP	-	expression tag	UNP Q584T8
CS	-15	VAL	-	expression tag	UNP Q584T8
CS	-14	LYS	-	expression tag	UNP Q584T8
CS	-13	LYS	-	expression tag	UNP Q584T8
CS	-12	LYS	-	expression tag	UNP Q584T8
CS	-11	ILE	-	expression tag	UNP Q584T8
CS	-10	VAL	-	expression tag	UNP Q584T8
CS	-9	TYR	-	expression tag	UNP Q584T8
CS	-8	PHE	-	expression tag	UNP Q584T8
CS	-7	HIS	-	expression tag	UNP Q584T8
CS	-6	CYS	-	expression tag	UNP Q584T8
CS	-5	CYS	-	expression tag	UNP Q584T8
CS	-4	THR	-	expression tag	UNP Q584T8
CS	-3	ARG	-	expression tag	UNP Q584T8
CS	-2	LYS	-	expression tag	UNP Q584T8
CS	-1	LYS	-	expression tag	UNP Q584T8
CS	0	SER	-	expression tag	UNP Q584T8

- Molecule 42 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	CU	184	Total	C	N	O	S	0	0
			1538	965	307	254	12		

- Molecule 43 is a protein called mt-IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	CZ	151	Total	C	N	O	S	0	0
			1212	759	231	215	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CZ	6	SER	GLY	conflict	UNP Q57WU2
CZ	30	THR	ILE	conflict	UNP Q57WU2
CZ	172	THR	ALA	conflict	UNP Q57WU2

- Molecule 44 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ca	592	Total	C	N	O	S	0	0
			5004	3201	898	882	23		

- Molecule 45 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Cb	252	Total	C	N	O	S	0	0
			2056	1300	368	380	8		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cb	244	SER	ASN	conflict	UNP Q57VB2
Cb	?	-	GLU	deletion	UNP Q57VB2
Cb	312	ALA	-	expression tag	UNP Q57VB2
Cb	313	CYS	-	expression tag	UNP Q57VB2
Cb	314	SER	-	expression tag	UNP Q57VB2
Cb	315	ARG	-	expression tag	UNP Q57VB2
Cb	316	ASP	-	expression tag	UNP Q57VB2
Cb	317	GLY	-	expression tag	UNP Q57VB2
Cb	318	PHE	-	expression tag	UNP Q57VB2
Cb	319	ALA	-	expression tag	UNP Q57VB2
Cb	320	LEU	-	expression tag	UNP Q57VB2
Cb	321	MET	-	expression tag	UNP Q57VB2
Cb	322	LYS	-	expression tag	UNP Q57VB2
Cb	323	ALA	-	expression tag	UNP Q57VB2
Cb	324	ASN	-	expression tag	UNP Q57VB2
Cb	325	LYS	-	expression tag	UNP Q57VB2

- Molecule 46 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Cd	291	Total	C	N	O	S	0	0
			2386	1491	442	443	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cd	299	UNK	GLY	conflict	UNP Q38DK6

- Molecule 47 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Cg	482	Total	C	N	O	S	0	0
			3904	2499	684	701	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	181	VAL	ALA	conflict	UNP Q585C2
Cg	498	ARG	-	expression tag	UNP Q585C2

- Molecule 48 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ci	165	Total	C	N	O	S	0	0
			1348	848	247	244	9		

- Molecule 49 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Cj	226	Total	C	N	O	S	0	0
			1792	1138	310	340	4		

- Molecule 50 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ck	703	Total	C	N	O	S	0	0
			5596	3503	1017	1050	26		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ck	107	SER	LEU	conflict	UNP Q387C7
Ck	144	PHE	LEU	conflict	UNP Q387C7
Ck	253	TYR	PHE	conflict	UNP Q387C7
Ck	339	GLU	VAL	conflict	UNP Q387C7
Ck	871	GLY	GLU	conflict	UNP Q387C7

- Molecule 51 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Cm	196	Total	C	N	O	S	0	0
			1577	975	304	289	9		

- Molecule 52 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Cn	110	Total	C	N	O	S	0	0
			912	585	181	143	3		

- Molecule 53 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Cp	175	Total	C	N	O	S	0	0
			1483	937	268	273	5		

- Molecule 54 is a protein called mS42.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Cq	252	Total	C	N	O	S	0	0
			2005	1285	342	369	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cq	48	THR	ALA	conflict	UNP Q586A1
Cq	167	MET	VAL	conflict	UNP Q586A1

- Molecule 55 is a protein called mS43.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Cr	257	Total	C	N	O	S	0	0
			1999	1261	368	356	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cr	351	LYS	GLU	conflict	UNP Q585I1

- Molecule 56 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Cv	1059	Total	C	N	O	S	0	0
			8557	5387	1535	1596	39		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cv	718	THR	ALA	conflict	UNP Q383R4
Cv	1179	GLU	GLY	conflict	UNP Q383R4

- Molecule 57 is a RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	CA	621	Total	C	N	O	P	0	0
			13122	5906	2227	4368	621		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	298	U	C	conflict	GB 343546
CA	473	U	G	conflict	GB 343546
CA	614	U	-	insertion	GB 343546
CA	615	U	-	insertion	GB 343546
CA	616	U	-	insertion	GB 343546
CA	617	U	-	insertion	GB 343546
CA	618	U	-	insertion	GB 343546
CA	619	U	-	insertion	GB 343546
CA	620	U	-	insertion	GB 343546
CA	621	U	-	insertion	GB 343546

- Molecule 58 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	UO	5	Total	C	N	O	0	0
			30	20	5	5		

- Molecule 59 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	UP	7	Total	C	N	O	0	0
			42	28	7	7		

- Molecule 60 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	UQ	32	Total	C	N	O	0	0
			192	128	32	32		

- Molecule 61 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	UR	8	Total	C	N	O	0	0
			48	32	8	8		

- Molecule 62 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	US	54	Total	C	N	O	0	0
			324	216	54	54		

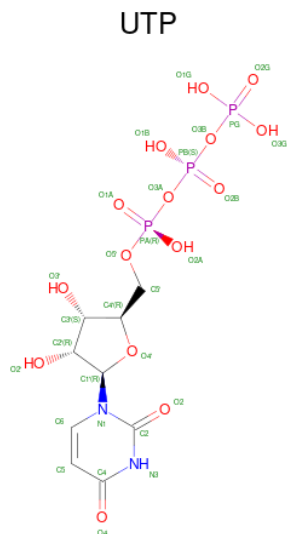
- Molecule 63 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	UT	44	Total	C	N	O	0	0
			264	176	44	44		

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
64	DA	1	Total	Zn	0
			1	1	
64	DS	2	Total	Zn	0
			2	2	
64	Cr	1	Total	Zn	0
			1	1	

- Molecule 65 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C₉H₁₅N₂O₁₅P₃).

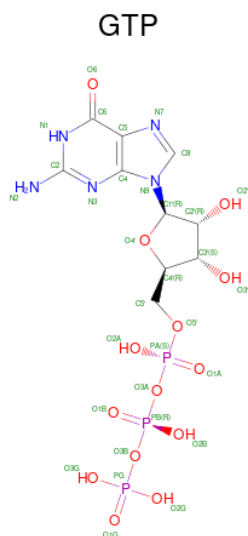


Mol	Chain	Residues	Atoms					AltConf
65	DJ	1	Total	C	N	O	P	0
			29	9	2	15	3	

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

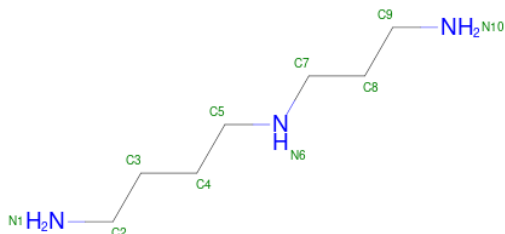
Mol	Chain	Residues	Atoms	AltConf
66	CQ	1	Total Mg 1 1	0
66	Ca	1	Total Mg 1 1	0
66	Cg	1	Total Mg 1 1	0
66	Cv	1	Total Mg 1 1	0
66	CA	35	Total Mg 35 35	0

- Molecule 67 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
67	Cg	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 68 is SPERMIDINE (CCD ID: SPD) (formula: $\text{C}_7\text{H}_{19}\text{N}_3$).



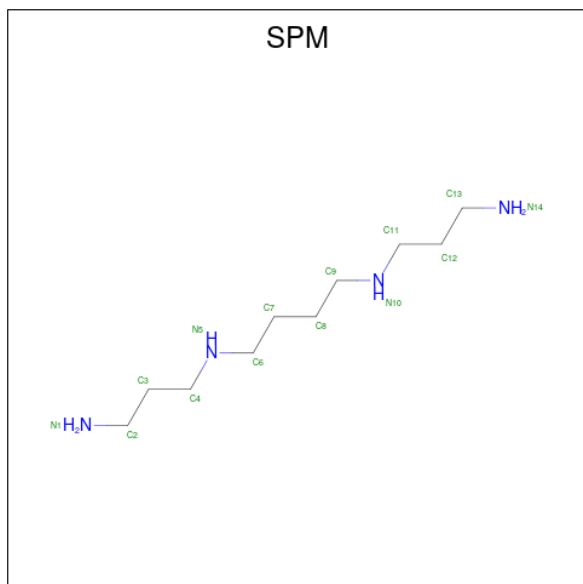
Mol	Chain	Residues	Atoms			AltConf
68	CA	1	Total 10	C 7	N 3	0
68	CA	1	Total 10	C 7	N 3	0
68	CA	1	Total 10	C 7	N 3	0

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Mol	Chain	Residues	Atoms			AltConf
68	CA	1	Total	C	N	0
			10	7	3	

- Molecule 69 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
69	CA	1	Total	C	N	0
			14	10	4	

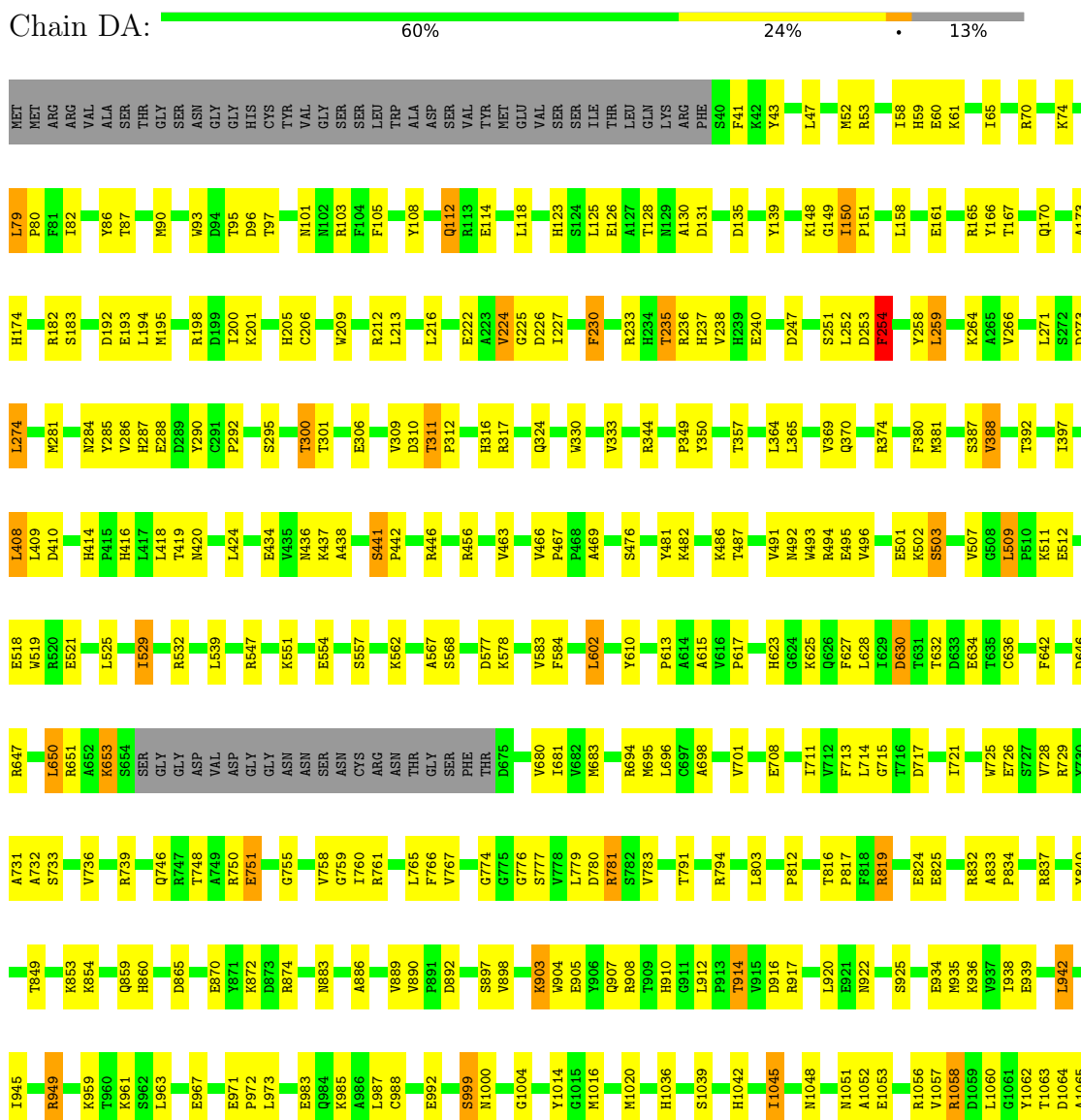
- Molecule 70 is water.

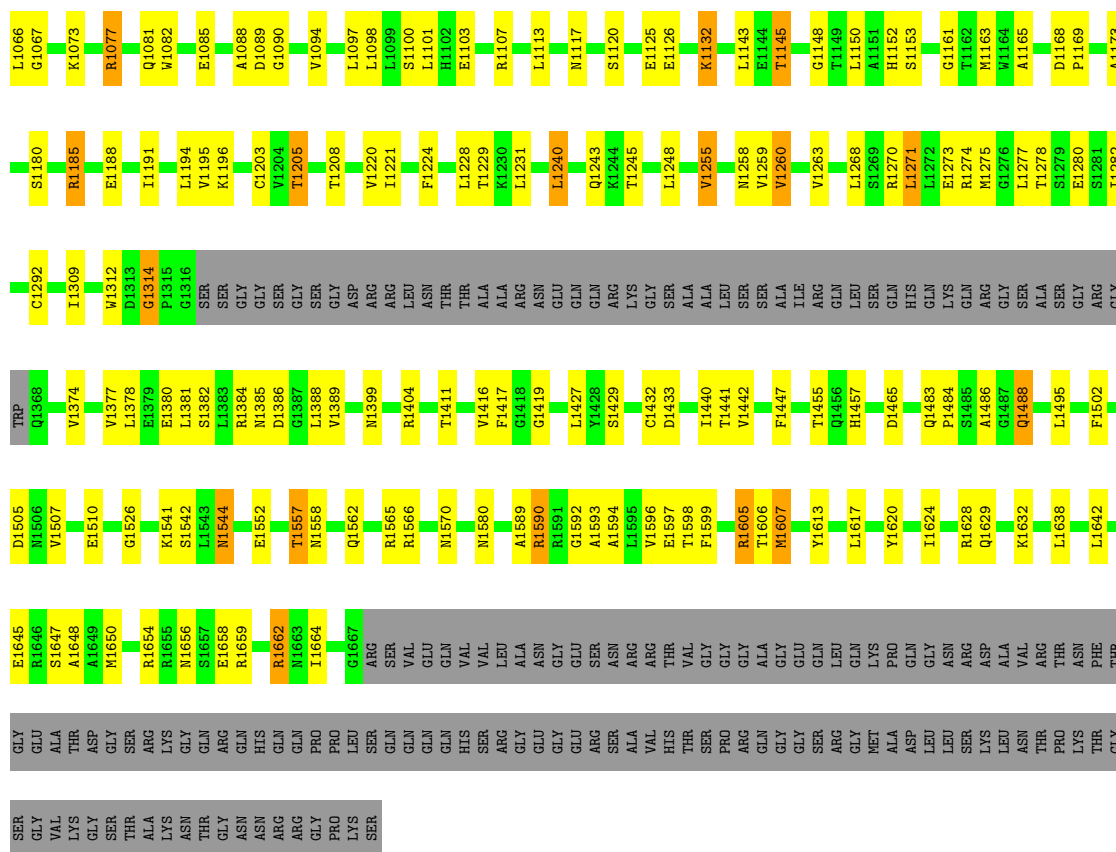
Mol	Chain	Residues	Atoms		AltConf
70	Cg	3	Total	O	0
			3	3	

