Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 08:34 am GMT

PDB ID	:	6HIY
EMDB ID	:	EMD-0232
Title	:	Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the body of the small mitoribosomal subunit in complex with mt-IF-3
Authors	:	Ramrath, D.J.F.; 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	:	3.27 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

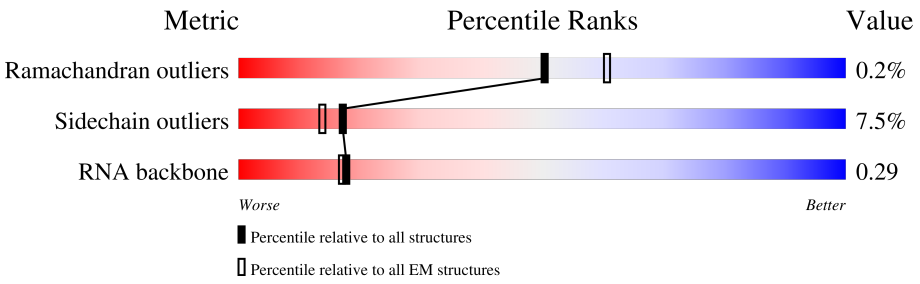
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.27 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)
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	DA	1788	75% 5% 20%
2	DD	812	92% 5% •
3	DI	407	90% 6% •
4	DL	307	44% • 54%
5	DM	294	94% 6%
6	DN	293	82% 5% 12%
7	DO	282	74% 5% 21%
8	DP	274	• 72% • 24%

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Mol	Chain	Length	Quality of chain
9	DQ	268	92%
10	DR	270	85% 7% 7%
11	DS	261	87% 5% 9%
12	DU	228	86% 8% 7%
13	DZ	94	84% 13%
14	Da	64	80% 6% 14%
15	CE	435	86% 9%
16	CF	160	95%
17	CH	282	88% 9%
18	CI	443	43% 54%
19	CK	326	68% 6% 26%
20	CL	87	90% 10%
21	CO	429	78% 6% 16%
22	CP	188	89% 7%
23	CQ	307	55% 7% 38%
24	CR	320	92% 6%
25	CU	193	90% 5% 5%
26	CZ	360	39% 58%
27	Ca	602	90% 8%
28	Cb	324	73% 5% 22%
29	Cd	440	61% 5% 34%
30	Cj	257	82% 6% 12%
31	Cm	215	80% 12% 9%
32	Cn	250	42% 56%
33	Cp	187	87% 6% 6%

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Mol	Chain	Length	Quality of chain
34	Cq	263	89% 6% •
35	Cr	439	53% 5% 41%
36	Cv	1211	82% 6% 13%
37	CA	621	42% 34% • 23%
38	UQ	32	100%
39	UR	8	100%
40	US	54	100%
41	UT	44	100%

2 Entry composition (i)

There are 45 unique types of molecules in this entry. The entry contains 100780 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
			Total	C	N	O	S		
1	DA	1426	11489	7252	2052	2151	34	0	0

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
			Total	C	N	O	S		
2	DD	791	6523	4127	1184	1171	41	0	0

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
			Total	C	N	O	S		
3	DI	390	3182	2020	554	594	14	0	0

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
			Total	C	N	O	S		
4	DL	140	1134	718	208	199	9	0	0

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
			Total	C	N	O	S		
5	DM	294	2430	1533	459	426	12	0	0

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
			Total	C	N	O	S		
6	DN	257	2091	1331	379	371	10	0	0

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
			Total	C	N	O	S		
7	DO	222	1804	1127	327	340	10	0	0

- Molecule 8 is a protein called mS63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	DP	207	1760	1132	312	307	9	0	0

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
			Total	C	N	O	S		
9	DQ	256	2061	1293	389	370	9	0	0

- Molecule 10 is a protein called mS65.

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

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
			Total	C	N	O	S		
11	DS	238	1904	1185	356	348	15	0	0

- Molecule 12 is a protein called mS68.

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

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
			Total	C	N	O	S		
13	DZ	82	697	457	113	123	4	0	0

- Molecule 14 is a protein called mS74.

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

- Molecule 15 is a protein called mS55m.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 16 is a protein called bS6m.

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

- Molecule 17 is a protein called uS8m.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	CI	202	1632	1035	281	309	7	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 19 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	CK	241	1980	1234	368	363	15	0	0

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 20 is a protein called uS12m.

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

- Molecule 21 is a protein called uS15m.

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

- Molecule 22 is a protein called bS16m.

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

- Molecule 23 is a protein called uS17m.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 24 is a protein called bS18m.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 25 is a protein called uS21m.

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

- Molecule 26 is a protein called mt-IF-3.

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

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 27 is a protein called mS22.

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

- Molecule 28 is a protein called mS23.

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

There are 15 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	CYS	-	expression tag	UNP Q57VB2
Cb	313	SER	-	expression tag	UNP Q57VB2
Cb	314	ARG	-	expression tag	UNP Q57VB2
Cb	315	ASP	-	expression tag	UNP Q57VB2
Cb	316	GLY	-	expression tag	UNP Q57VB2
Cb	317	PHE	-	expression tag	UNP Q57VB2
Cb	318	ALA	-	expression tag	UNP Q57VB2
Cb	319	LEU	-	expression tag	UNP Q57VB2
Cb	320	MET	-	expression tag	UNP Q57VB2
Cb	321	LYS	-	expression tag	UNP Q57VB2
Cb	322	ALA	-	expression tag	UNP Q57VB2
Cb	323	ASN	-	expression tag	UNP Q57VB2
Cb	324	LYS	-	expression tag	UNP Q57VB2

- Molecule 29 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Cd	291	2389	1491	442	446	10	0	0

- Molecule 30 is a protein called mS34.

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

- Molecule 31 is a protein called mS37.

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

- Molecule 32 is a protein called mS38.

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

- Molecule 33 is a protein called mS41.

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

- Molecule 34 is a protein called mS42.

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

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 35 is a protein called mS43.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 36 is a protein called mS47.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cv	16	CYS	PRO	conflict	UNP Q383R4
Cv	718	THR	ALA	conflict	UNP Q383R4
Cv	1179	GLU	GLY	conflict	UNP Q383R4

- Molecule 37 is a RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	CA	478	10092	4542	1705	3367	478	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	298	U	C	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 38 is a protein called Unknown protein.

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

- Molecule 39 is a protein called Unknown protein.

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

- Molecule 40 is a protein called Unknown protein.

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

- Molecule 41 is a protein called Unknown protein.

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

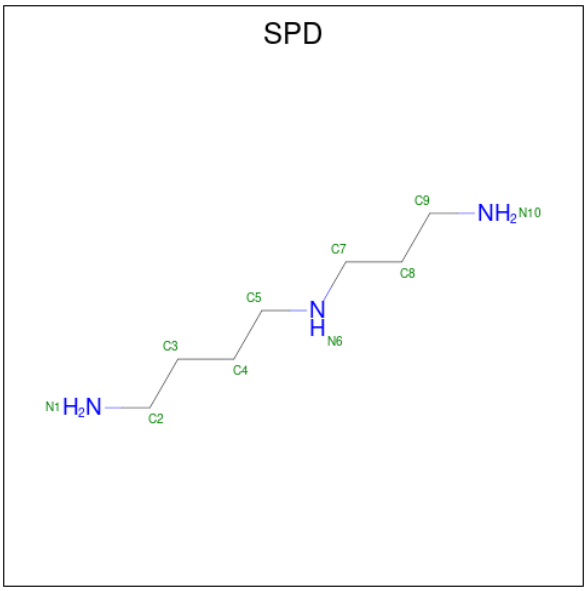
- Molecule 42 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

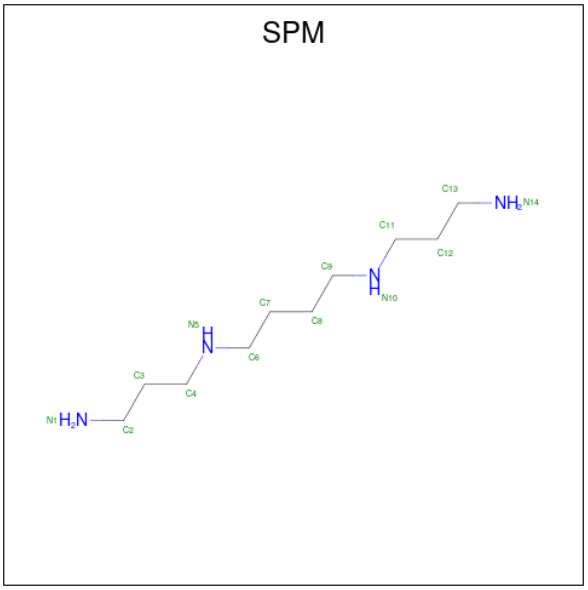
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
43	CO	1	1	1	0
43	CQ	1	1	1	0
43	Ca	1	1	1	0
43	Cv	1	1	1	0
43	CA	32	32	32	0