3 Residue-property plots

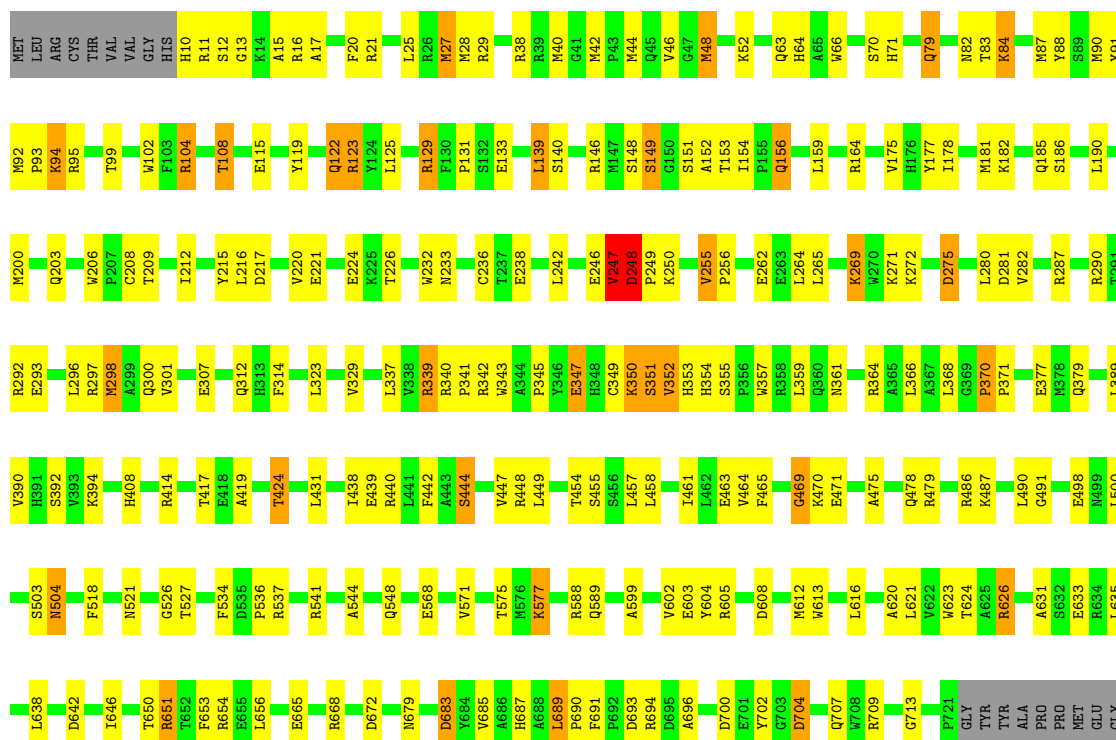
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: mS48





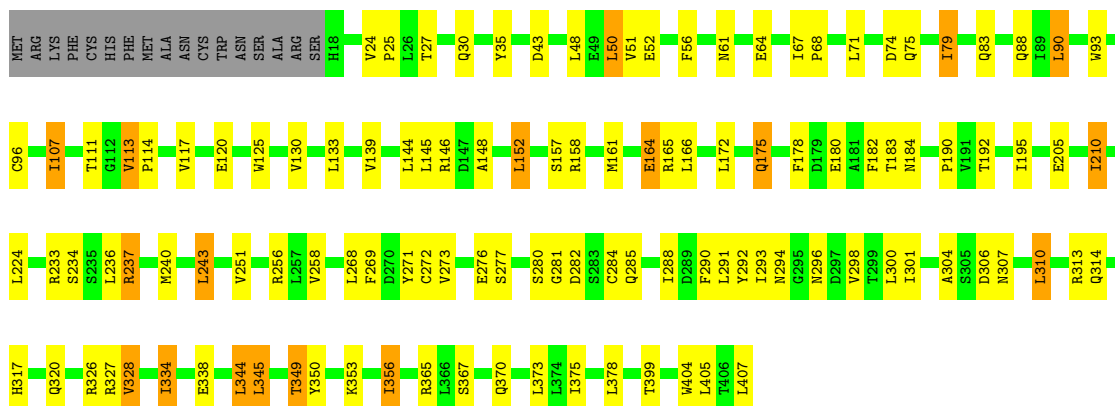
• Molecule 2: mS51





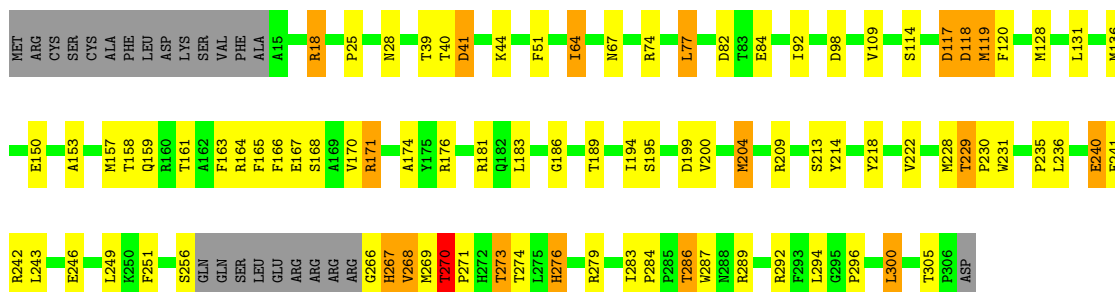
• Molecule 3: mS56

Chain DI: 67% 25%



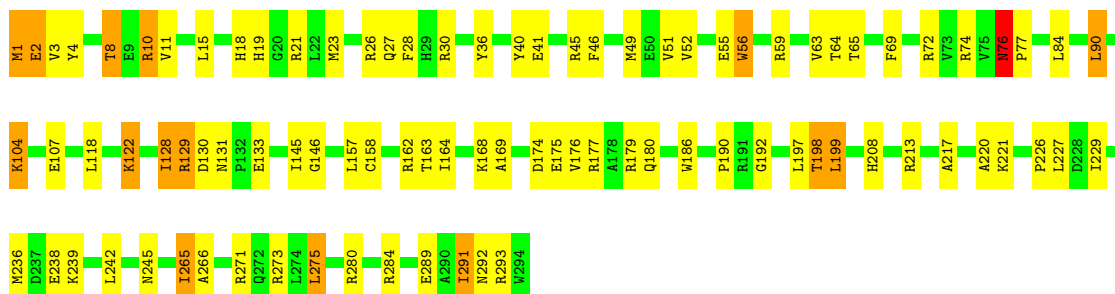
• Molecule 4: mS59

Chain DL: 63% 23% 6% 8%



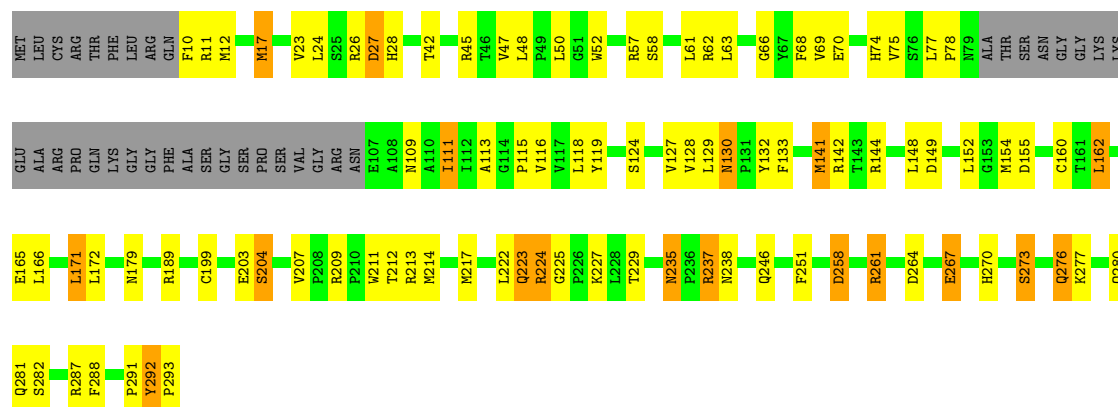
• Molecule 5: mS60

Chain DM: 69% 26% 5%



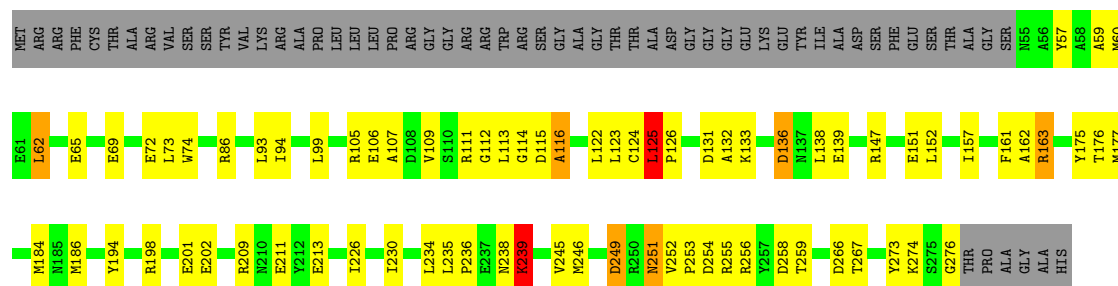
• Molecule 6: mS61

Chain DN: 55% 26% 6% 12%



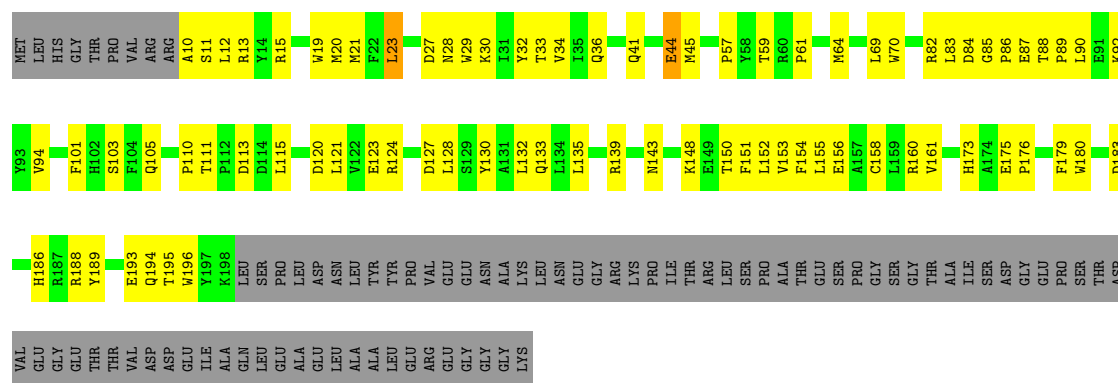
• Molecule 7: mS62

Chain DO: 52% (green), 24% (yellow), 21% (grey).



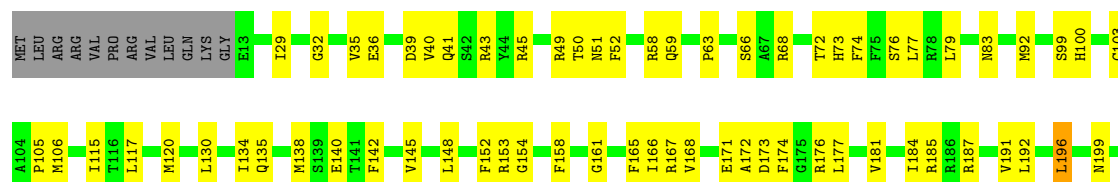
• Molecule 8: mS63

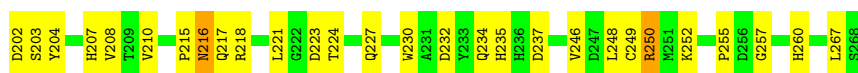
Chain DP: 40% (green), 28% (yellow), 31% (grey).



• Molecule 9: mS64

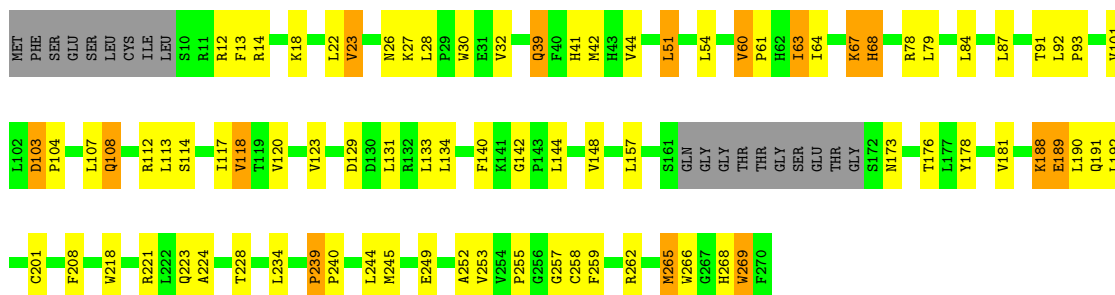
Chain DQ: 61% (green), 34% (yellow), 5% (grey).





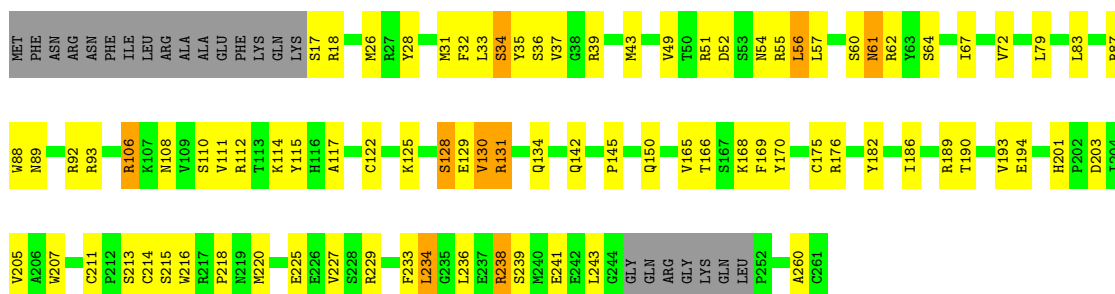
• Molecule 10: mS65

Chain DR: 62% 26% 6% 7%



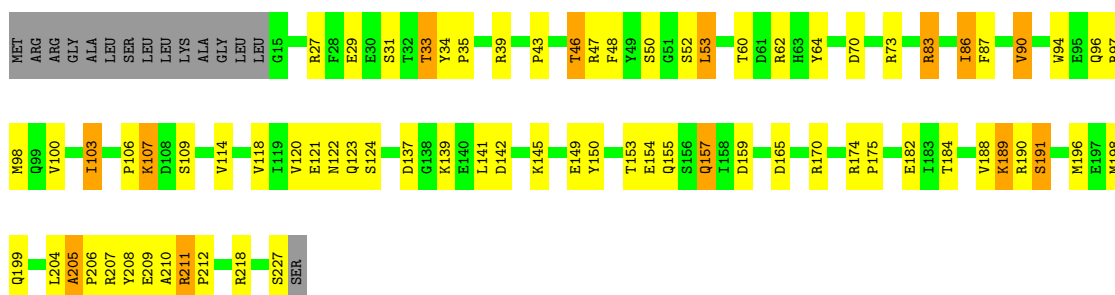
• Molecule 11: mS66

Chain DS: 58% 30% 9%



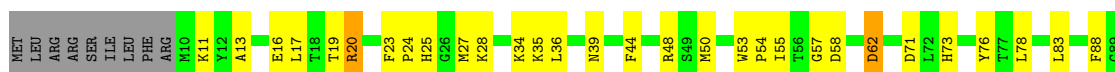
• Molecule 12: mS68

Chain DU: 61% 27% 6% 7%

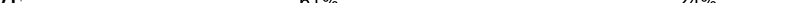


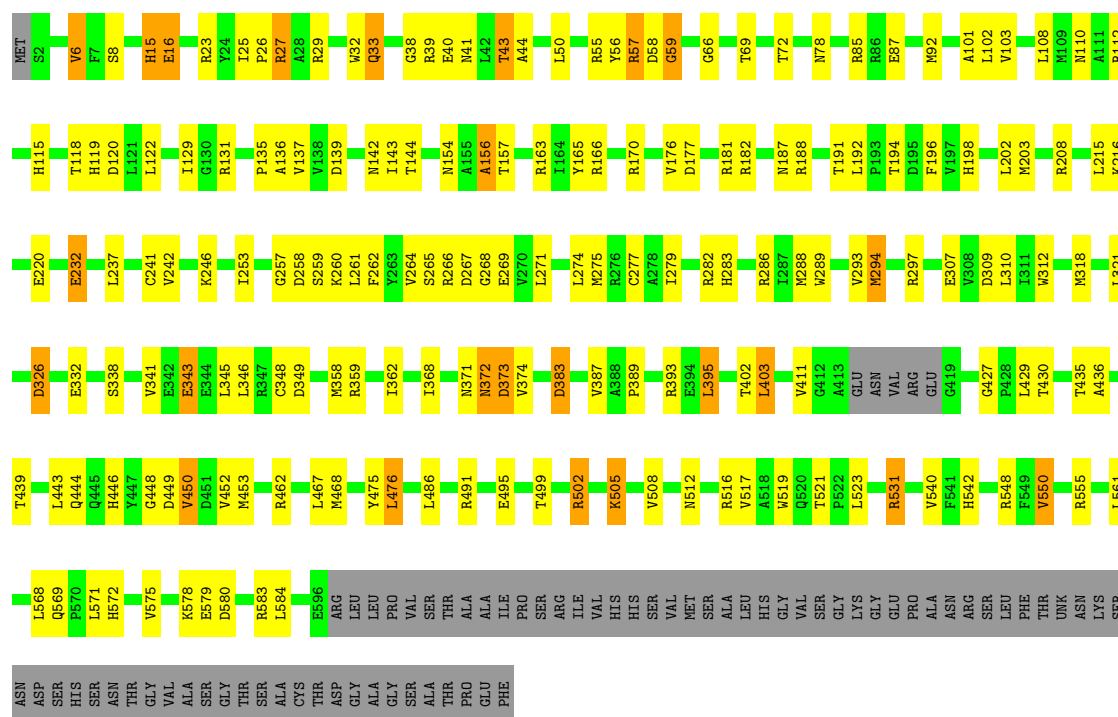
• Molecule 13: mS73

Chain DZ: 54% 31% 13%



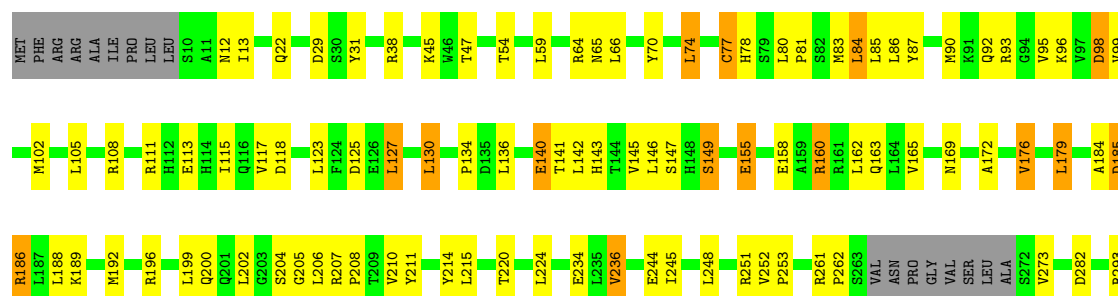
- Molecule 18: mS53

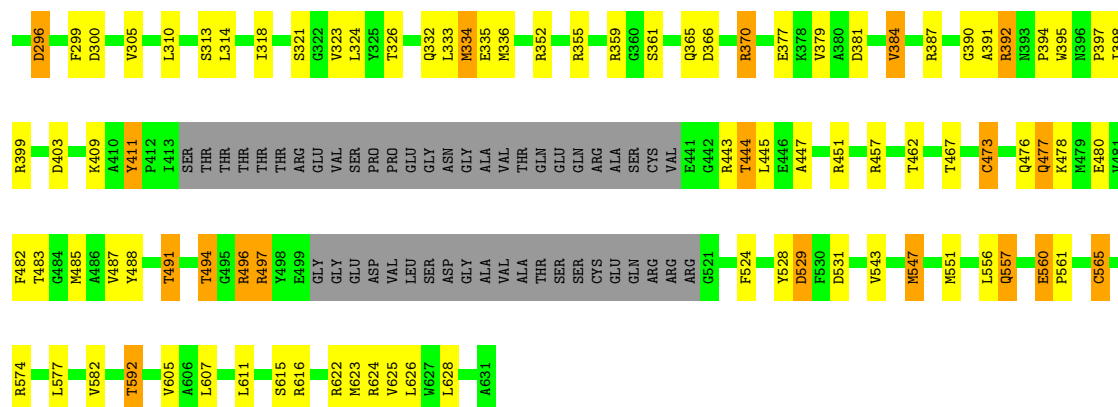
Chain DF: 



- Molecule 19: mS54

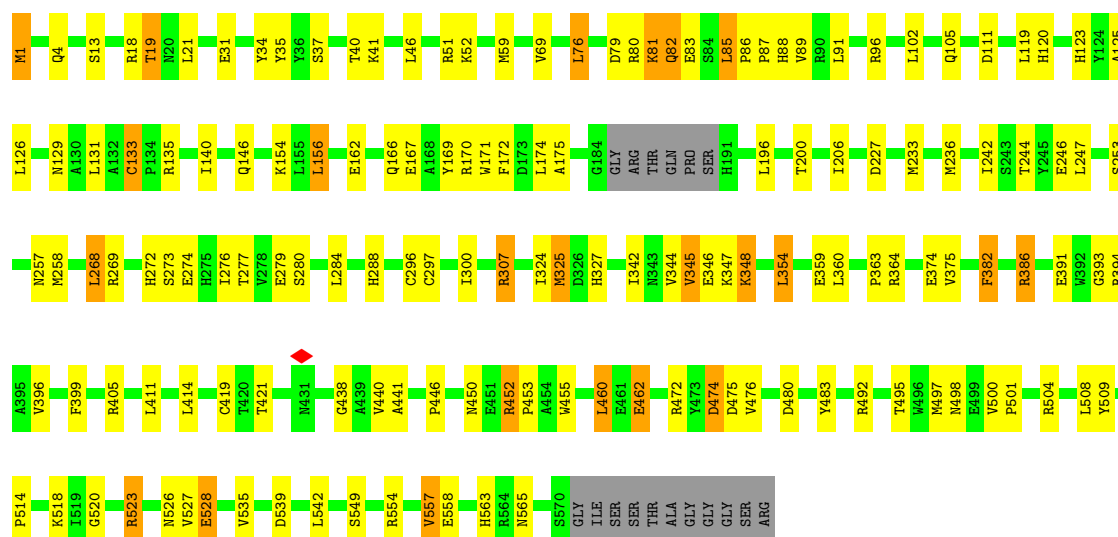
Chain DG:





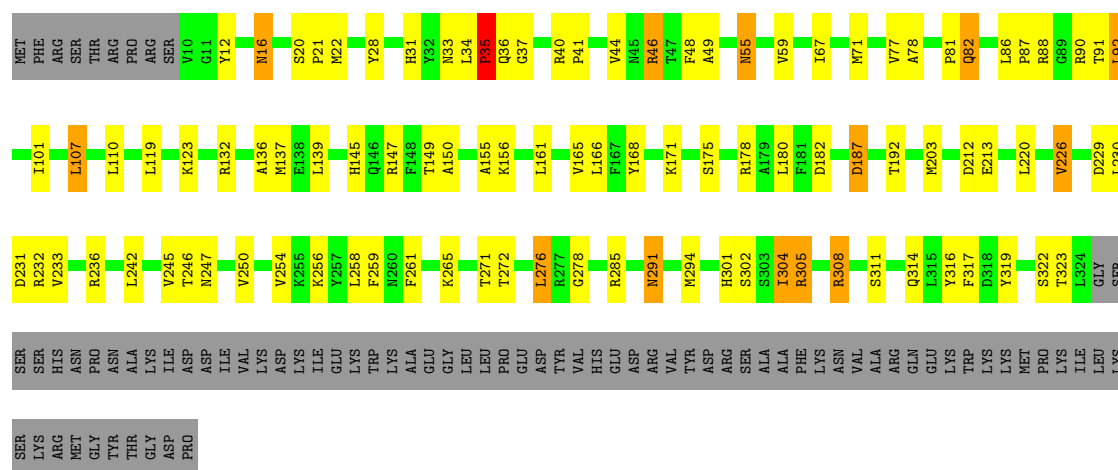
• Molecule 20: mS55

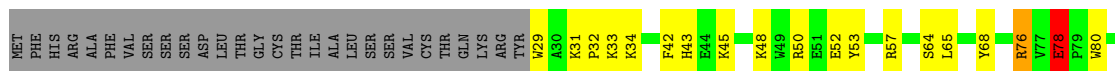
Chain DH: 71% 22%



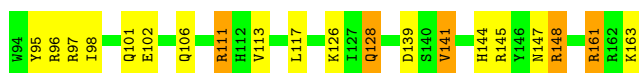
• Molecule 21: mS57

Chain DJ: 55% 21% 20%

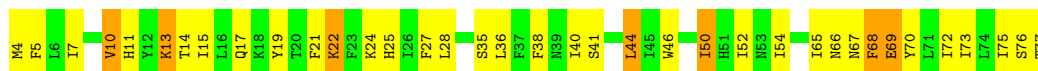




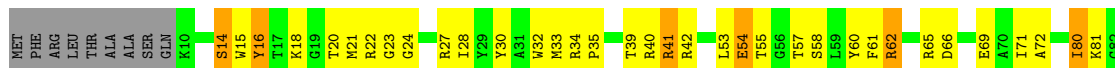
• Molecule 27: mS72



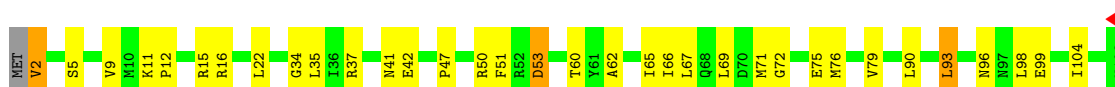
• Molecule 28: uS3m

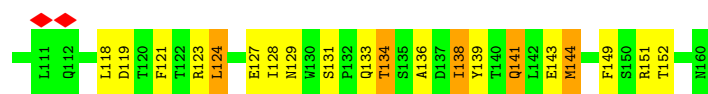


• Molecule 29: uS5m



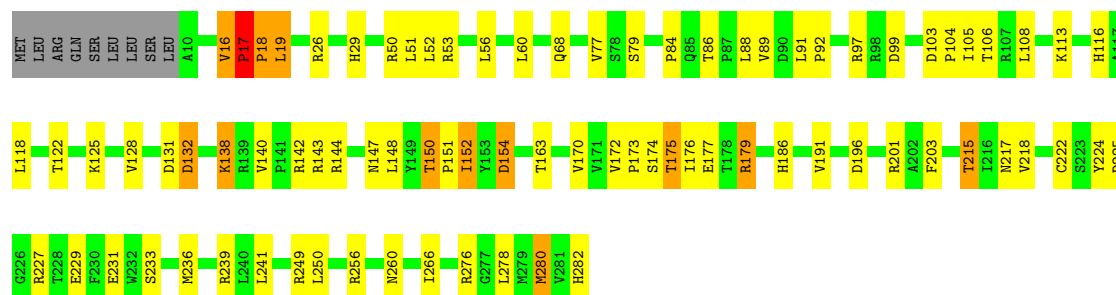
• Molecule 30: bS6m





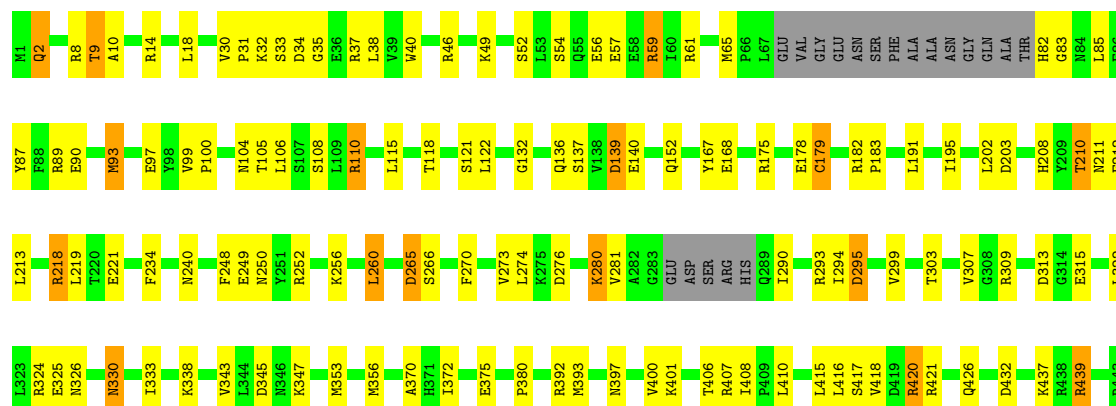
• Molecule 31: uS8m

Chain CH: 67% 25%



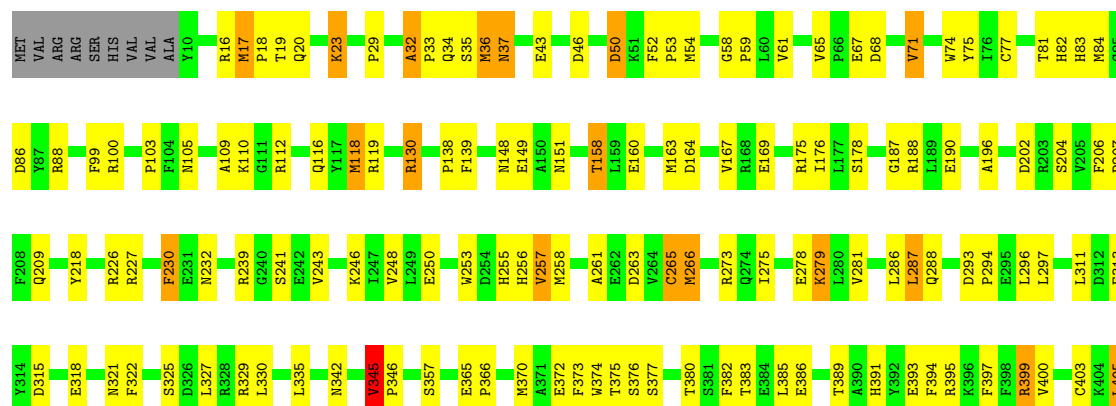
• Molecule 32: uS9m

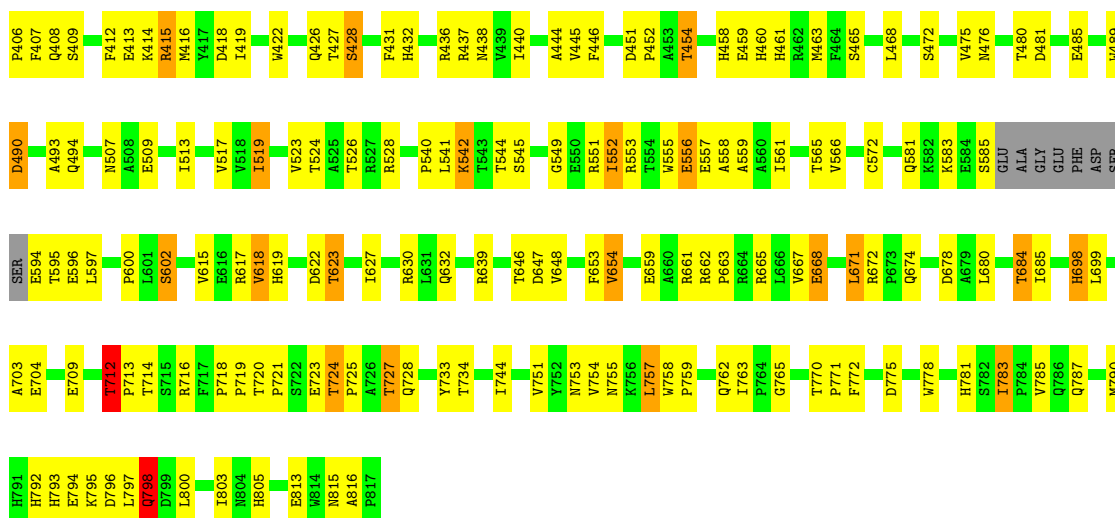
Chain CI: 67% 26%



• Molecule 33: uS10m

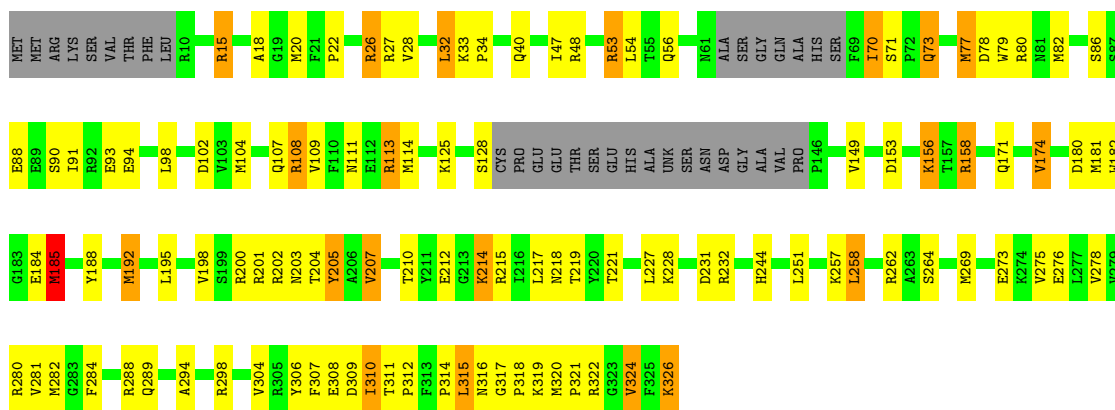
Chain CJ: 61% 32% 5%





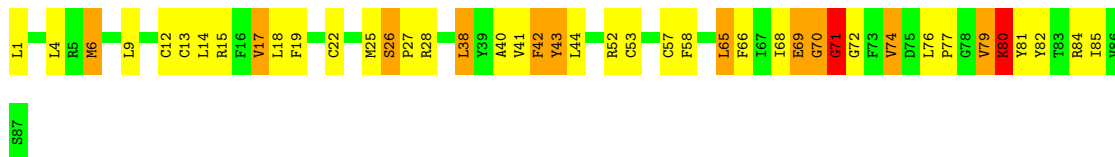
• Molecule 34: uS11m

Chain CK: 55% 28% 6% 10%



• Molecule 35: uS12m

Chain CL: 52% 33% 13% .