- Molecule 44 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
44	CA	1	20	14	6	0
			Total	C	N	
44	CA	1	20	14	6	0

- Molecule 45 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



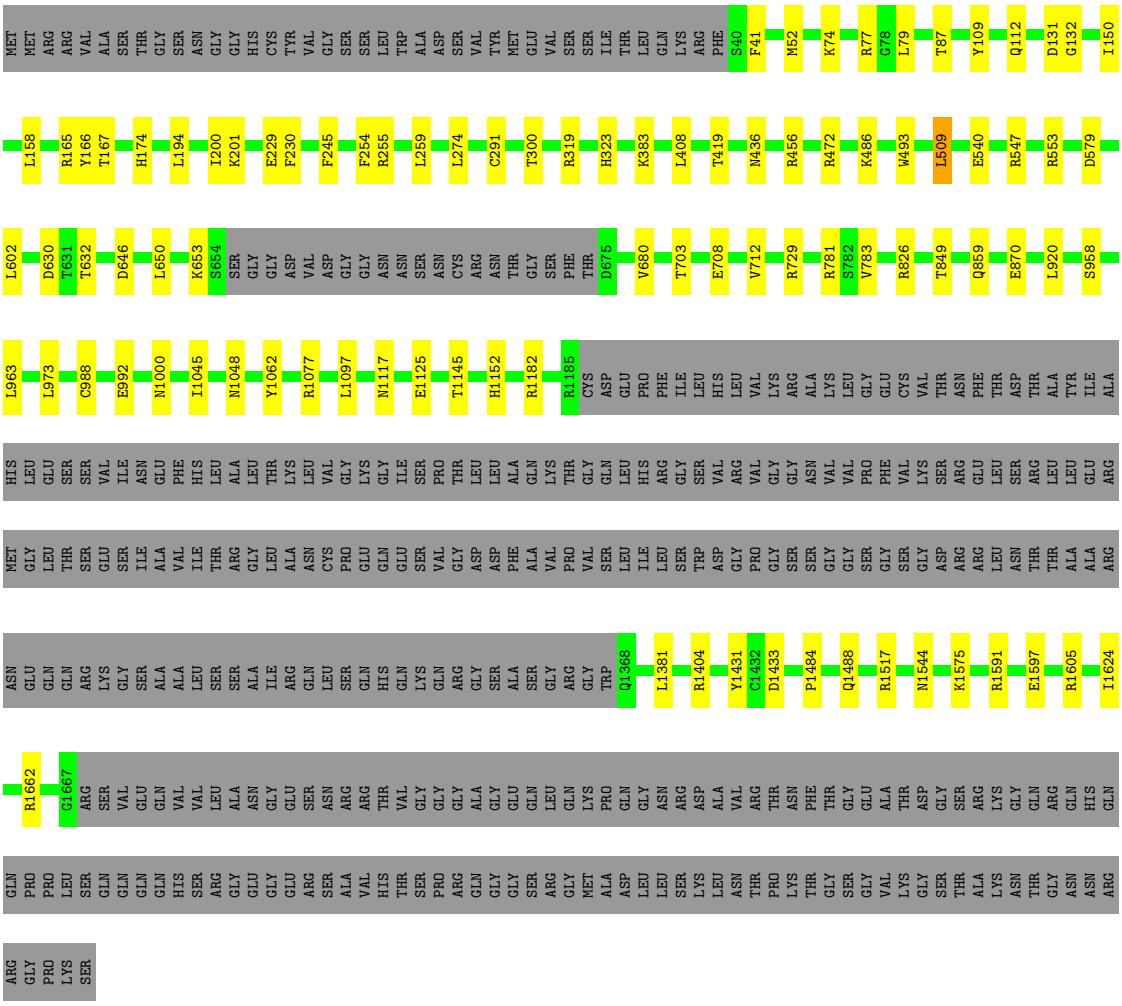
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
45	CA	1	14	10	4	0

3 Residue-property plots (i)

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

- Molecule 1: mS48

Chain DA: 75% 5% 20%



- Molecule 2: mS51

Chain DD: 92% 5%

MET LEU ARG CYS THR VAL VAL GLY HIS H10 R11 S12 M27 M48 D72 Q79 K94 T108 Q122 R123 R129 R146 S151 Q173 E201 E221 T226 N233 D248 V255 P256 M298 R358 E377 M378 Q379 K394 L452

N453 T454 N504 N521 R541 K577 W592 T624 R634 I646 R651 T652 F653 R654 N679 D704 P721 GLY TYR TYR ALA PRO PRO MET GLU GLY GLU HIS GLN R734 R741 S770 R787 D799 Y812

- Molecule 3: mS56

Chain DI: 90% 6% •

MET ARG LYS PHE CYS HIS PHE MET ALA ASN CYS TRP ASN SER ALA ARG SER H18 I79 L90 V113 D116 D159 E164 Q175 F178 D179 E180 P190 V191 T192 Y232 R233 R237 D261 D282 L310 R313 L344 L345 K353 I362

R365 T399 L407

- Molecule 4: mS59

Chain DL: 44% • 54%

MET ARG CYS SER CYS ALA PHE LEU ASP LYS SER VAL PHE ALA ALA LYS ARG ARG VAL ILE VAL PRO ILE HIS PRO THR PRO ASN PHE PRO ALA HIS PHE ILE LYS SER ALA PHE THR THR ASP PRO LEU LYS GLU LYS GLN LYS ALA ARG PHE SER SER GLY GLY GLU ALA MET ARG GLU

VAL GLN ASP ILE PRO LYS ASN LEU GLU GLY GLU ARG SER ARG ARG ARG ASP LEU ALA SER ARG GLY ASP THR GLU PHE GLN ALA LEU VAL GLU PHE ILE GLU GLY ALA SER TYR ASP GLN LEU ILE SER GLY ARG ARG PHE LYS LYS VAL TYR ASP VAL LEU SER GLU ASN D117 M136

L145 T158 F165 S256 GLN GLN SER LEU GLU ARG ARG ARG ARG GLY HIS VAL MET THR PRO HIS THR THR LEU HIS GLY ARG ARG ILE PHE PHE TRP ILE PRO PRO THR TRP ASN ARG ALA GLY ARG PHE LEU GLY PRO HIS VAL THR LEU TYR PRO GLY MET THR PRO ASP

- Molecule 5: mS60

Chain DM: 94% 6%

M1 L15 R30 F46 W56 R59 R72 N76 L90 R103 I128 R129 D130 N131 L157 R179 K185 L199 K253 L275 W294

- Molecule 6: mS61

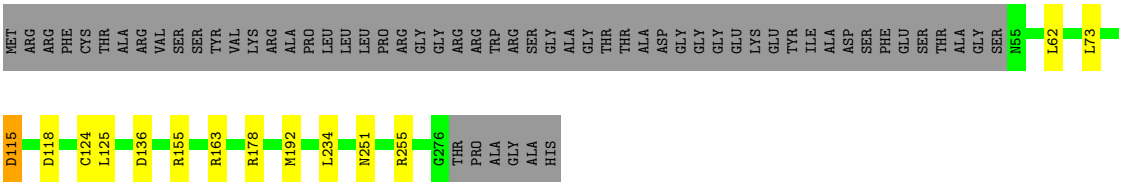
Chain DN: 82% 5% 12%

MET LEU CYS ARG THR PHE LEU ARG GLN F10 R11 V23 T42 N79 ALA THR SER ASN GLY GLY LYS LYS GLU ALA ARG PRO GLN LYS GLY GLY PHE ALA SER GLY SER PRO SER VAL GLY ARG ASN E107 A108 N109 M141 R142 L152 L162 Q223 R224 R237

Q246 Q276 F288 Y292 P293

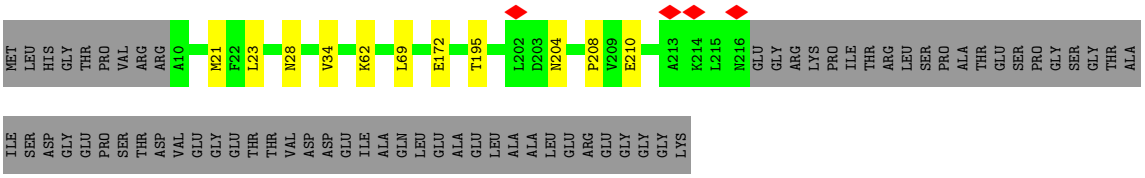
- Molecule 7: mS62

Chain DO: 74% 5% 21%



• Molecule 8: mS63

Chain DP:

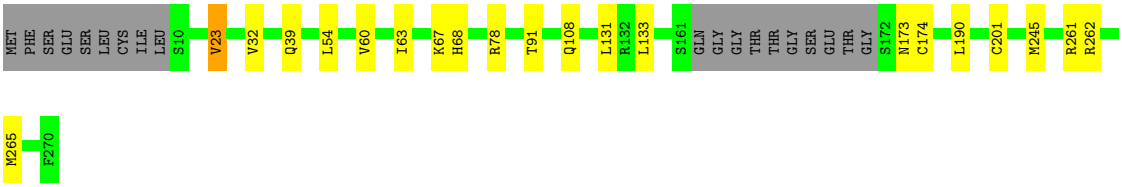


• Molecule 9: mS64

Chain DQ:

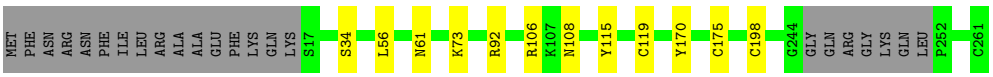
• Molecule 10: mS65

Chain DR:



• Molecule 11: mS66

Chain DS:

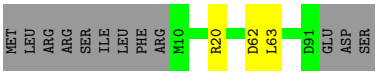


• Molecule 12: mS68

Chain DU:

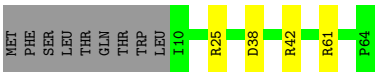
• Molecule 13: mS73

Chain DZ:



- Molecule 14: mS74

Chain Da:

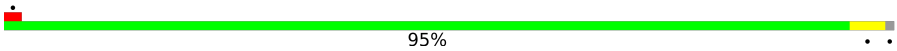


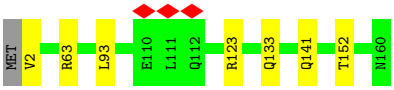
- Molecule 15: mS55m

Chain CE:

- Molecule 16: bS6m

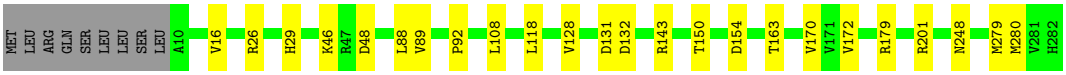
Chain CF:





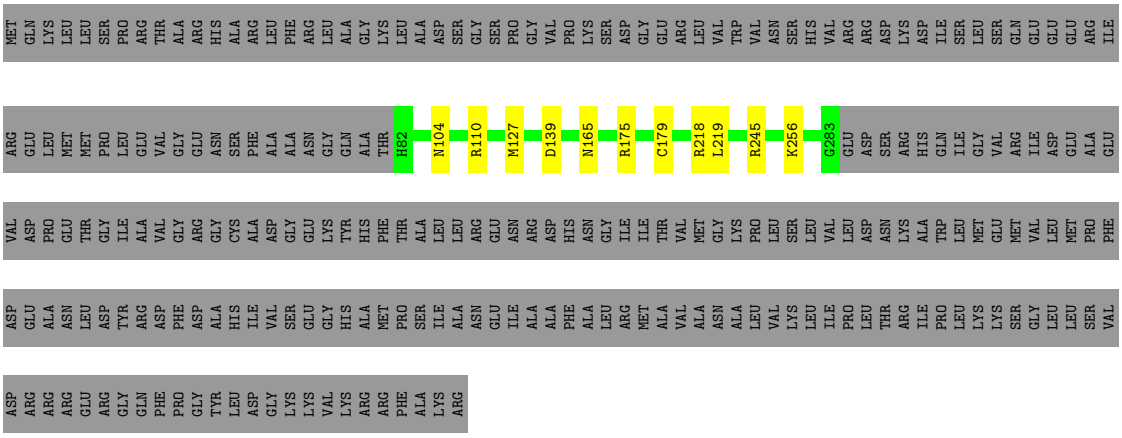
- Molecule 17: uS8m

Chain CH:



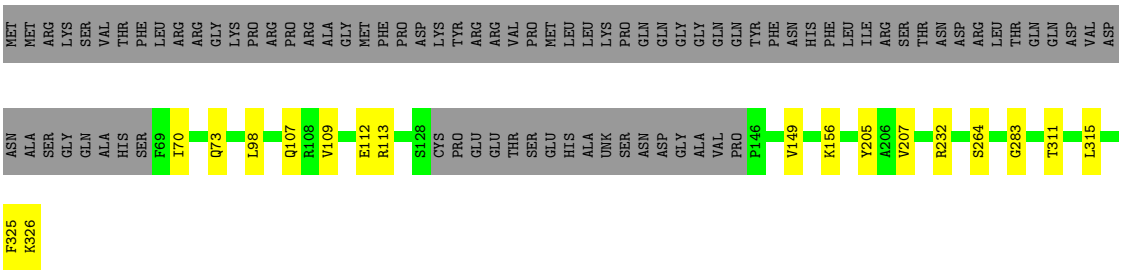
- Molecule 18: uS9m

Chain CI:



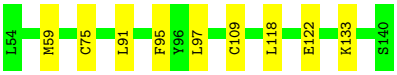
- Molecule 19: uS11m

Chain CK:



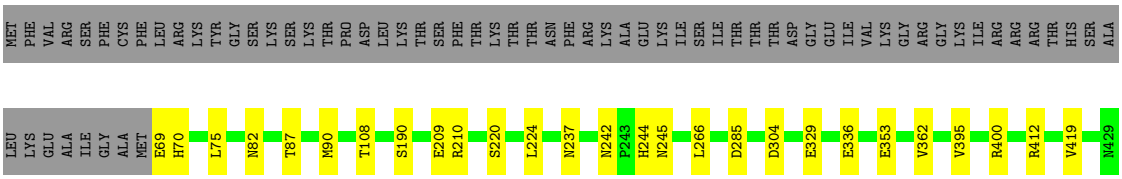
- Molecule 20: uS12m

Chain CL:



- Molecule 21: uS15m

Chain CO:

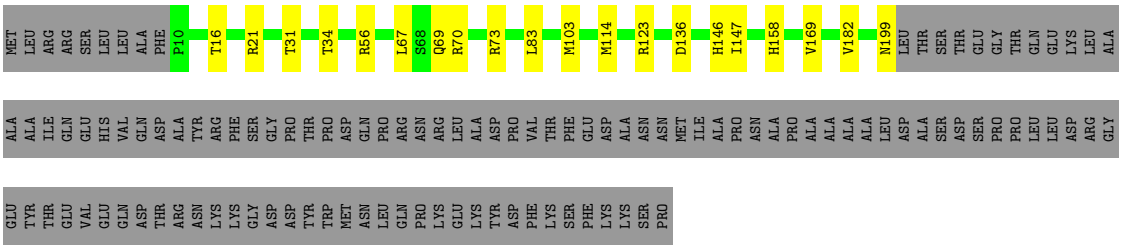


- Molecule 22: bS16m

Chain CP:

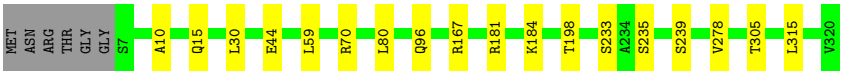
- Molecule 23: uS17m

Chain CQ:



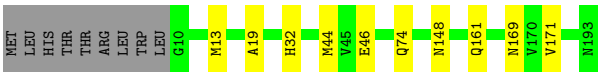
- Molecule 24: bS18m

Chain CR:



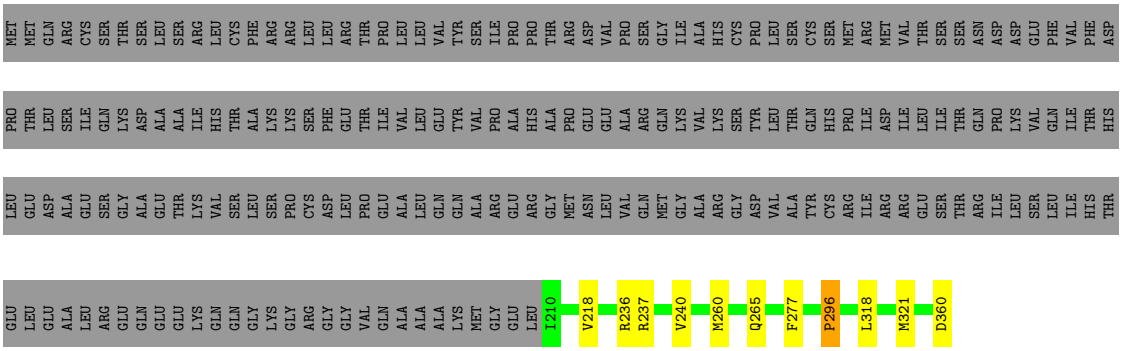
- Molecule 25: uS21m

Chain CU:



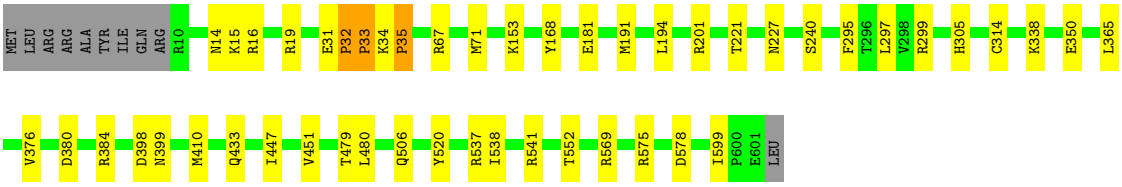
- Molecule 26: mt-IF-3

Chain CZ:



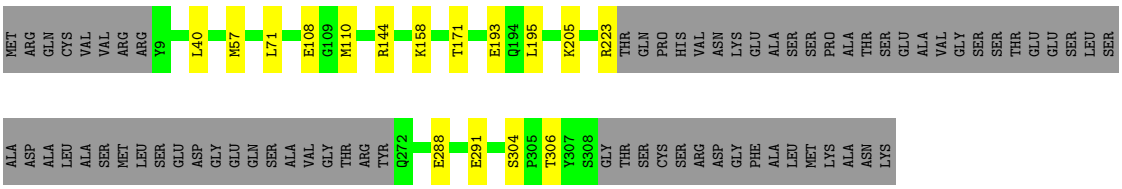
- Molecule 27: mS22

Chain Ca:



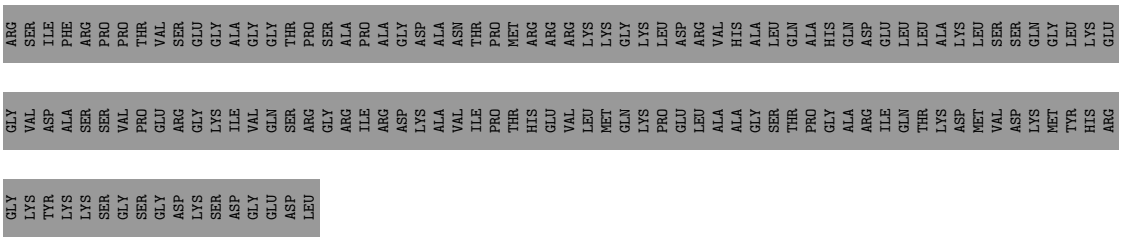
- Molecule 28: mS23

Chain Cb:



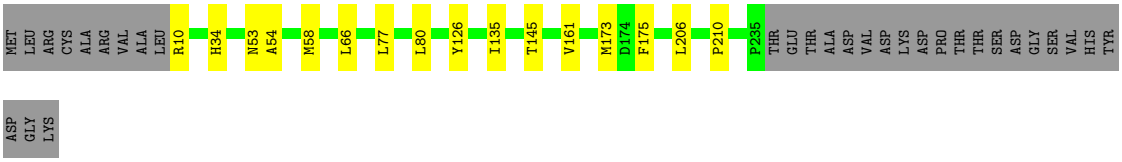
- Molecule 29: mS26

Chain Cd:



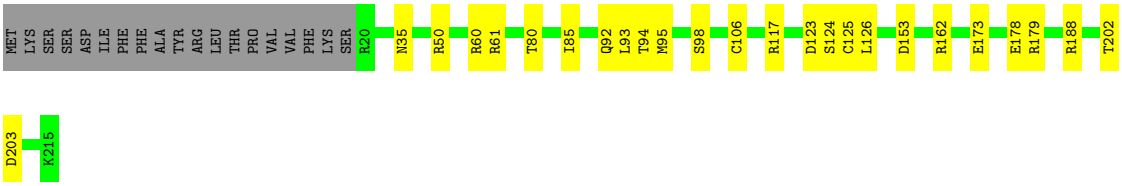
- Molecule 30: mS34

Chain Cj:



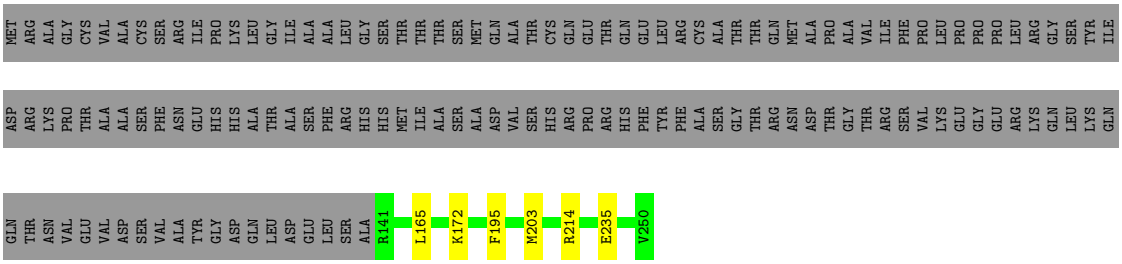
- Molecule 31: mS37

Chain Cm:



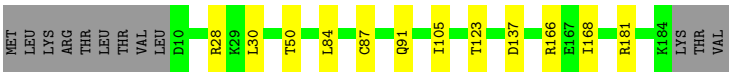
- Molecule 32: mS38

Chain Cn:



- Molecule 33: mS41

Chain Cp:

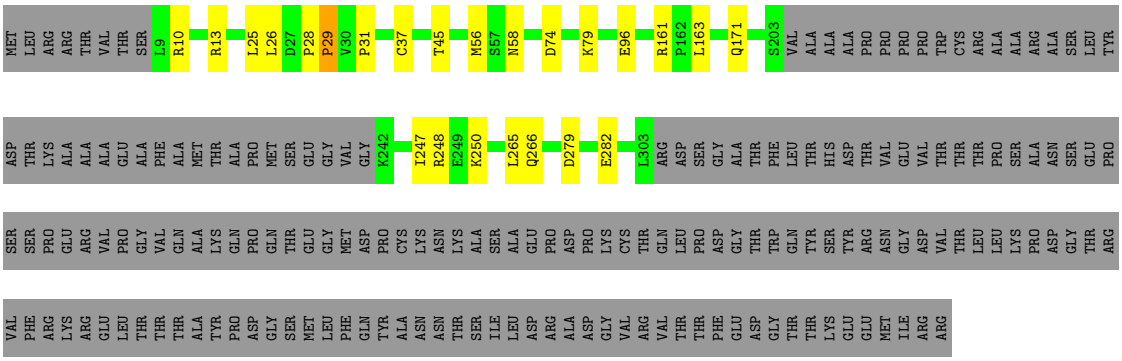


- Molecule 34: mS42

Chain Cq:

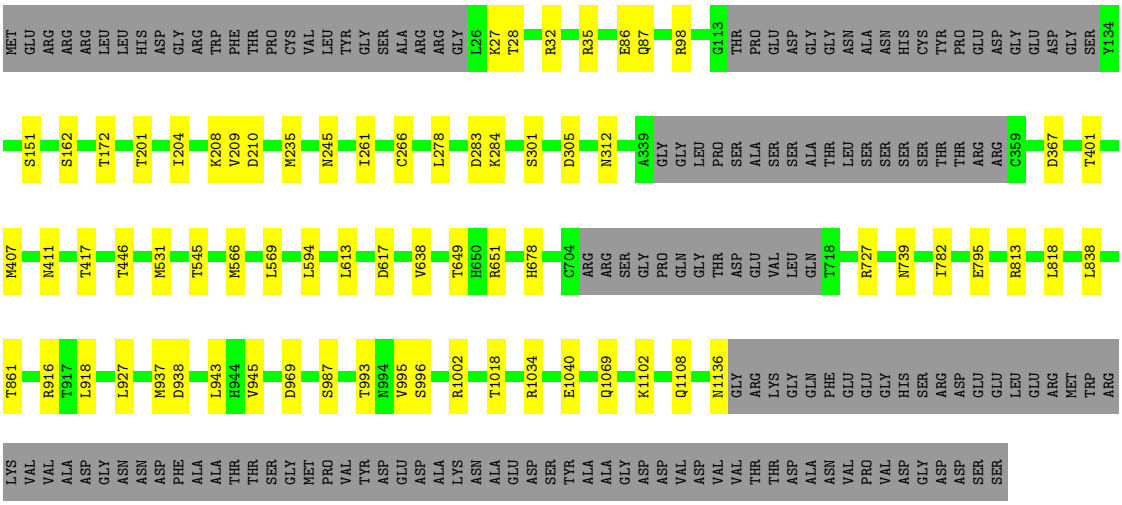
- Molecule 35: mS43

Chain Cr:



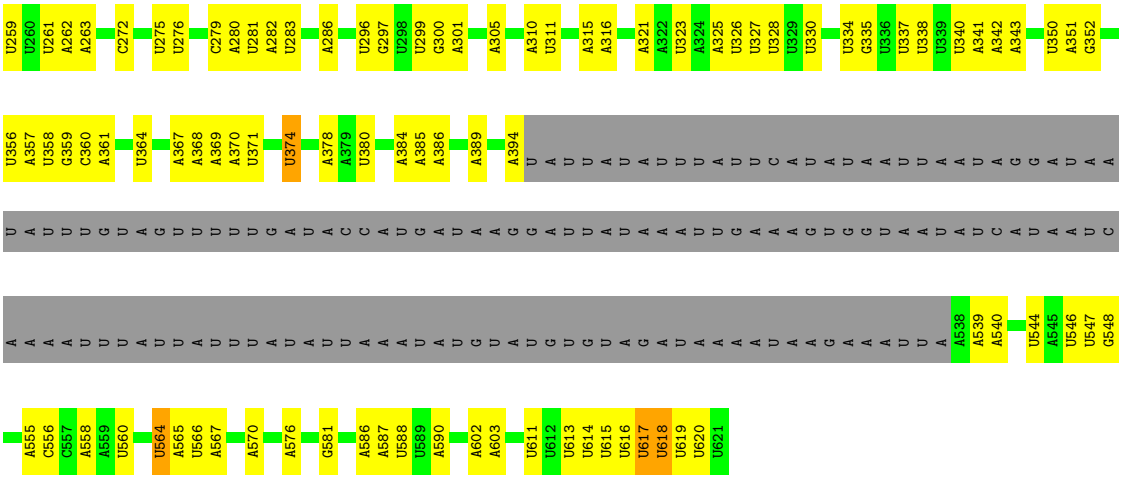
- Molecule 36: mS47

Chain Cv:



- Molecule 37: 9S rRNA

Chain CA:



- Molecule 38: Unknown protein

Chain UQ: 100%

There are no outlier residues recorded for this chain.