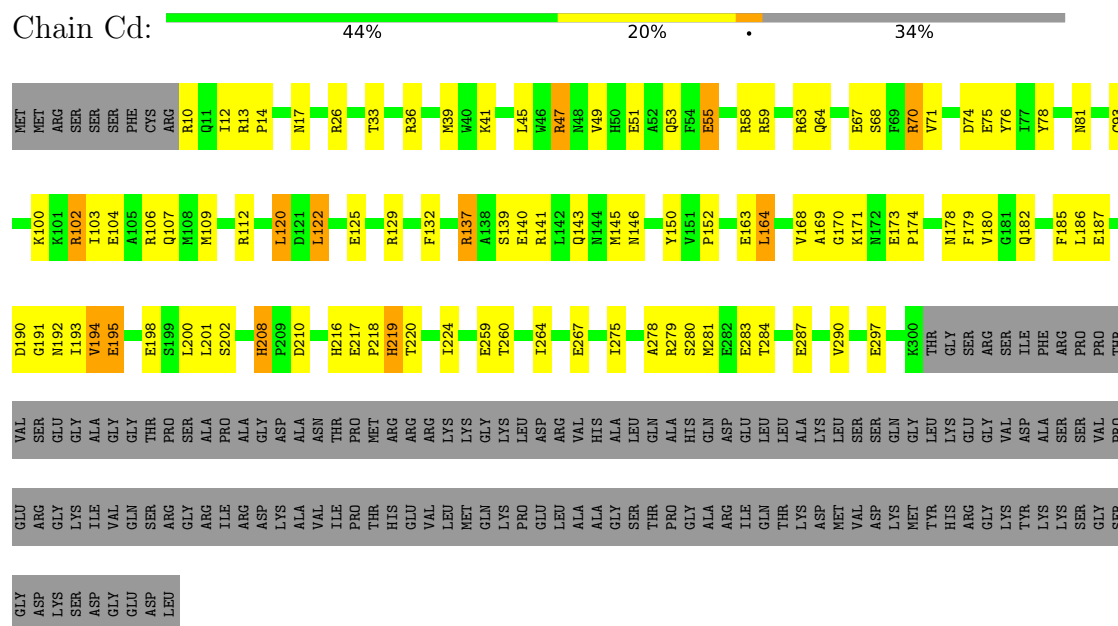


• Molecule 36: uS14m

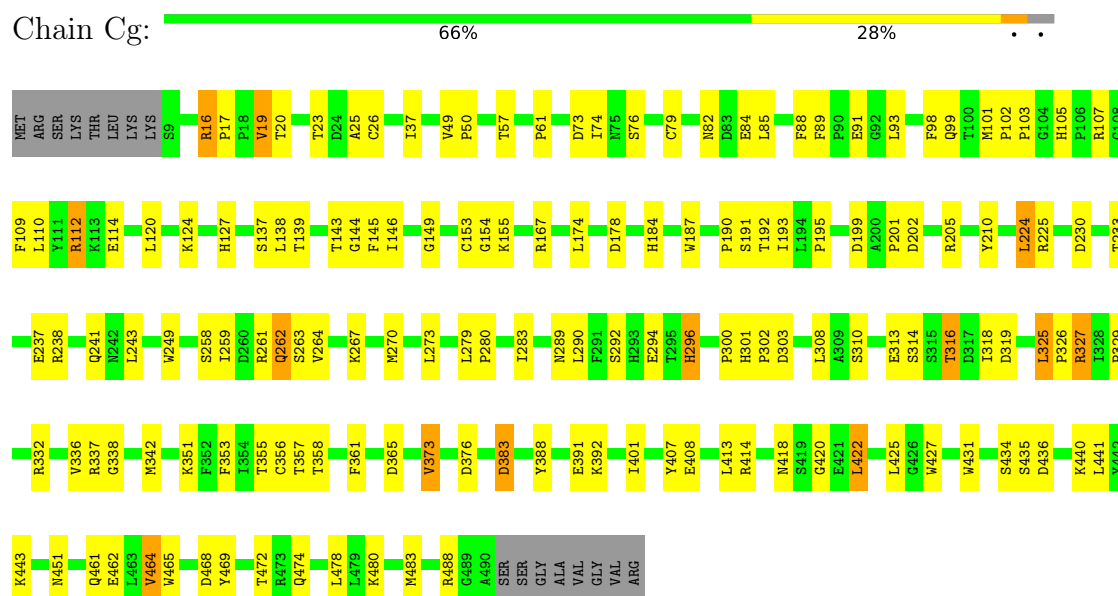
Chain CN: 58% 29% 8% 5%



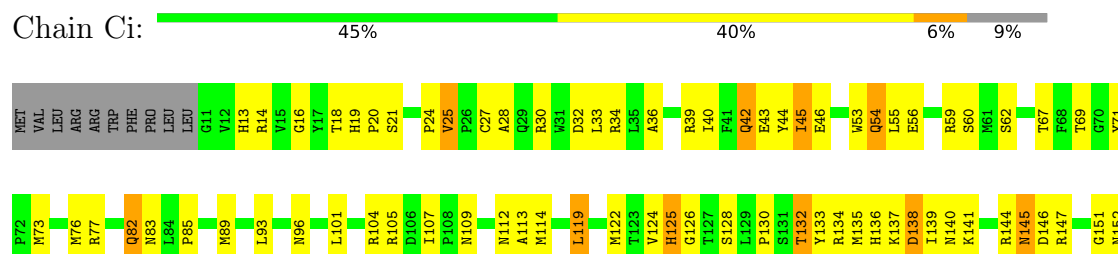
- Molecule 46: mS26



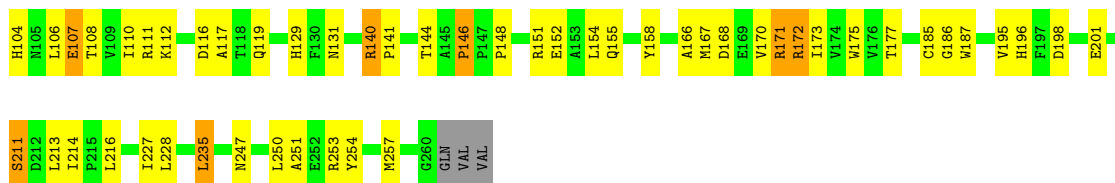
- Molecule 47: mS29



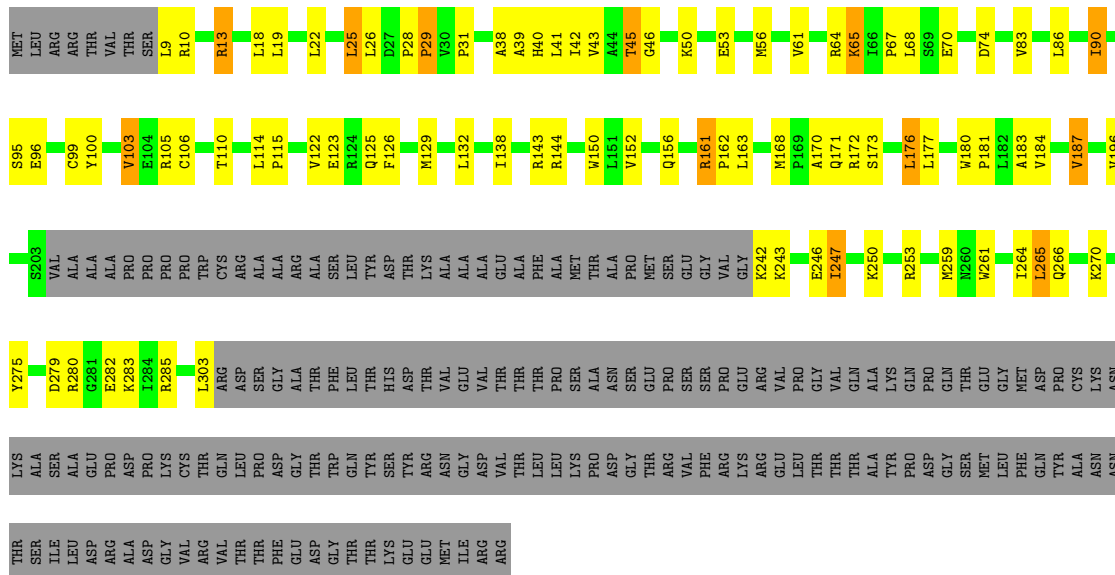
- Molecule 48: mS33



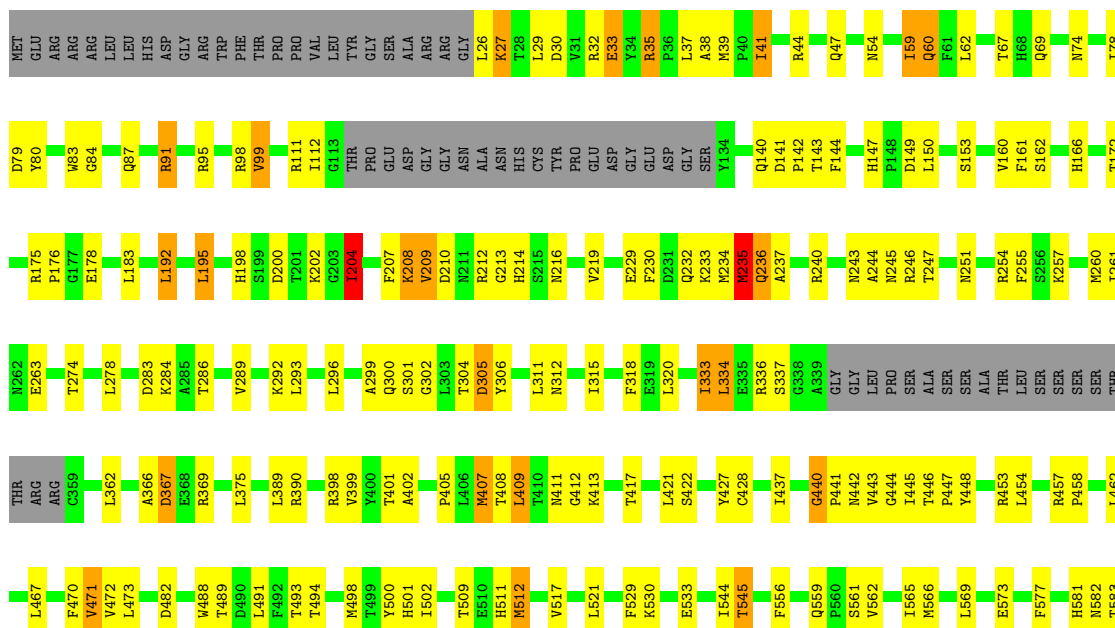
MET	ARG	LEU	CYS	ARG	ARG	LEU	SER	Y9
V10	M21	T24	M26	P27	I30	R36	T52	F55
S56	Q57	P58	R59	N61	Y62	P63	V64	S65
Q76	F77	D78	M79	Q80	Y81	S82	L83	F84
H85	R86	N92	L93	R94	H95	T96	L97	G98
T99	P100	L101						

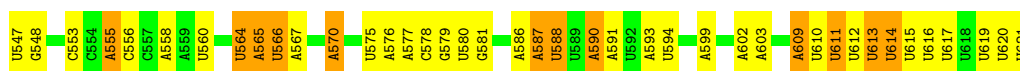


• Molecule 55: mS43



• Molecule 56: mS47





- Molecule 58: Unknown Protein



- Molecule 59: Unknown Protein



- Molecule 60: Unknown Protein



There are no outlier residues recorded for this chain.

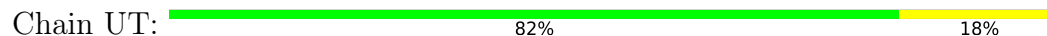
- Molecule 61: Unknown Protein



- Molecule 62: Unknown Protein



- Molecule 63: Unknown Protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31911	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.538	Depositor
Minimum map value	-0.316	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0114	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, MG, SPM, UTP, ZN, GTP

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	DA	0.47	1/12780 (0.0%)	0.89	34/17297 (0.2%)
2	DD	0.48	0/6710	0.94	24/9087 (0.3%)
3	DI	0.47	0/3248	0.86	1/4401 (0.0%)
4	DL	0.54	0/2346	0.97	8/3164 (0.3%)
5	DM	0.51	0/2488	0.92	6/3362 (0.2%)
6	DN	0.50	0/2148	1.01	14/2916 (0.5%)
7	DO	0.47	0/1840	0.95	7/2482 (0.3%)
8	DP	0.43	0/1662	0.81	1/2249 (0.0%)
9	DQ	0.48	0/2111	0.93	4/2863 (0.1%)
10	DR	0.46	0/2090	0.96	8/2849 (0.3%)
11	DS	0.45	0/1950	0.87	1/2633 (0.0%)
12	DU	0.45	0/1799	0.85	2/2438 (0.1%)
13	DZ	0.46	0/725	0.89	2/984 (0.2%)
14	Da	0.46	0/520	0.87	0/694
15	DB	0.45	0/9369	0.88	17/12692 (0.1%)
16	DC	0.44	0/8952	0.88	19/12145 (0.2%)
17	DE	0.41	0/4955	0.92	20/6708 (0.3%)
18	DF	0.46	0/4856	0.88	12/6581 (0.2%)
19	DG	0.43	0/4674	0.88	12/6333 (0.2%)
20	DH	0.46	0/4684	0.88	6/6347 (0.1%)
21	DJ	0.47	0/2649	0.89	9/3598 (0.3%)
22	DK	0.41	0/2045	0.84	2/2759 (0.1%)
23	DT	0.42	0/2133	0.89	7/2889 (0.2%)
24	DV	0.47	0/1382	0.95	7/1871 (0.4%)
25	DW	0.45	0/1407	0.93	2/1916 (0.1%)
26	DX	0.43	0/1231	0.88	5/1654 (0.3%)
27	DY	0.54	0/1334	0.96	5/1810 (0.3%)
28	CC	0.49	0/666	0.95	4/900 (0.4%)
29	CE	0.54	0/3484	0.96	7/4708 (0.1%)
30	CF	0.48	0/1319	0.87	1/1783 (0.1%)
31	CH	0.56	0/2276	0.97	7/3071 (0.2%)
32	CI	0.51	0/3453	0.88	2/4655 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	CJ	0.52	0/6705	0.97	32/9124 (0.4%)
34	CK	0.47	0/2472	0.89	2/3315 (0.1%)
35	CL	0.48	0/759	0.96	4/1026 (0.4%)
36	CN	0.50	0/1361	0.90	2/1840 (0.1%)
37	CO	0.51	0/3085	0.94	11/4165 (0.3%)
38	CP	0.54	0/1533	1.02	8/2074 (0.4%)
39	CQ	0.58	0/1631	1.07	5/2203 (0.2%)
40	CR	0.52	0/2640	0.97	2/3572 (0.1%)
41	CS	0.47	0/1209	0.95	5/1626 (0.3%)
42	CU	0.48	0/1576	0.85	0/2115
43	CZ	0.46	0/1237	0.90	3/1659 (0.2%)
44	Ca	0.51	0/5159	0.94	19/6980 (0.3%)
45	Cb	0.53	0/2105	0.94	4/2842 (0.1%)
46	Cd	0.52	0/2438	0.86	4/3288 (0.1%)
47	Cg	0.47	0/4025	0.95	11/5467 (0.2%)
48	Ci	0.51	0/1388	1.00	5/1878 (0.3%)
49	Cj	0.45	0/1842	0.89	4/2511 (0.2%)
50	Ck	0.49	0/5696	0.90	6/7705 (0.1%)
51	Cm	0.59	0/1616	1.02	4/2175 (0.2%)
52	Cn	0.51	0/934	0.96	5/1248 (0.4%)
53	Cp	0.46	0/1528	0.88	2/2072 (0.1%)
54	Cq	0.52	0/2066	0.91	5/2815 (0.2%)
55	Cr	0.45	0/2038	0.91	6/2759 (0.2%)
56	Cv	0.51	0/8780	0.96	25/11901 (0.2%)
57	CA	0.27	0/14679	0.45	0/22827
All	All	0.47	1/181788 (0.0%)	0.89	430/249026 (0.2%)

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	DA	0	2
2	DD	0	3
6	DN	0	1
7	DO	0	2
10	DR	0	2
16	DC	0	2
19	DG	0	2
21	DJ	0	1
23	DT	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	DX	0	1
31	CH	0	2
33	CJ	0	2
35	CL	0	3
37	CO	0	2
46	Cd	0	1
47	Cg	0	1
50	Ck	0	1
56	Cv	0	2
All	All	0	31

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DA	529	ILE	C-O	5.61	1.30	1.24

The worst 5 of 430 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DD	255	VAL	CA-C-N	13.36	136.54	119.84
2	DD	255	VAL	C-N-CA	13.36	136.54	119.84
17	DE	327	ASN	CA-C-N	-11.05	109.00	120.38
17	DE	327	ASN	C-N-CA	-11.05	109.00	120.38
56	Cv	945	VAL	CA-C-N	-9.94	110.19	120.03

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DA	166	TYR	Peptide
1	DA	273	ASP	Peptide
2	DD	247	VAL	Peptide
2	DD	255	VAL	Peptide
2	DD	351	SER	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	DA	12482	0	12152	306	0
2	DD	6523	0	6307	195	0
3	DI	3182	0	3153	69	0
4	DL	2287	0	2275	61	0
5	DM	2430	0	2427	68	0
6	DN	2091	0	2076	77	0
7	DO	1804	0	1752	58	0
8	DP	1613	0	1581	52	0
9	DQ	2061	0	2041	69	0
10	DR	2025	0	2029	62	0
11	DS	1904	0	1855	65	0
12	DU	1754	0	1687	61	0
13	DZ	697	0	644	28	0
14	Da	501	0	473	26	0
15	DB	9148	0	8834	223	0
16	DC	8748	0	8532	180	0
17	DE	4831	0	4789	115	0
18	DF	4747	0	4723	128	0
19	DG	4575	0	4490	130	0
20	DH	4578	0	4520	100	0
21	DJ	2572	0	2495	75	0
22	DK	2007	0	1998	41	0
23	DT	2058	0	1928	86	0
24	DV	1346	0	1335	38	0
25	DW	1359	0	1342	41	0
26	DX	1196	0	1189	30	0
27	DY	1293	0	1287	33	0
28	CC	646	0	679	29	0
29	CE	3399	0	3376	139	0
30	CF	1292	0	1261	44	0
31	CH	2228	0	2204	59	0
32	CI	3386	0	3374	103	0
33	CJ	6516	0	6261	207	0
34	CK	2418	0	2360	118	0
35	CL	733	0	741	29	0
36	CN	1322	0	1304	60	0
37	CO	3003	0	2995	115	0
38	CP	1489	0	1510	66	0
39	CQ	1584	0	1601	55	0
40	CR	2567	0	2508	101	0
41	CS	1175	0	1191	43	0
42	CU	1538	0	1539	74	0
43	CZ	1212	0	1178	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Ca	5004	0	4776	219	0
45	Cb	2056	0	2031	79	0
46	Cd	2386	0	2220	79	0
47	Cg	3904	0	3786	92	0
48	Ci	1348	0	1306	65	0
49	Cj	1792	0	1744	73	0
50	Ck	5596	0	5613	182	0
51	Cm	1577	0	1505	71	0
52	Cn	912	0	969	49	0
53	Cp	1483	0	1438	66	0
54	Cq	2005	0	1916	47	0
55	Cr	1999	0	2007	53	0
56	Cv	8557	0	8252	262	0
57	CA	13122	0	6563	279	0
58	UO	30	0	33	3	0
59	UP	42	0	46	1	0
60	UQ	192	0	194	0	0
61	UR	48	0	50	4	0
62	US	324	0	326	5	0
63	UT	264	0	268	4	0
64	Cr	1	0	0	0	0
64	DA	1	0	0	0	0
64	DS	2	0	0	0	0
65	DJ	29	0	11	2	0
66	CA	35	0	0	0	0
66	CQ	1	0	0	0	0
66	Ca	1	0	0	0	0
66	Cg	1	0	0	0	0
66	Cv	1	0	0	0	0
67	Cg	32	0	12	6	0
68	CA	40	0	76	3	0
69	CA	14	0	26	0	0
70	Cg	3	0	0	1	0
All	All	177122	0	167164	4189	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 12.

The worst 5 of 4189 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)
46:Cd:137:ARG:HG2	46:Cd:137:ARG:HH11	1.23	1.03
44:Ca:536:ARG:NH1	44:Ca:539:GLN:OE1	1.94	0.99
30:CF:129:ASN:HB3	40:CR:125:ASN:HD22	1.31	0.96
19:DG:628:LEU:O	47:Cg:124:LYS:NZ	2.00	0.95
57:CA:564:U:H3	57:CA:570:A:H61	1.06	0.95

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	DA	1551/1788 (87%)	1490 (96%)	59 (4%)	2 (0%)	48	77
2	DD	787/812 (97%)	740 (94%)	44 (6%)	3 (0%)	30	58
3	DI	388/407 (95%)	365 (94%)	22 (6%)	1 (0%)	36	64
4	DL	279/307 (91%)	261 (94%)	18 (6%)	0	100	100
5	DM	292/294 (99%)	280 (96%)	12 (4%)	0	100	100
6	DN	253/293 (86%)	238 (94%)	15 (6%)	0	100	100
7	DO	220/282 (78%)	209 (95%)	10 (4%)	1 (0%)	24	53
8	DP	187/274 (68%)	176 (94%)	11 (6%)	0	100	100
9	DQ	254/268 (95%)	244 (96%)	9 (4%)	1 (0%)	30	58
10	DR	247/270 (92%)	236 (96%)	10 (4%)	1 (0%)	30	58
11	DS	234/261 (90%)	222 (95%)	11 (5%)	1 (0%)	30	58
12	DU	211/228 (92%)	198 (94%)	11 (5%)	2 (1%)	14	41
13	DZ	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
14	Da	53/64 (83%)	52 (98%)	1 (2%)	0	100	100
15	DB	1109/1181 (94%)	1073 (97%)	35 (3%)	1 (0%)	48	77
16	DC	1087/1165 (93%)	1053 (97%)	33 (3%)	1 (0%)	48	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	DE	576/747 (77%)	564 (98%)	12 (2%)	0	100	100
18	DF	586/666 (88%)	568 (97%)	18 (3%)	0	100	100
19	DG	558/631 (88%)	543 (97%)	15 (3%)	0	100	100
20	DH	560/581 (96%)	539 (96%)	21 (4%)	0	100	100
21	DJ	313/396 (79%)	299 (96%)	13 (4%)	1 (0%)	36	64
22	DK	249/324 (77%)	238 (96%)	11 (4%)	0	100	100
23	DT	237/247 (96%)	232 (98%)	5 (2%)	0	100	100
24	DV	158/183 (86%)	152 (96%)	6 (4%)	0	100	100
25	DW	159/179 (89%)	153 (96%)	6 (4%)	0	100	100
26	DX	139/169 (82%)	130 (94%)	9 (6%)	0	100	100
27	DY	152/163 (93%)	147 (97%)	5 (3%)	0	100	100
28	CC	72/74 (97%)	67 (93%)	5 (7%)	0	100	100
29	CE	413/435 (95%)	386 (94%)	26 (6%)	1 (0%)	43	70
30	CF	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
31	CH	271/282 (96%)	259 (96%)	11 (4%)	1 (0%)	30	58
32	CI	418/443 (94%)	405 (97%)	13 (3%)	0	100	100
33	CJ	796/817 (97%)	755 (95%)	39 (5%)	2 (0%)	36	64
34	CK	287/326 (88%)	267 (93%)	20 (7%)	0	100	100
35	CL	85/87 (98%)	79 (93%)	5 (6%)	1 (1%)	10	34
36	CN	155/166 (93%)	148 (96%)	7 (4%)	0	100	100
37	CO	359/429 (84%)	342 (95%)	16 (4%)	1 (0%)	36	64
38	CP	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
39	CQ	188/307 (61%)	178 (95%)	10 (5%)	0	100	100
40	CR	312/320 (98%)	297 (95%)	14 (4%)	1 (0%)	36	64
41	CS	140/244 (57%)	132 (94%)	8 (6%)	0	100	100
42	CU	182/193 (94%)	173 (95%)	8 (4%)	1 (0%)	24	53
43	CZ	149/360 (41%)	142 (95%)	6 (4%)	1 (1%)	18	46
44	Ca	590/602 (98%)	551 (93%)	34 (6%)	5 (1%)	16	44
45	Cb	248/325 (76%)	241 (97%)	7 (3%)	0	100	100
46	Cd	288/440 (66%)	277 (96%)	10 (4%)	1 (0%)	36	64
47	Cg	480/498 (96%)	462 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	Ci	163/181 (90%)	154 (94%)	9 (6%)	0	100	100
49	Cj	224/257 (87%)	215 (96%)	8 (4%)	1 (0%)	30	58
50	Ck	699/874 (80%)	676 (97%)	22 (3%)	1 (0%)	48	77
51	Cm	194/215 (90%)	182 (94%)	12 (6%)	0	100	100
52	Cn	108/250 (43%)	103 (95%)	5 (5%)	0	100	100
53	Cp	173/187 (92%)	167 (96%)	6 (4%)	0	100	100
54	Cq	250/263 (95%)	242 (97%)	8 (3%)	0	100	100
55	Cr	253/439 (58%)	241 (95%)	11 (4%)	1 (0%)	30	58
56	Cv	1051/1211 (87%)	1010 (96%)	41 (4%)	0	100	100
All	All	19802/22847 (87%)	18951 (96%)	818 (4%)	33 (0%)	44	70

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	CZ	296	PRO
44	Ca	32	PRO
44	Ca	33	PRO
44	Ca	35	PRO
2	DD	352	VAL

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	DA	1322/1514 (87%)	1195 (90%)	127 (10%)	8	28
2	DD	694/711 (98%)	618 (89%)	76 (11%)	6	22
3	DI	350/365 (96%)	312 (89%)	38 (11%)	6	23
4	DL	241/263 (92%)	209 (87%)	32 (13%)	4	16
5	DM	252/252 (100%)	223 (88%)	29 (12%)	5	21
6	DN	229/256 (90%)	206 (90%)	23 (10%)	7	26
7	DO	186/229 (81%)	172 (92%)	14 (8%)	12	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	DP	170/239 (71%)	157 (92%)	13 (8%)	12	38
9	DQ	228/239 (95%)	220 (96%)	8 (4%)	32	56
10	DR	220/235 (94%)	193 (88%)	27 (12%)	4	19
11	DS	209/228 (92%)	194 (93%)	15 (7%)	13	39
12	DU	190/201 (94%)	169 (89%)	21 (11%)	6	22
13	DZ	72/84 (86%)	67 (93%)	5 (7%)	14	40
14	Da	50/59 (85%)	42 (84%)	8 (16%)	2	10
15	DB	976/1030 (95%)	870 (89%)	106 (11%)	6	23
16	DC	927/985 (94%)	827 (89%)	100 (11%)	6	23
17	DE	519/644 (81%)	466 (90%)	53 (10%)	7	25
18	DF	500/560 (89%)	442 (88%)	58 (12%)	5	21
19	DG	490/543 (90%)	430 (88%)	60 (12%)	5	19
20	DH	493/504 (98%)	437 (89%)	56 (11%)	5	21
21	DJ	275/347 (79%)	246 (90%)	29 (10%)	6	24
22	DK	209/261 (80%)	186 (89%)	23 (11%)	6	22
23	DT	220/228 (96%)	192 (87%)	28 (13%)	4	17
24	DV	145/165 (88%)	133 (92%)	12 (8%)	10	35
25	DW	148/163 (91%)	132 (89%)	16 (11%)	6	23
26	DX	124/149 (83%)	111 (90%)	13 (10%)	6	24
27	DY	137/146 (94%)	117 (85%)	20 (15%)	3	13
28	CC	73/73 (100%)	64 (88%)	9 (12%)	4	19
29	CE	358/372 (96%)	309 (86%)	49 (14%)	3	15
30	CF	136/144 (94%)	121 (89%)	15 (11%)	6	22
31	CH	237/246 (96%)	207 (87%)	30 (13%)	4	17
32	CI	357/371 (96%)	319 (89%)	38 (11%)	6	23
33	CJ	709/723 (98%)	619 (87%)	90 (13%)	4	17
34	CK	257/283 (91%)	220 (86%)	37 (14%)	3	13
35	CL	79/79 (100%)	63 (80%)	16 (20%)	1	4
36	CN	142/150 (95%)	122 (86%)	20 (14%)	3	14
37	CO	318/377 (84%)	267 (84%)	51 (16%)	2	10
38	CP	160/168 (95%)	142 (89%)	18 (11%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	CQ	171/270 (63%)	145 (85%)	26 (15%)	3	11
40	CR	275/279 (99%)	244 (89%)	31 (11%)	5	21
41	CS	126/220 (57%)	116 (92%)	10 (8%)	11	37
42	CU	160/169 (95%)	146 (91%)	14 (9%)	9	31
43	CZ	121/313 (39%)	108 (89%)	13 (11%)	6	23
44	Ca	516/543 (95%)	463 (90%)	53 (10%)	7	25
45	Cb	219/277 (79%)	194 (89%)	25 (11%)	5	21
46	Cd	237/381 (62%)	209 (88%)	28 (12%)	5	20
47	Cg	424/437 (97%)	383 (90%)	41 (10%)	8	28
48	Ci	144/160 (90%)	118 (82%)	26 (18%)	2	7
49	Cj	193/219 (88%)	171 (89%)	22 (11%)	5	21
50	Ck	608/747 (81%)	542 (89%)	66 (11%)	6	23
51	Cm	165/184 (90%)	140 (85%)	25 (15%)	3	11
52	Cn	95/210 (45%)	83 (87%)	12 (13%)	4	18
53	Cp	163/175 (93%)	146 (90%)	17 (10%)	7	24
54	Cq	210/221 (95%)	182 (87%)	28 (13%)	4	16
55	Cr	211/369 (57%)	183 (87%)	28 (13%)	4	16
56	Cv	912/1034 (88%)	797 (87%)	115 (13%)	4	18
All	All	17352/19794 (88%)	15389 (89%)	1963 (11%)	8	21

5 of 1963 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	DT	91	GLN
52	Cn	235	GLU
32	CI	406	THR
51	Cm	137	SER
56	Cv	530	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 490 such sidechains are listed below:

Mol	Chain	Res	Type
20	DH	275	HIS
51	Cm	73	HIS
29	CE	161	GLN

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Mol	Chain	Res	Type
50	Ck	682	ASN
56	Cv	535	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
57	CA	619/621 (99%)	287 (46%)	9 (1%)