- Molecule 39: Unknown protein

Chain UR: 100%

There are no outlier residues recorded for this chain.

- Molecule 40: Unknown protein

Chain US: 100%

There are no outlier residues recorded for this chain.

- Molecule 41: Unknown protein

Chain UT: 100%

There are no outlier residues recorded for this chain.

4 Experimental information (i)

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 ($e^-/Å^2$)	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	0.514	Depositor
Minimum map value	-0.265	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0115	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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	DA	0.38	1/11769 (0.0%)	0.55	2/15925 (0.0%)
2	DD	0.38	0/6710	0.56	1/9087 (0.0%)
3	DI	0.37	0/3248	0.57	2/4401 (0.0%)
4	DL	0.41	0/1160	0.56	0/1560
5	DM	0.39	0/2488	0.55	0/3362
6	DN	0.40	0/2148	0.59	0/2916
7	DO	0.38	0/1840	0.56	0/2482
8	DP	0.52	1/1813 (0.1%)	0.56	0/2457
9	DQ	0.37	0/2111	0.56	0/2863
10	DR	0.36	0/2090	0.56	0/2849
11	DS	0.35	0/1950	0.52	0/2633
12	DU	0.38	0/1799	0.54	0/2438
13	DZ	0.38	0/725	0.55	0/984
14	Da	0.40	0/520	0.54	0/694
15	CE	0.40	0/3484	0.56	0/4708
16	CF	0.38	0/1319	0.53	0/1783
17	CH	0.42	0/2276	0.55	0/3071
18	CI	0.37	0/1670	0.51	0/2260
19	CK	0.37	0/2024	0.56	1/2715 (0.0%)
20	CL	0.42	0/759	0.55	0/1026
21	CO	0.38	0/3085	0.54	0/4165
22	CP	0.42	0/1533	0.57	0/2074
23	CQ	0.46	0/1631	0.59	0/2203
24	CR	0.39	0/2640	0.55	0/3572
25	CU	0.38	0/1576	0.52	0/2115
26	CZ	0.39	0/1237	0.54	1/1659 (0.1%)
27	Ca	0.40	0/5159	0.55	3/6980 (0.0%)
28	Cb	0.39	0/2105	0.54	0/2842
29	Cd	0.40	0/2446	0.51	0/3299
30	Cj	0.35	0/1842	0.55	0/2511
31	Cm	0.42	0/1616	0.60	1/2175 (0.0%)
32	Cn	0.40	0/934	0.57	0/1248

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Cp	0.36	0/1528	0.51	0/2072
34	Cq	0.40	0/2066	0.54	0/2815
35	Cr	0.36	0/2038	0.56	3/2759 (0.1%)
36	Cv	0.37	0/8780	0.55	0/11901
37	CA	0.51	1/11286 (0.0%)	0.96	16/17548 (0.1%)
All	All	0.40	3/103405 (0.0%)	0.62	30/142152 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	DA	0	1
2	DD	0	2
6	DN	0	2
7	DO	0	2
10	DR	0	1
17	CH	0	1
27	Ca	0	1
30	Cj	0	1
36	Cv	0	2
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DA	323	HIS	CG-CD2	6.72	1.47	1.35
37	CA	310	A	N9-C4	5.63	1.41	1.37
8	DP	210	GLU	CD-OE2	5.46	1.31	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	CK	283	GLY	N-CA-C	7.77	132.53	113.10
37	CA	188	U	C2-N1-C1'	7.02	126.12	117.70
27	Ca	35	PRO	N-CA-CB	6.53	111.13	103.30
27	Ca	33	PRO	N-CA-CB	6.41	110.99	103.30
27	Ca	32	PRO	N-CA-CB	6.40	110.98	103.30
37	CA	63	G	N3-C4-C5	6.30	131.75	128.60
3	DI	345	LEU	CA-CB-CG	6.23	129.63	115.30
37	CA	617	U	C2-N1-C1'	6.23	125.17	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	CA	618	U	O5'-P-OP2	-6.10	100.21	105.70
35	Cr	28	PRO	N-CA-CB	6.09	110.60	103.30
37	CA	152	U	C5-C6-N1	6.08	125.74	122.70
37	CA	617	U	N1-C2-O2	5.95	126.97	122.80
35	Cr	31	PRO	N-CA-CB	5.94	110.43	103.30
37	CA	310	A	C2-N3-C4	5.88	113.54	110.60
37	CA	69	U	N3-C2-O2	-5.84	118.11	122.20
37	CA	617	U	N3-C2-O2	-5.83	118.12	122.20
26	CZ	296	PRO	N-CA-CB	5.68	110.11	103.30
37	CA	374	U	C2-N1-C1'	5.58	124.39	117.70
2	DD	255	VAL	C-N-CD	-5.56	108.37	120.60
37	CA	370	A	O4'-C1'-N9	5.53	112.63	108.20
1	DA	1484	PRO	N-CA-CB	5.50	109.90	103.30
37	CA	188	U	N1-C2-O2	5.45	126.62	122.80
37	CA	87	U	N3-C2-O2	-5.36	118.45	122.20
1	DA	509	LEU	CA-CB-CG	5.25	127.38	115.30
35	Cr	29	PRO	N-CA-CB	5.22	109.57	103.30
31	Cm	203	ASP	CB-CG-OD2	5.19	122.97	118.30
37	CA	564	U	C5-C6-N1	5.16	125.28	122.70
3	DI	116	ASP	CB-CG-OD2	5.15	122.94	118.30
37	CA	66	U	C2-N1-C1'	5.13	123.86	117.70
37	CA	87	U	N1-C2-O2	5.03	126.32	122.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	CH	92	PRO	Peptide
27	Ca	599	ILE	Peptide
30	Cj	53	ASN	Peptide
36	Cv	545	THR	Peptide
36	Cv	943	LEU	Peptide
1	DA	166	TYR	Peptide
2	DD	248	ASP	Peptide
2	DD	255	VAL	Peptide
6	DN	142	ARG	Peptide
6	DN	292	TYR	Peptide
7	DO	124	CYS	Peptide
7	DO	251	ASN	Peptide
10	DR	23	VAL	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1420/1788 (79%)	1370 (96%)	48 (3%)	2 (0%)	51	82
2	DD	787/812 (97%)	747 (95%)	38 (5%)	2 (0%)	41	72
3	DI	388/407 (95%)	366 (94%)	21 (5%)	1 (0%)	41	72
4	DL	138/307 (45%)	130 (94%)	8 (6%)	0	100	100
5	DM	292/294 (99%)	283 (97%)	9 (3%)	0	100	100
6	DN	253/293 (86%)	242 (96%)	11 (4%)	0	100	100
7	DO	220/282 (78%)	213 (97%)	6 (3%)	1 (0%)	29	62
8	DP	205/274 (75%)	195 (95%)	9 (4%)	1 (0%)	29	62
9	DQ	254/268 (95%)	246 (97%)	6 (2%)	2 (1%)	19	52
10	DR	247/270 (92%)	239 (97%)	8 (3%)	0	100	100
11	DS	234/261 (90%)	227 (97%)	7 (3%)	0	100	100
12	DU	211/228 (92%)	202 (96%)	7 (3%)	2 (1%)	17	50
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	CE	413/435 (95%)	395 (96%)	18 (4%)	0	100	100
16	CF	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
17	CH	271/282 (96%)	265 (98%)	5 (2%)	1 (0%)	34	67
18	CI	200/443 (45%)	196 (98%)	4 (2%)	0	100	100
19	CK	237/326 (73%)	225 (95%)	12 (5%)	0	100	100
20	CL	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
21	CO	359/429 (84%)	343 (96%)	14 (4%)	2 (1%)	25	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	CP	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
23	CQ	188/307 (61%)	182 (97%)	6 (3%)	0	100	100
24	CR	312/320 (98%)	297 (95%)	14 (4%)	1 (0%)	41	72
25	CU	182/193 (94%)	177 (97%)	4 (2%)	1 (0%)	29	62
26	CZ	149/360 (41%)	142 (95%)	6 (4%)	1 (1%)	22	56
27	Ca	590/602 (98%)	556 (94%)	29 (5%)	5 (1%)	19	52
28	Cb	248/324 (76%)	242 (98%)	6 (2%)	0	100	100
29	Cd	289/440 (66%)	281 (97%)	6 (2%)	2 (1%)	22	56
30	Cj	224/257 (87%)	216 (96%)	7 (3%)	1 (0%)	34	67
31	Cm	194/215 (90%)	184 (95%)	10 (5%)	0	100	100
32	Cn	108/250 (43%)	103 (95%)	5 (5%)	0	100	100
33	Cp	173/187 (92%)	169 (98%)	4 (2%)	0	100	100
34	Cq	250/263 (95%)	243 (97%)	7 (3%)	0	100	100
35	Cr	253/439 (58%)	243 (96%)	9 (4%)	1 (0%)	34	67
36	Cv	1051/1211 (87%)	1011 (96%)	40 (4%)	0	100	100
All	All	10893/13360 (82%)	10460 (96%)	407 (4%)	26 (0%)	50	77