5 of 287 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
57	CA	2	A
57	CA	3	A
57	CA	4	A
57	CA	5	U
57	CA	6	U

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	CA	527	A
57	CA	547	U
57	CA	275	U
57	CA	350	U
57	CA	361	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 43 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	SPD	CA	738	-	9,9,9	0.53	0	8,8,8	0.48	0
69	SPM	CA	740	-	13,13,13	0.34	0	12,12,12	0.81	0
68	SPD	CA	739	-	9,9,9	0.40	0	8,8,8	0.58	0
67	GTP	Cg	501	66	33,34,34	1.15	3 (9%)	50,54,54	1.61	12 (24%)
68	SPD	CA	737	-	9,9,9	0.34	0	8,8,8	0.71	0
68	SPD	CA	736	-	9,9,9	0.33	0	8,8,8	0.73	0
65	UTP	DJ	401	-	29,30,30	1.74	6 (20%)	43,47,47	1.84	11 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	SPD	CA	738	-	-	2/7/7/7	-
69	SPM	CA	740	-	-	4/11/11/11	-
68	SPD	CA	739	-	-	2/7/7/7	-
67	GTP	Cg	501	66	-	4/22/38/38	0/3/3/3
68	SPD	CA	737	-	-	0/7/7/7	-
68	SPD	CA	736	-	-	4/7/7/7	-
65	UTP	DJ	401	-	-	11/22/38/38	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	DJ	401	UTP	PA-O3A	4.48	1.64	1.59
67	Cg	501	GTP	PA-O3A	3.25	1.63	1.59
67	Cg	501	GTP	PB-O3A	3.10	1.62	1.59
65	DJ	401	UTP	PB-O3A	3.09	1.62	1.59
65	DJ	401	UTP	PB-O3B	2.92	1.62	1.59

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	DJ	401	UTP	C1'-N1-C2	4.91	126.40	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	DJ	401	UTP	N3-C2-N1	4.50	120.75	114.89
65	DJ	401	UTP	C4-N3-C2	-4.34	121.22	126.61
67	Cg	501	GTP	C5-C4-N3	-3.92	122.15	128.39
67	Cg	501	GTP	C2-N3-C4	3.59	118.48	112.30

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

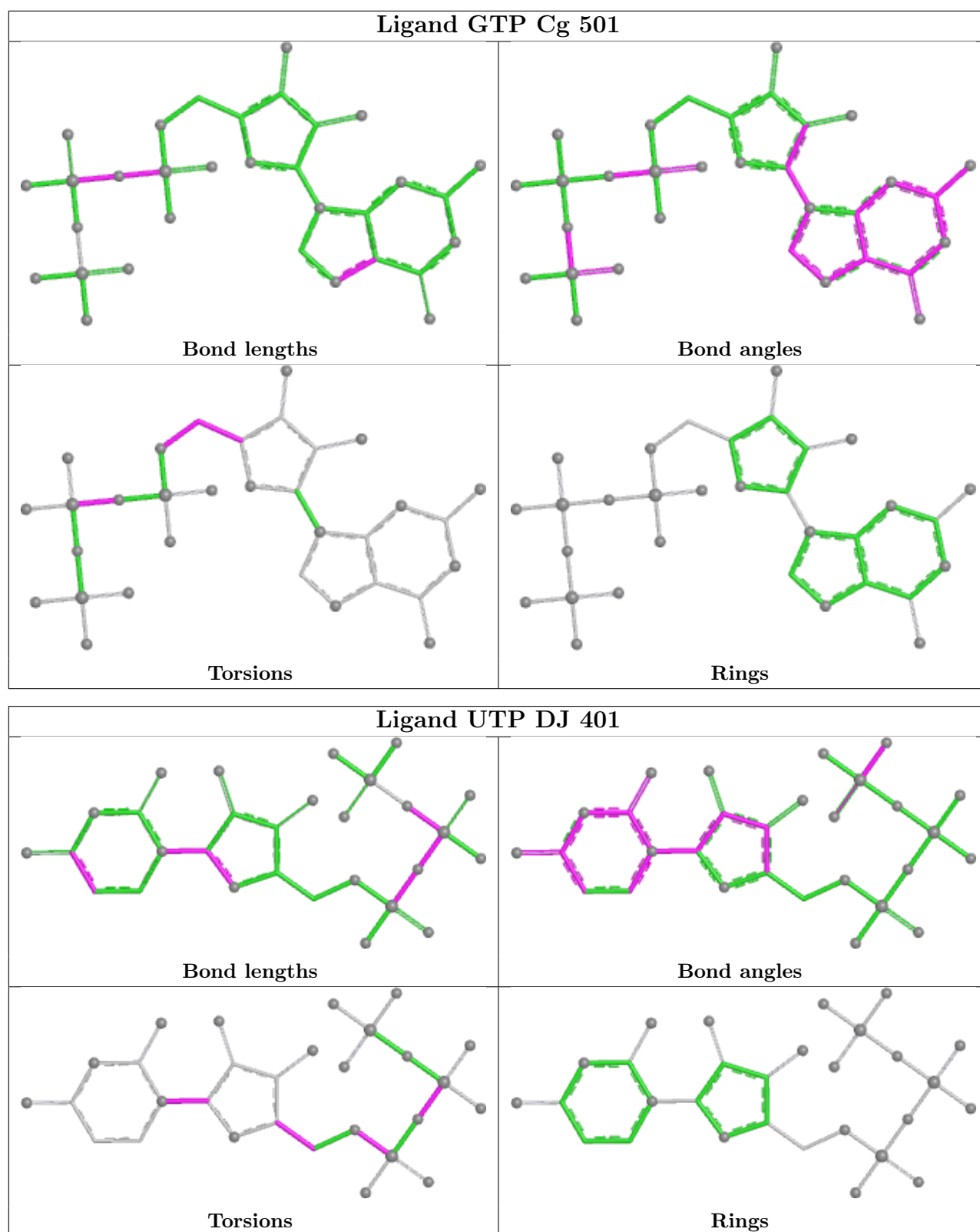
Mol	Chain	Res	Type	Atoms
65	DJ	401	UTP	C5'-O5'-PA-O1A
65	DJ	401	UTP	C5'-O5'-PA-O2A
65	DJ	401	UTP	C5'-O5'-PA-O3A
65	DJ	401	UTP	O4'-C4'-C5'-O5'
68	CA	738	SPD	C3-C4-C5-N6

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	CA	738	SPD	1	0
67	Cg	501	GTP	6	0
68	CA	737	SPD	1	0
68	CA	736	SPD	1	0
65	DJ	401	UTP	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
57	CA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CA	80:U	O3'	81:U	P	6.49

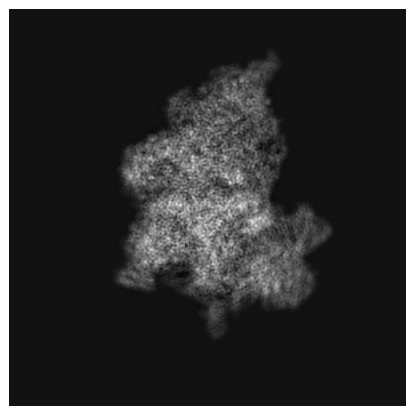
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0230. These allow visual inspection of the internal detail of the map and identification of artifacts.

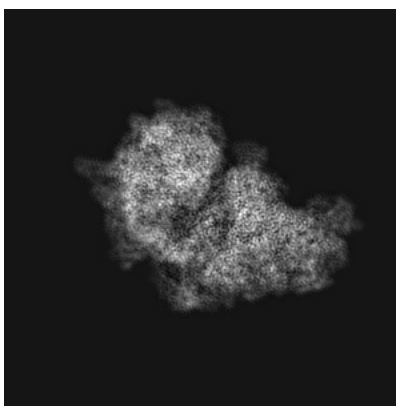
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

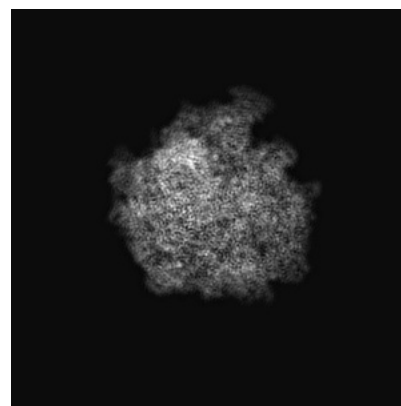
6.1.1 Primary map



X

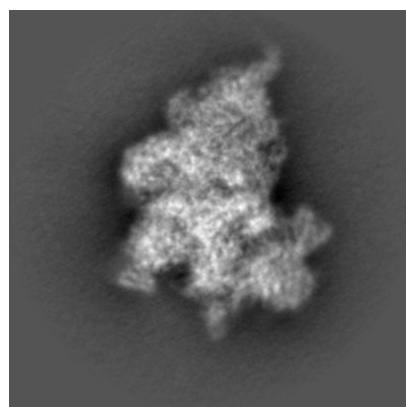


Y

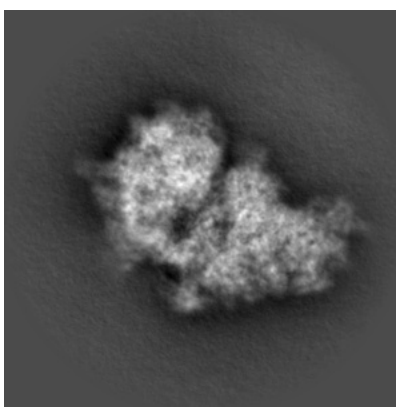


Z

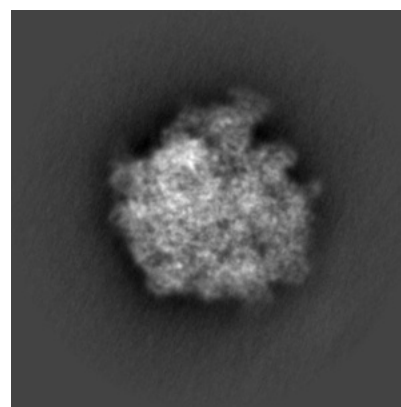
6.1.2 Raw map



X



Y

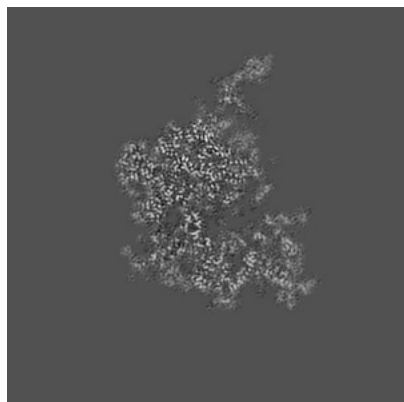


Z

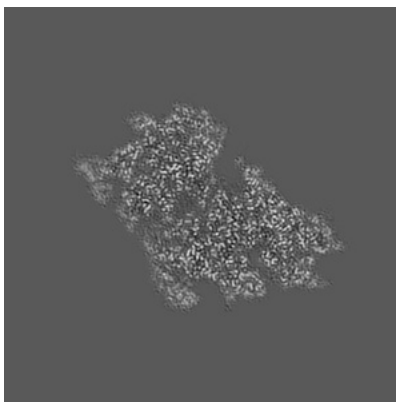
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

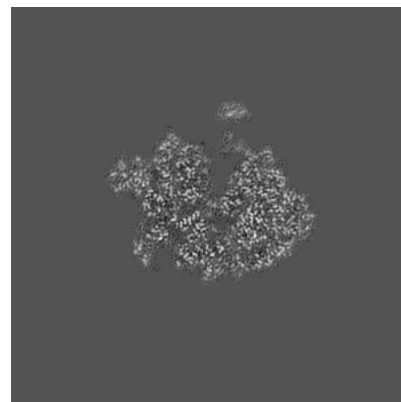
6.2.1 Primary map



X Index: 160

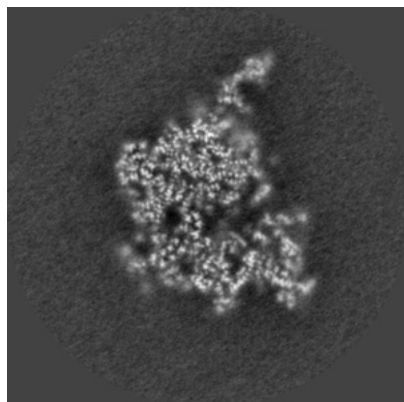


Y Index: 160

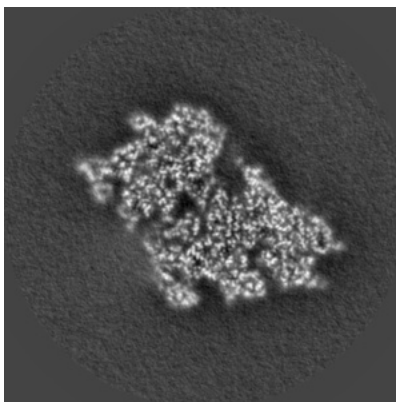


Z Index: 160

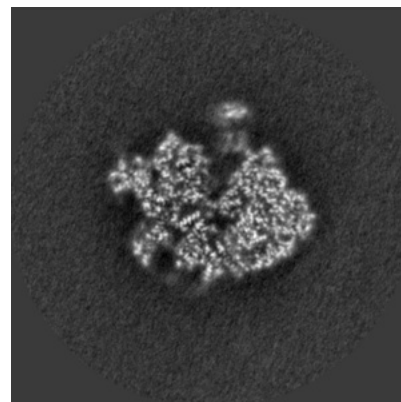
6.2.2 Raw map



X Index: 160



Y Index: 160

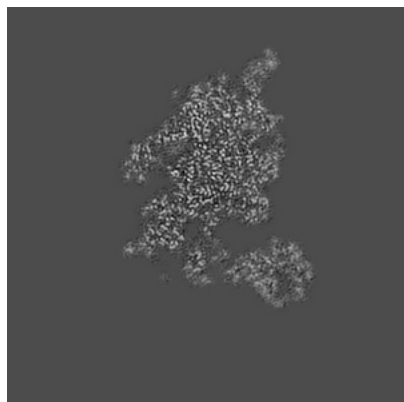


Z Index: 160

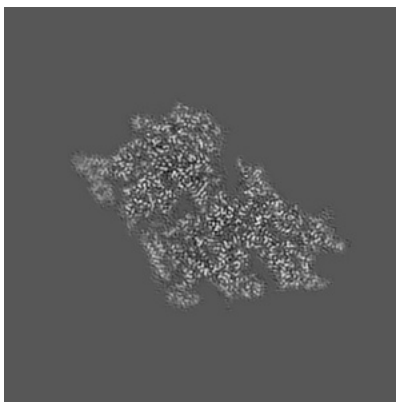
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

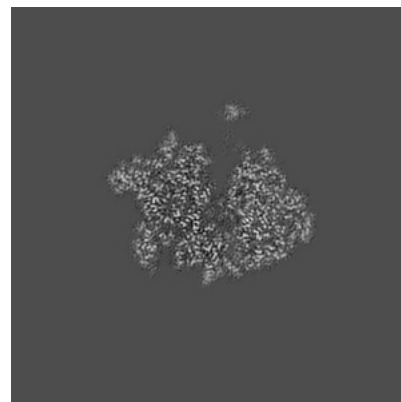
6.3.1 Primary map



X Index: 143

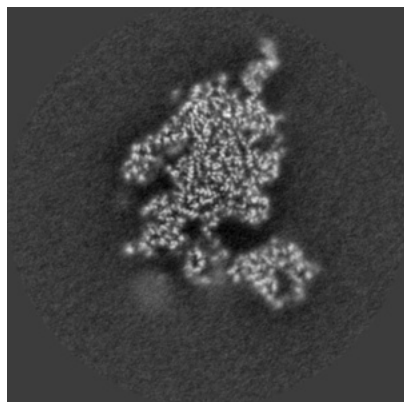


Y Index: 162

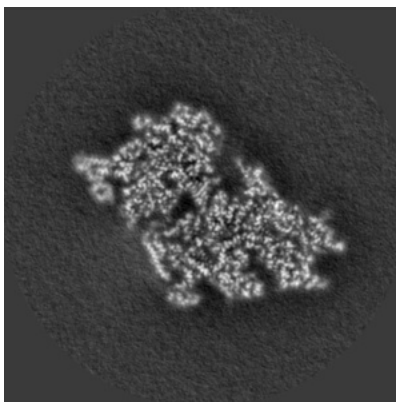


Z Index: 162

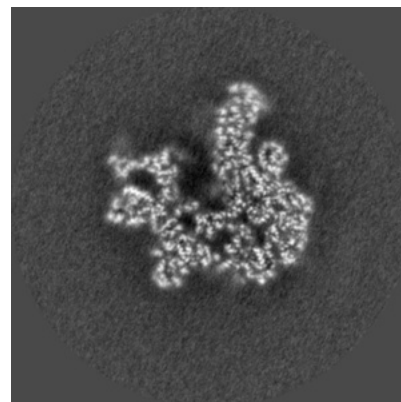
6.3.2 Raw map



X Index: 143



Y Index: 162

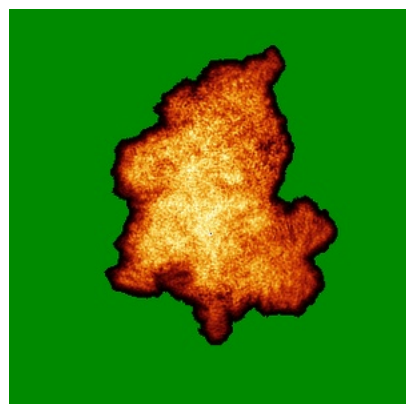


Z Index: 143

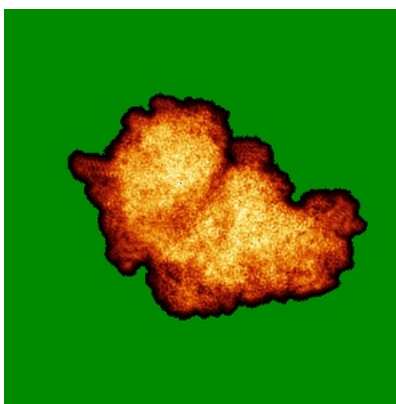
The images above show the largest variance slices of the map in three orthogonal directions.

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

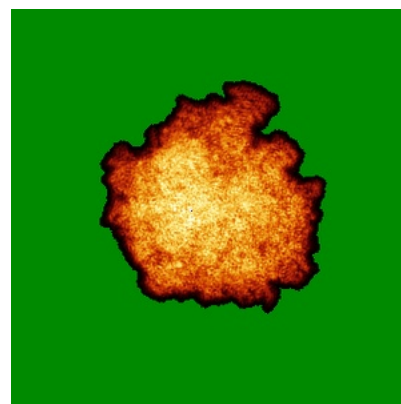
6.4.1 Primary map



X

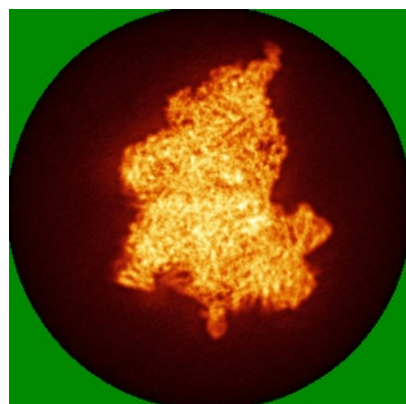


Y

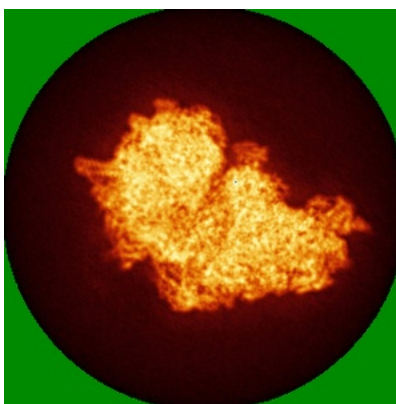


Z

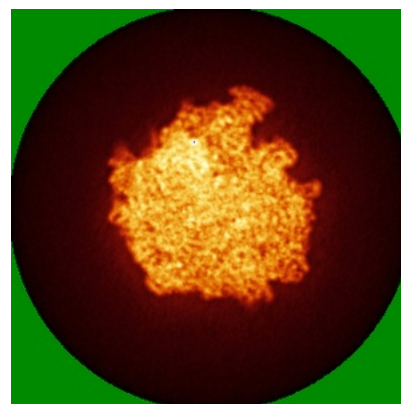
6.4.2 Raw map



X



Y

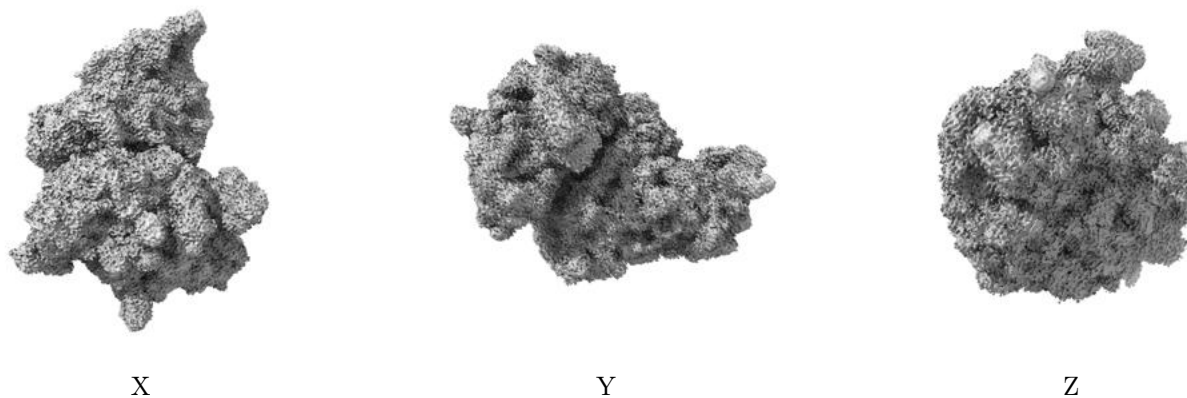


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0114. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

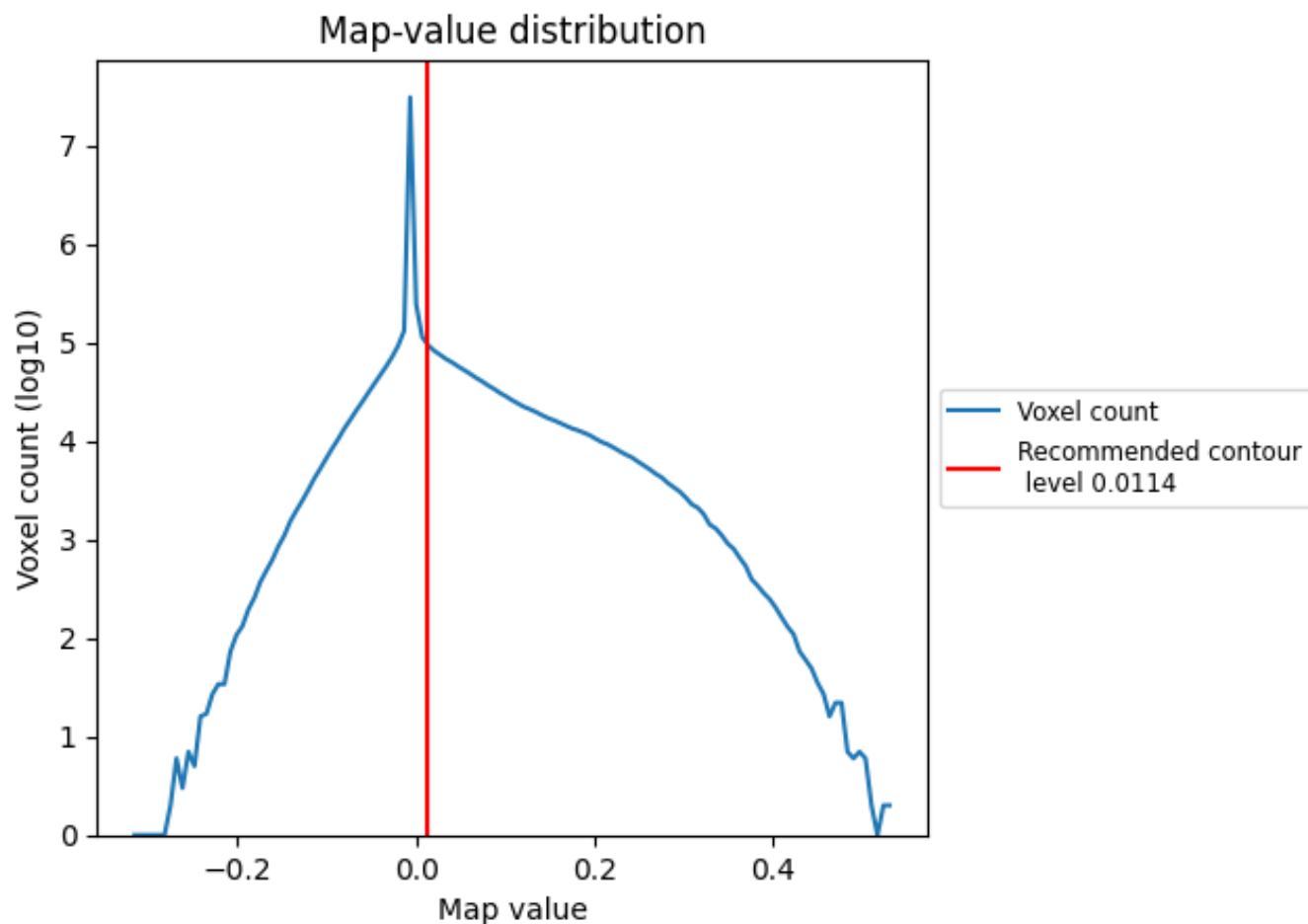
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

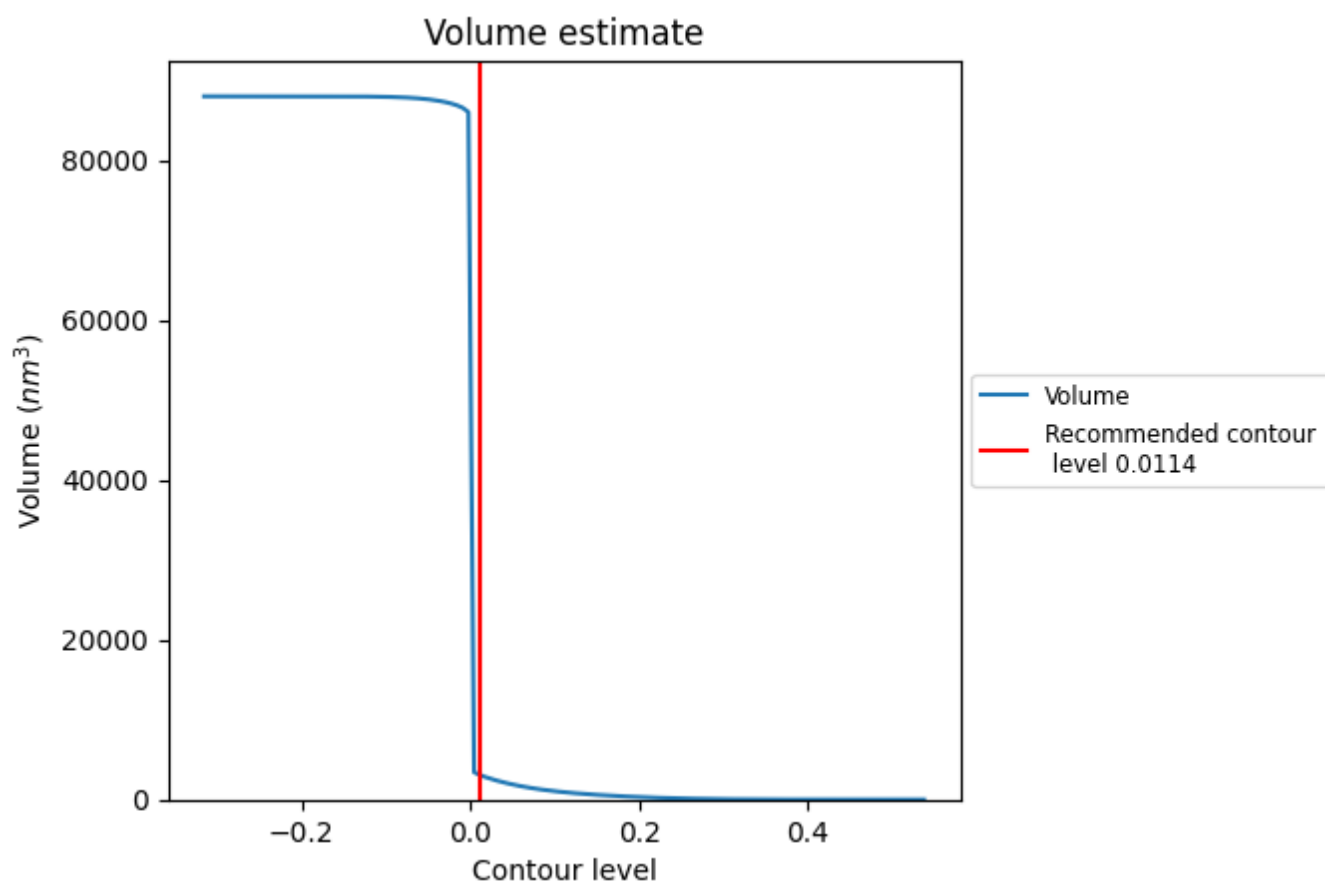
This section contains the results of statistical analysis of the map.

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.

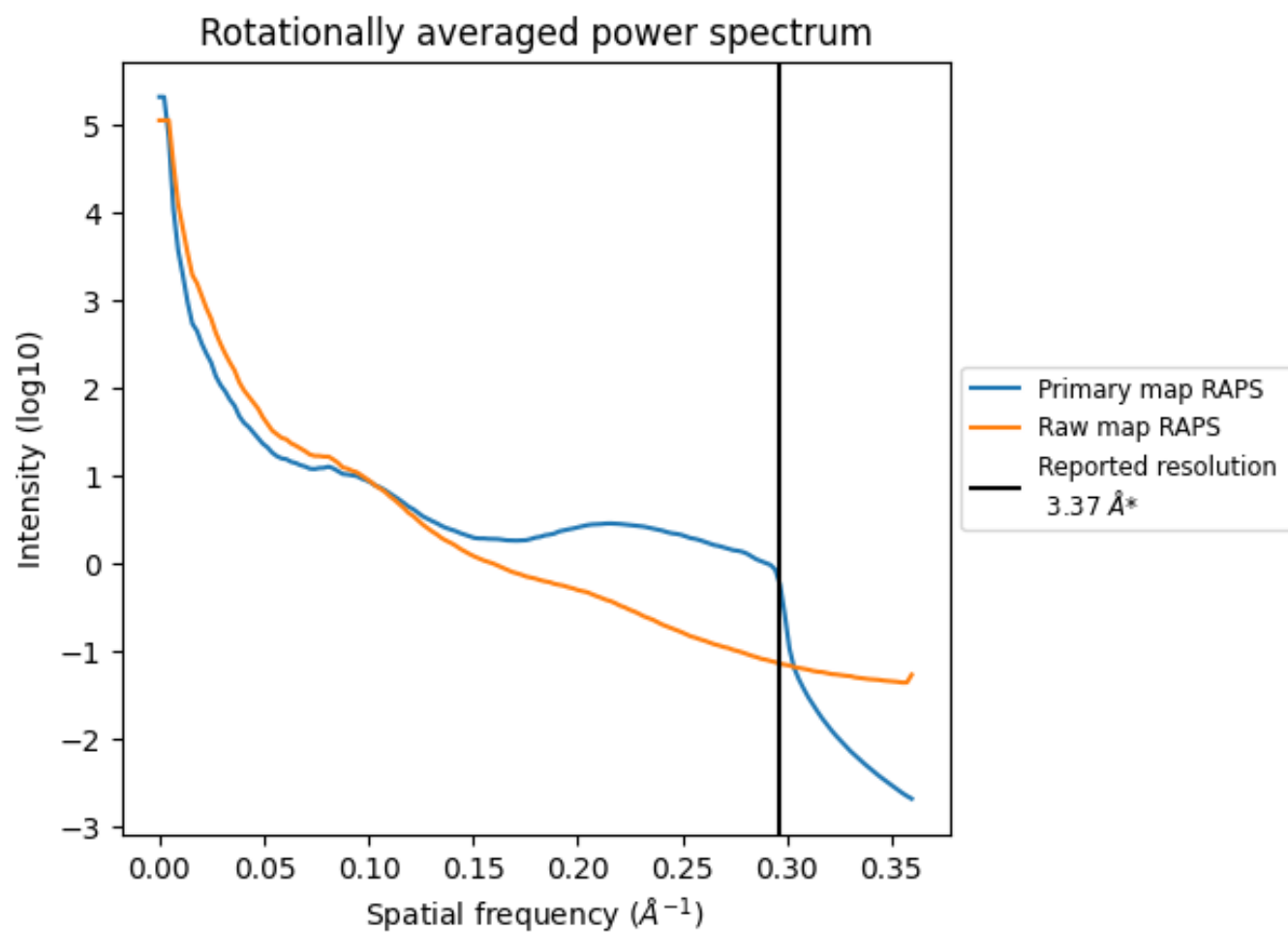
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3069 nm³; this corresponds to an approximate mass of 2773 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 ⓘ