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	CZ	296	PRO
27	Ca	32	PRO
27	Ca	33	PRO
27	Ca	35	PRO
24	CR	10	ALA
27	Ca	34	LYS
2	DD	256	PRO
12	DU	191	SER
17	CH	16	VAL
30	Cj	54	ALA
1	DA	132	GLY
3	DI	190	PRO
8	DP	62	LYS
25	CU	19	ALA
29	Cd	224	ILE
29	Cd	247	LYS
2	DD	248	ASP

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Mol	Chain	Res	Type
7	DO	115	ASP
9	DQ	173	ASP
12	DU	205	ALA
21	CO	70	HIS
1	DA	229	GLU
27	Ca	31	GLU
9	DQ	254	SER
21	CO	90	MET
35	Cr	29	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DA	1211/1514 (80%)	1125 (93%)	86 (7%)	14	42
2	DD	694/711 (98%)	652 (94%)	42 (6%)	18	48
3	DI	350/365 (96%)	328 (94%)	22 (6%)	18	47
4	DL	118/263 (45%)	114 (97%)	4 (3%)	37	65
5	DM	252/252 (100%)	233 (92%)	19 (8%)	13	39
6	DN	229/256 (90%)	215 (94%)	14 (6%)	18	48
7	DO	186/229 (81%)	174 (94%)	12 (6%)	17	46
8	DP	187/239 (78%)	178 (95%)	9 (5%)	25	56
9	DQ	228/239 (95%)	220 (96%)	8 (4%)	36	64
10	DR	220/235 (94%)	199 (90%)	21 (10%)	8	29
11	DS	209/228 (92%)	197 (94%)	12 (6%)	20	51
12	DU	190/201 (94%)	174 (92%)	16 (8%)	11	35
13	DZ	72/84 (86%)	69 (96%)	3 (4%)	30	60
14	Da	50/59 (85%)	46 (92%)	4 (8%)	12	37
15	CE	358/372 (96%)	317 (88%)	41 (12%)	5	22
16	CF	136/144 (94%)	129 (95%)	7 (5%)	24	54
17	CH	237/246 (96%)	215 (91%)	22 (9%)	9	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	CI	171/371 (46%)	160 (94%)	11 (6%)	17	47
19	CK	210/283 (74%)	193 (92%)	17 (8%)	11	36
20	CL	79/79 (100%)	70 (89%)	9 (11%)	5	23
21	CO	318/377 (84%)	293 (92%)	25 (8%)	12	37
22	CP	160/168 (95%)	147 (92%)	13 (8%)	11	36
23	CQ	171/270 (63%)	151 (88%)	20 (12%)	5	22
24	CR	275/279 (99%)	258 (94%)	17 (6%)	18	48
25	CU	160/169 (95%)	151 (94%)	9 (6%)	21	51
26	CZ	121/313 (39%)	111 (92%)	10 (8%)	11	35
27	Ca	516/543 (95%)	473 (92%)	43 (8%)	11	35
28	Cb	219/277 (79%)	203 (93%)	16 (7%)	14	40
29	Cd	240/381 (63%)	219 (91%)	21 (9%)	10	33
30	Cj	193/219 (88%)	179 (93%)	14 (7%)	14	40
31	Cm	165/184 (90%)	141 (86%)	24 (14%)	3	15
32	Cn	95/210 (45%)	89 (94%)	6 (6%)	18	47
33	Cp	163/175 (93%)	151 (93%)	12 (7%)	13	40
34	Cq	210/221 (95%)	193 (92%)	17 (8%)	11	36
35	Cr	211/369 (57%)	190 (90%)	21 (10%)	7	28
36	Cv	912/1034 (88%)	844 (92%)	68 (8%)	13	39
All	All	9516/11559 (82%)	8801 (92%)	715 (8%)	17	39

All (715) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DA	41	PHE
1	DA	52	MET
1	DA	74	LYS
1	DA	77	ARG
1	DA	79	LEU
1	DA	87	THR
1	DA	109	TYR
1	DA	112	GLN
1	DA	131	ASP
1	DA	150	ILE
1	DA	158	LEU

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Mol	Chain	Res	Type
1	DA	165	ARG
1	DA	167	THR
1	DA	174	HIS
1	DA	194	LEU
1	DA	200	ILE
1	DA	201	LYS
1	DA	230	PHE
1	DA	245	PHE
1	DA	254	PHE
1	DA	255	ARG
1	DA	259	LEU
1	DA	274	LEU
1	DA	291	CYS
1	DA	300	THR
1	DA	319	ARG
1	DA	383	LYS
1	DA	408	LEU
1	DA	419	THR
1	DA	436	ASN
1	DA	456	ARG
1	DA	472	ARG
1	DA	486	LYS
1	DA	493	TRP
1	DA	509	LEU
1	DA	540	GLU
1	DA	547	ARG
1	DA	553	ARG
1	DA	579	ASP
1	DA	602	LEU
1	DA	630	ASP
1	DA	632	THR
1	DA	646	ASP
1	DA	650	LEU
1	DA	653	LYS
1	DA	680	VAL
1	DA	703	THR
1	DA	708	GLU
1	DA	712	VAL
1	DA	729	ARG
1	DA	781	ARG
1	DA	783	VAL
1	DA	826	ARG

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Mol	Chain	Res	Type
1	DA	849	THR
1	DA	859	GLN
1	DA	870	GLU
1	DA	920	LEU
1	DA	958	SER
1	DA	963	LEU
1	DA	973	LEU
1	DA	988	CYS
1	DA	992	GLU
1	DA	1000	ASN
1	DA	1045	ILE
1	DA	1048	ASN
1	DA	1062	TYR
1	DA	1077	ARG
1	DA	1097	LEU
1	DA	1117	ASN
1	DA	1125	GLU
1	DA	1145	THR
1	DA	1152	HIS
1	DA	1182	ARG
1	DA	1381	LEU
1	DA	1404	ARG
1	DA	1431	TYR
1	DA	1433	ASP
1	DA	1488	GLN
1	DA	1517	ARG
1	DA	1544	ASN
1	DA	1575	LYS
1	DA	1591	ARG
1	DA	1597	GLU
1	DA	1605	ARG
1	DA	1624	ILE
1	DA	1662	ARG
2	DD	12	SER
2	DD	27	MET
2	DD	48	MET
2	DD	72	ASP
2	DD	79	GLN
2	DD	94	LYS
2	DD	108	THR
2	DD	122	GLN
2	DD	123	ARG

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Mol	Chain	Res	Type
2	DD	129	ARG
2	DD	146	ARG
2	DD	151	SER
2	DD	173	GLN
2	DD	201	GLU
2	DD	221	GLU
2	DD	226	THR
2	DD	233	ASN
2	DD	298	MET
2	DD	358	ARG
2	DD	377	GLU
2	DD	379	GLN
2	DD	394	LYS
2	DD	452	LEU
2	DD	454	THR
2	DD	504	ASN
2	DD	521	ASN
2	DD	541	ARG
2	DD	577	LYS
2	DD	592	TRP
2	DD	624	THR
2	DD	634	ARG
2	DD	646	ILE
2	DD	651	ARG
2	DD	653	PHE
2	DD	654	ARG
2	DD	679	ASN
2	DD	704	ASP
2	DD	741	ARG
2	DD	770	SER
2	DD	787	ARG
2	DD	799	ASP
2	DD	812	TYR
3	DI	79	ILE
3	DI	90	LEU
3	DI	113	VAL
3	DI	159	ASP
3	DI	164	GLU
3	DI	175	GLN
3	DI	178	PHE
3	DI	180	GLU
3	DI	192	THR

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Mol	Chain	Res	Type
3	DI	232	TYR
3	DI	233	ARG
3	DI	237	ARG
3	DI	261	ASP
3	DI	282	ASP
3	DI	310	LEU
3	DI	313	ARG
3	DI	344	LEU
3	DI	345	LEU
3	DI	353	LYS
3	DI	362	ILE
3	DI	365	ARG
3	DI	399	THR
4	DL	136	MET
4	DL	145	LEU
4	DL	158	THR
4	DL	165	PHE
5	DM	1	MET
5	DM	15	LEU
5	DM	30	ARG
5	DM	46	PHE
5	DM	56	TRP
5	DM	59	ARG
5	DM	72	ARG
5	DM	76	ASN
5	DM	90	LEU
5	DM	103	ARG
5	DM	128	ILE
5	DM	129	ARG
5	DM	131	ASN
5	DM	157	LEU
5	DM	179	ARG
5	DM	185	LYS
5	DM	199	LEU
5	DM	253	LYS
5	DM	275	LEU
6	DN	11	ARG
6	DN	23	VAL
6	DN	42	THR
6	DN	79	ASN
6	DN	109	ASN
6	DN	141	MET

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Mol	Chain	Res	Type
6	DN	152	LEU
6	DN	162	LEU
6	DN	223	GLN
6	DN	224	ARG
6	DN	237	ARG
6	DN	246	GLN
6	DN	276	GLN
6	DN	288	PHE
7	DO	62	LEU
7	DO	73	LEU
7	DO	115	ASP
7	DO	118	ASP
7	DO	125	LEU
7	DO	136	ASP
7	DO	155	ARG
7	DO	163	ARG
7	DO	178	ARG
7	DO	192	MET
7	DO	234	LEU
7	DO	255	ARG
8	DP	21	MET
8	DP	23	LEU
8	DP	28	ASN
8	DP	34	VAL
8	DP	69	LEU
8	DP	172	GLU
8	DP	195	THR
8	DP	204	ASN
8	DP	208	PRO
9	DQ	41	GLN
9	DQ	120	MET
9	DQ	127	ARG
9	DQ	177	LEU
9	DQ	192	LEU
9	DQ	214	ARG
9	DQ	216	ASN
9	DQ	250	ARG
10	DR	23	VAL
10	DR	32	VAL
10	DR	39	GLN
10	DR	54	LEU
10	DR	60	VAL

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Mol	Chain	Res	Type
10	DR	63	ILE
10	DR	67	LYS
10	DR	68	HIS
10	DR	78	ARG
10	DR	91	THR
10	DR	108	GLN
10	DR	131	LEU
10	DR	133	LEU
10	DR	173	ASN
10	DR	174	CYS
10	DR	190	LEU
10	DR	201	CYS
10	DR	245	MET
10	DR	261	ARG
10	DR	262	ARG
10	DR	265	MET
11	DS	34	SER
11	DS	56	LEU
11	DS	61	ASN
11	DS	73	LYS
11	DS	92	ARG
11	DS	106	ARG
11	DS	108	ASN
11	DS	115	TYR
11	DS	119	CYS
11	DS	170	TYR
11	DS	175	CYS
11	DS	198	CYS
12	DU	33	THR
12	DU	46	THR
12	DU	47	ARG
12	DU	73	ARG
12	DU	83	ARG
12	DU	86	ILE
12	DU	90	VAL
12	DU	103	ILE
12	DU	124	SER
12	DU	153	THR
12	DU	165	ASP
12	DU	176	ARG
12	DU	189	LYS
12	DU	207	ARG

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Mol	Chain	Res	Type
12	DU	211	ARG
12	DU	218	ARG
13	DZ	20	ARG
13	DZ	62	ASP
13	DZ	63	LEU
14	Da	25	ARG
14	Da	38	ASP
14	Da	42	ARG
14	Da	61	ARG
15	CE	10	LYS
15	CE	13	ASN
15	CE	16	TYR
15	CE	17	THR
15	CE	27	ARG
15	CE	41	ARG
15	CE	48	ASN
15	CE	58	SER
15	CE	64	THR
15	CE	65	ARG
15	CE	80	ILE
15	CE	83	MET
15	CE	87	ILE
15	CE	112	THR
15	CE	121	THR
15	CE	124	THR
15	CE	137	LEU
15	CE	157	LYS
15	CE	163	ILE
15	CE	165	CYS
15	CE	188	GLU
15	CE	201	ILE
15	CE	223	ARG
15	CE	231	ARG
15	CE	232	ILE
15	CE	279	LEU
15	CE	313	MET
15	CE	314	MET
15	CE	332	ASP
15	CE	334	ARG
15	CE	364	ARG
15	CE	365	MET
15	CE	370	ASP

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Mol	Chain	Res	Type
15	CE	391	THR
15	CE	395	THR
15	CE	396	LEU
15	CE	405	LYS
15	CE	410	LEU
15	CE	417	ASN
15	CE	422	VAL
15	CE	424	LEU
16	CF	2	VAL
16	CF	63	ARG
16	CF	93	LEU
16	CF	123	ARG
16	CF	133	GLN
16	CF	141	GLN
16	CF	152	THR
17	CH	26	ARG
17	CH	29	HIS
17	CH	46	LYS
17	CH	48	ASP
17	CH	88	LEU
17	CH	89	VAL
17	CH	108	LEU
17	CH	118	LEU
17	CH	128	VAL
17	CH	131	ASP
17	CH	132	ASP
17	CH	143	ARG
17	CH	150	THR
17	CH	154	ASP
17	CH	163	THR
17	CH	170	VAL
17	CH	172	VAL
17	CH	179	ARG
17	CH	201	ARG
17	CH	248	ASN
17	CH	279	MET
17	CH	280	MET
18	CI	104	ASN
18	CI	110	ARG
18	CI	127	MET
18	CI	139	ASP
18	CI	165	ASN

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Mol	Chain	Res	Type
18	CI	175	ARG
18	CI	179	CYS
18	CI	218	ARG
18	CI	219	LEU
18	CI	245	ARG
18	CI	256	LYS
19	CK	70	ILE
19	CK	73	GLN
19	CK	98	LEU
19	CK	107	GLN
19	CK	109	VAL
19	CK	112	GLU
19	CK	113	ARG
19	CK	149	VAL
19	CK	156	LYS
19	CK	205	TYR
19	CK	207	VAL
19	CK	232	ARG
19	CK	264	SER
19	CK	311	THR
19	CK	315	LEU
19	CK	325	PHE
19	CK	326	LYS
20	CL	59	MET
20	CL	75	CYS
20	CL	91	LEU
20	CL	95	PHE
20	CL	97	LEU
20	CL	109	CYS
20	CL	118	LEU
20	CL	122	GLU
20	CL	133	LYS
21	CO	69	GLU
21	CO	75	LEU
21	CO	82	ASN
21	CO	87	THR
21	CO	108	THR
21	CO	190	SER
21	CO	209	GLU
21	CO	210	ARG
21	CO	220	SER
21	CO	224	LEU

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Mol	Chain	Res	Type
21	CO	237	ASN
21	CO	242	ASN
21	CO	244	HIS
21	CO	245	ASN
21	CO	266	LEU
21	CO	285	ASP
21	CO	304	ASP
21	CO	329	GLU
21	CO	336	GLU
21	CO	353	GLU
21	CO	362	VAL
21	CO	395	VAL
21	CO	400	ARG
21	CO	412	ARG
21	CO	419	VAL
22	CP	14	LYS
22	CP	15	ARG
22	CP	36	VAL
22	CP	40	PHE
22	CP	59	ARG
22	CP	68	CYS
22	CP	90	MET
22	CP	93	THR
22	CP	129	THR
22	CP	152	ASN
22	CP	163	LYS
22	CP	170	SER
22	CP	188	LEU
23	CQ	16	THR
23	CQ	21	ARG
23	CQ	31	THR
23	CQ	34	THR
23	CQ	56	ARG
23	CQ	67	LEU
23	CQ	69	GLN
23	CQ	70	ARG
23	CQ	73	ARG
23	CQ	83	LEU
23	CQ	103	MET
23	CQ	114	MET
23	CQ	123	ARG
23	CQ	136	ASP

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Mol	Chain	Res	Type
23	CQ	146	HIS
23	CQ	147	ILE
23	CQ	158	HIS
23	CQ	169	VAL
23	CQ	182	VAL
23	CQ	199	ASN
24	CR	15	GLN
24	CR	30	LEU
24	CR	44	GLU
24	CR	59	LEU
24	CR	70	ARG
24	CR	80	LEU
24	CR	96	GLN
24	CR	167	ARG
24	CR	181	ARG
24	CR	184	LYS
24	CR	198	THR
24	CR	233	SER
24	CR	235	SER
24	CR	239	SER
24	CR	278	VAL
24	CR	305	THR
24	CR	315	LEU
25	CU	13	MET
25	CU	32	HIS
25	CU	44	MET
25	CU	46	GLU
25	CU	74	GLN
25	CU	148	ASN
25	CU	161	GLN
25	CU	169	ASN
25	CU	171	VAL
26	CZ	218	VAL
26	CZ	236	ARG
26	CZ	237	ARG
26	CZ	240	VAL
26	CZ	260	MET
26	CZ	265	GLN
26	CZ	277	PHE
26	CZ	318	LEU
26	CZ	321	MET
26	CZ	360	ASP