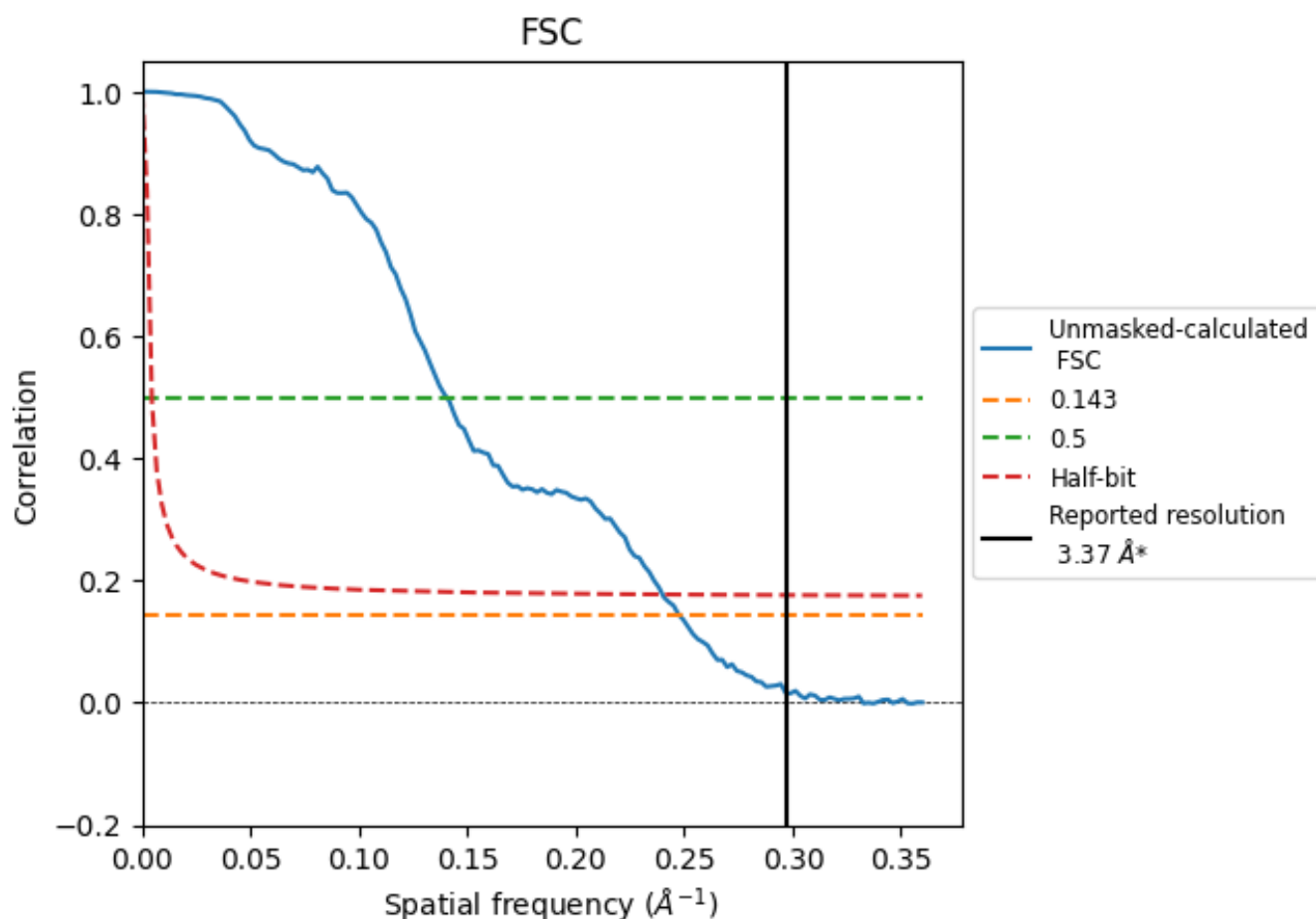


*Reported resolution corresponds to spatial frequency of $0.297 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.297 Å⁻¹

8.2 Resolution estimates [i](#)

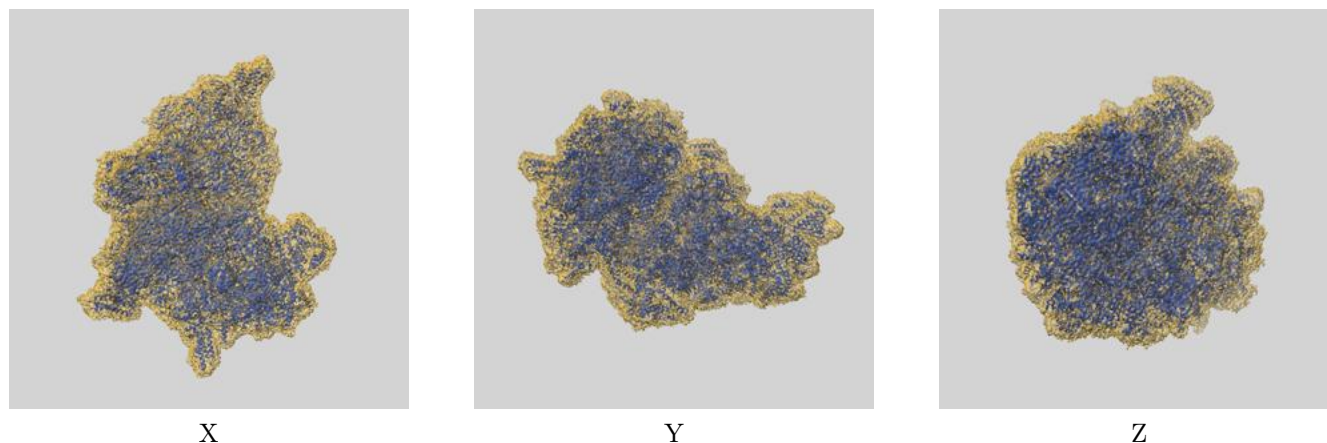
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	7.13	4.17

*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 4.04 differs from the reported value 3.37 by more than 10 %

9 Map-model fit [i](#)

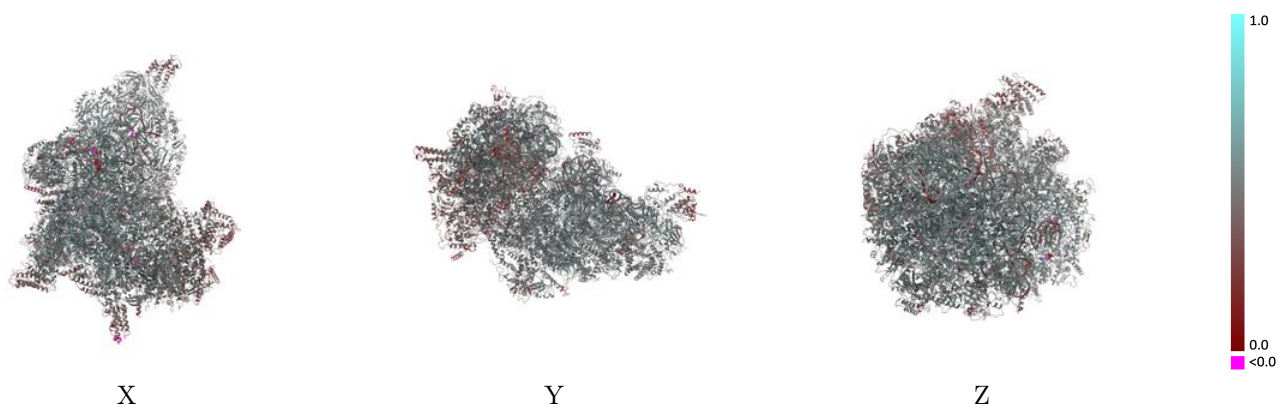
This section contains information regarding the fit between EMDB map EMD-0230 and PDB model 6HIW. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)



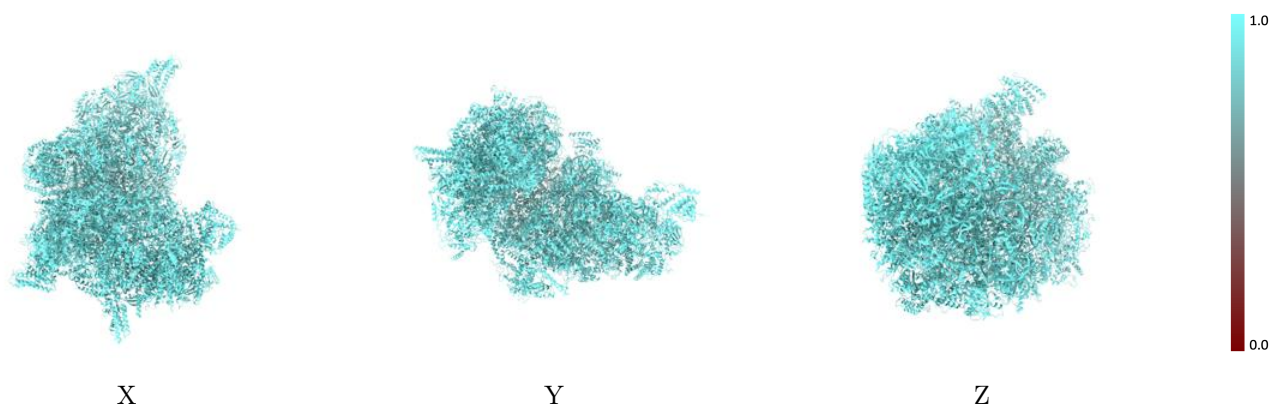
The images above show the 3D surface view of the map at the recommended contour level 0.0114 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



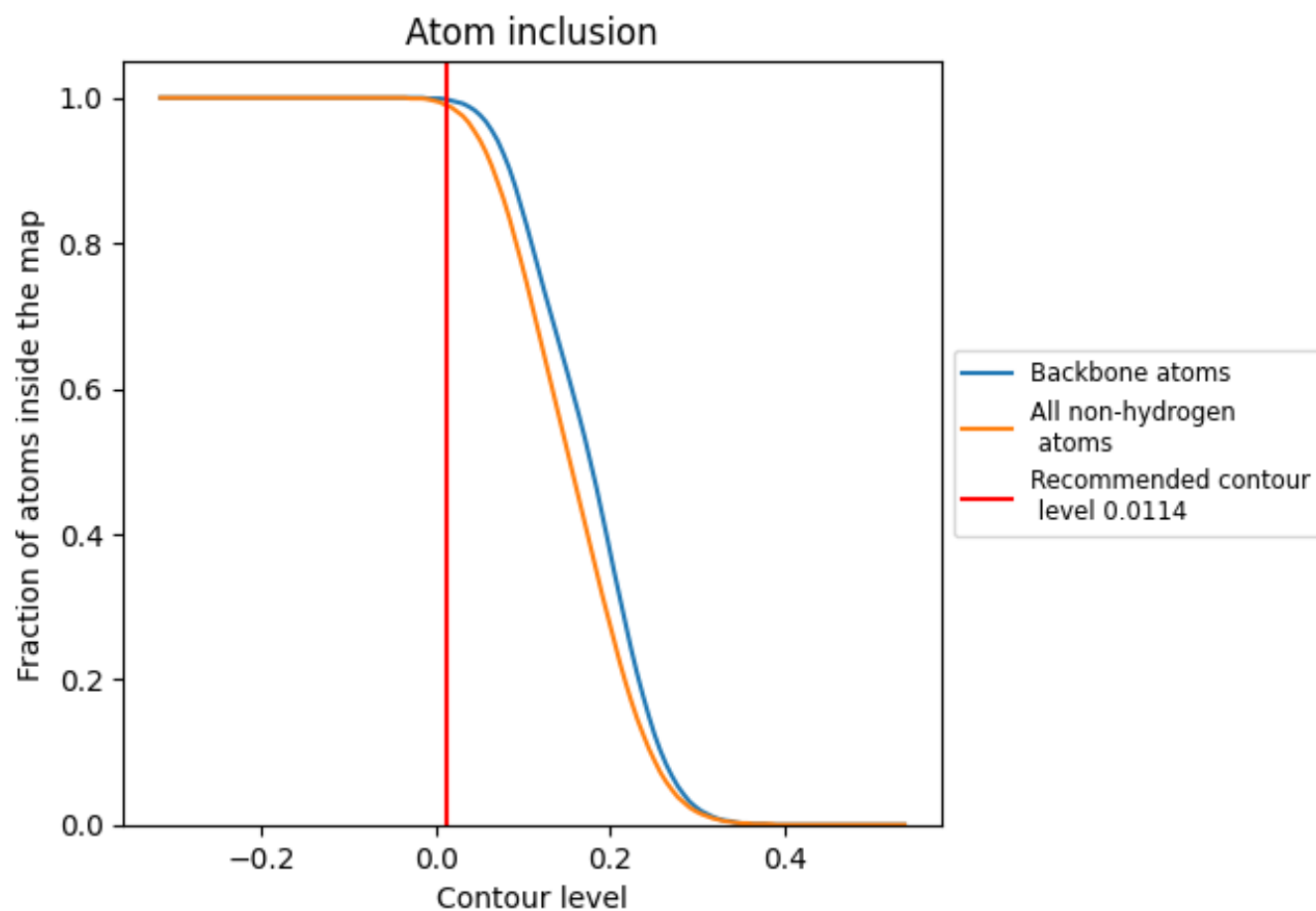
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0114).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0114) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9900	 0.4880
CA	 0.9940	 0.5000
CC	 0.9730	 0.5070
CE	 0.9920	 0.5330
CF	 0.9840	 0.4870
CH	 0.9830	 0.5160
CI	 0.9870	 0.5190
CJ	 0.9860	 0.5010
CK	 0.9940	 0.4860
CL	 0.9940	 0.5200
CN	 0.9910	 0.5310
CO	 0.9960	 0.5210
CP	 0.9960	 0.5250
CQ	 0.9970	 0.5500
CR	 0.9860	 0.5100
CS	 0.9950	 0.5120
CU	 0.9940	 0.5090
CZ	 0.9860	 0.3940
Ca	 0.9900	 0.5130
Cb	 0.9930	 0.4990
Cd	 0.9900	 0.4760
Cg	 0.9920	 0.5000
Ci	 0.9880	 0.5170
Cj	 0.9990	 0.4810
Ck	 0.9800	 0.4500
Cm	 0.9820	 0.5070
Cn	 0.9980	 0.5270
Cp	 0.9970	 0.4630
Cq	 0.9940	 0.5180
Cr	 0.9950	 0.4560
Cv	 0.9940	 0.5120
DA	 0.9920	 0.4800
DB	 0.9850	 0.4860
DC	 0.9880	 0.3980
DD	 0.9920	 0.5080



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Chain	Atom inclusion	Q-score
DE	 0.9910	 0.4280
DF	 0.9940	 0.4900
DG	 0.9890	 0.4560
DH	 0.9890	 0.4870
DI	 0.9960	 0.4970
DJ	 0.9920	 0.4820
DK	 0.9890	 0.4680
DL	 0.9750	 0.5140
DM	 0.9940	 0.5260
DN	 0.9900	 0.5130
DO	 0.9940	 0.4740
DP	 0.9970	 0.4270
DQ	 0.9960	 0.4900
DR	 0.9980	 0.4740
DS	 0.9990	 0.4800
DT	 0.9920	 0.4960
DU	 0.9920	 0.5000
DV	 0.9870	 0.5200
DW	 0.9910	 0.5100
DX	 0.9890	 0.5040
DY	 0.9890	 0.5170
DZ	 0.9880	 0.5220
Da	 1.0000	 0.5490
UO	 1.0000	 0.4330
UP	 1.0000	 0.3640
UQ	 0.9900	 0.4000
UR	 1.0000	 0.3800
US	 0.9940	 0.4110
UT	 0.9660	 0.3610