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Mol	Chain	Res	Type
27	Ca	14	ASN
27	Ca	15	LYS
27	Ca	16	ARG
27	Ca	19	ARG
27	Ca	67	ARG
27	Ca	71	MET
27	Ca	153	LYS
27	Ca	168	TYR
27	Ca	181	GLU
27	Ca	191	MET
27	Ca	194	LEU
27	Ca	201	ARG
27	Ca	221	THR
27	Ca	227	ASN
27	Ca	240	SER
27	Ca	295	PHE
27	Ca	297	LEU
27	Ca	299	ARG
27	Ca	305	HIS
27	Ca	314	CYS
27	Ca	338	LYS
27	Ca	350	GLU
27	Ca	365	LEU
27	Ca	376	VAL
27	Ca	380	ASP
27	Ca	384	ARG
27	Ca	398	ASP
27	Ca	399	ASN
27	Ca	410	MET
27	Ca	433	GLN
27	Ca	447	ILE
27	Ca	451	VAL
27	Ca	479	THR
27	Ca	480	LEU
27	Ca	506	GLN
27	Ca	520	TYR
27	Ca	537	ARG
27	Ca	538	ILE
27	Ca	541	ARG
27	Ca	552	THR
27	Ca	569	ARG
27	Ca	575	ARG

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Mol	Chain	Res	Type
27	Ca	578	ASP
28	Cb	40	LEU
28	Cb	57	MET
28	Cb	71	LEU
28	Cb	108	GLU
28	Cb	110	MET
28	Cb	144	ARG
28	Cb	158	LYS
28	Cb	171	THR
28	Cb	193	GLU
28	Cb	195	LEU
28	Cb	205	LYS
28	Cb	223	ARG
28	Cb	288	GLU
28	Cb	291	GLU
28	Cb	304	SER
28	Cb	306	THR
29	Cd	13	ARG
29	Cd	44	GLU
29	Cd	63	ARG
29	Cd	74	ASP
29	Cd	102	ARG
29	Cd	106	ARG
29	Cd	108	MET
29	Cd	120	LEU
29	Cd	122	LEU
29	Cd	125	GLU
29	Cd	164	LEU
29	Cd	168	VAL
29	Cd	180	VAL
29	Cd	208	HIS
29	Cd	210	ASP
29	Cd	216	HIS
29	Cd	217	GLU
29	Cd	219	HIS
29	Cd	222	SER
29	Cd	259	GLU
29	Cd	284	THR
30	Cj	10	ARG
30	Cj	34	HIS
30	Cj	58	MET
30	Cj	66	LEU

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Mol	Chain	Res	Type
30	Cj	77	LEU
30	Cj	80	LEU
30	Cj	126	TYR
30	Cj	135	ILE
30	Cj	145	THR
30	Cj	161	VAL
30	Cj	173	MET
30	Cj	175	PHE
30	Cj	206	LEU
30	Cj	210	PRO
31	Cm	35	ASN
31	Cm	50	ARG
31	Cm	60	ARG
31	Cm	61	ARG
31	Cm	80	THR
31	Cm	85	ILE
31	Cm	92	GLN
31	Cm	93	LEU
31	Cm	94	THR
31	Cm	95	MET
31	Cm	98	SER
31	Cm	106	CYS
31	Cm	117	ARG
31	Cm	123	ASP
31	Cm	124	SER
31	Cm	125	CYS
31	Cm	126	LEU
31	Cm	153	ASP
31	Cm	162	ARG
31	Cm	173	GLU
31	Cm	178	GLU
31	Cm	179	ARG
31	Cm	188	ARG
31	Cm	202	THR
32	Cn	165	LEU
32	Cn	172	LYS
32	Cn	195	PHE
32	Cn	203	MET
32	Cn	214	ARG
32	Cn	235	GLU
33	Cp	28	ARG
33	Cp	30	LEU

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Mol	Chain	Res	Type
33	Cp	50	THR
33	Cp	84	LEU
33	Cp	87	CYS
33	Cp	91	GLN
33	Cp	105	ILE
33	Cp	123	THR
33	Cp	137	ASP
33	Cp	166	ARG
33	Cp	168	ILE
33	Cp	181	ARG
34	Cq	19	VAL
34	Cq	30	ILE
34	Cq	64	VAL
34	Cq	65	SER
34	Cq	78	ASP
34	Cq	79	MET
34	Cq	96	THR
34	Cq	106	LEU
34	Cq	107	GLU
34	Cq	111	ARG
34	Cq	144	THR
34	Cq	185	CYS
34	Cq	207	CYS
34	Cq	227	ILE
34	Cq	235	LEU
34	Cq	250	LEU
34	Cq	253	ARG
35	Cr	10	ARG
35	Cr	13	ARG
35	Cr	25	LEU
35	Cr	26	LEU
35	Cr	37	CYS
35	Cr	45	THR
35	Cr	56	MET
35	Cr	58	ASN
35	Cr	74	ASP
35	Cr	79	LYS
35	Cr	96	GLU
35	Cr	161	ARG
35	Cr	163	LEU
35	Cr	171	GLN
35	Cr	247	ILE

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Mol	Chain	Res	Type
35	Cr	248	ARG
35	Cr	250	LYS
35	Cr	265	LEU
35	Cr	266	GLN
35	Cr	279	ASP
35	Cr	282	GLU
36	Cv	27	LYS
36	Cv	28	THR
36	Cv	32	ARG
36	Cv	35	ARG
36	Cv	86	GLU
36	Cv	87	GLN
36	Cv	98	ARG
36	Cv	151	SER
36	Cv	162	SER
36	Cv	172	THR
36	Cv	201	THR
36	Cv	204	ILE
36	Cv	208	LYS
36	Cv	209	VAL
36	Cv	210	ASP
36	Cv	235	MET
36	Cv	245	ASN
36	Cv	261	ILE
36	Cv	266	CYS
36	Cv	278	LEU
36	Cv	283	ASP
36	Cv	284	LYS
36	Cv	301	SER
36	Cv	305	ASP
36	Cv	312	ASN
36	Cv	367	ASP
36	Cv	401	THR
36	Cv	407	MET
36	Cv	411	ASN
36	Cv	417	THR
36	Cv	446	THR
36	Cv	531	MET
36	Cv	566	MET
36	Cv	569	LEU
36	Cv	594	LEU
36	Cv	613	LEU

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Mol	Chain	Res	Type
36	Cv	617	ASP
36	Cv	638	VAL
36	Cv	649	THR
36	Cv	651	ARG
36	Cv	678	HIS
36	Cv	727	ARG
36	Cv	739	ASN
36	Cv	782	ILE
36	Cv	795	GLU
36	Cv	813	ARG
36	Cv	818	LEU
36	Cv	838	LEU
36	Cv	861	THR
36	Cv	916	ARG
36	Cv	918	LEU
36	Cv	927	LEU
36	Cv	937	MET
36	Cv	938	ASP
36	Cv	945	VAL
36	Cv	969	ASP
36	Cv	987	SER
36	Cv	993	THR
36	Cv	995	VAL
36	Cv	996	SER
36	Cv	1002	ARG
36	Cv	1018	THR
36	Cv	1034	ARG
36	Cv	1040	GLU
36	Cv	1069	GLN
36	Cv	1102	LYS
36	Cv	1108	GLN
36	Cv	1136	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (197) such sidechains are listed below:

Mol	Chain	Res	Type
1	DA	49	HIS
1	DA	59	HIS
1	DA	91	ASN
1	DA	112	GLN
1	DA	123	HIS
1	DA	196	GLN

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Mol	Chain	Res	Type
1	DA	237	HIS
1	DA	287	HIS
1	DA	414	HIS
1	DA	436	ASN
1	DA	457	GLN
1	DA	746	GLN
1	DA	882	GLN
1	DA	907	GLN
1	DA	910	HIS
1	DA	979	GLN
1	DA	984	GLN
1	DA	1038	HIS
1	DA	1048	ASN
1	DA	1081	GLN
1	DA	1117	ASN
1	DA	1175	HIS
1	DA	1179	GLN
1	DA	1399	ASN
1	DA	1488	GLN
1	DA	1513	GLN
1	DA	1562	GLN
1	DA	1570	ASN
1	DA	1629	GLN
2	DD	76	ASN
2	DD	137	HIS
2	DD	156	GLN
2	DD	174	HIS
2	DD	176	HIS
2	DD	203	GLN
2	DD	300	GLN
2	DD	312	GLN
2	DD	313	HIS
2	DD	348	HIS
2	DD	353	HIS
2	DD	379	GLN
2	DD	387	GLN
2	DD	404	HIS
2	DD	408	HIS
2	DD	453	ASN
2	DD	499	ASN
2	DD	507	GLN
2	DD	521	ASN

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Mol	Chain	Res	Type
2	DD	542	HIS
2	DD	669	HIS
2	DD	679	ASN
2	DD	687	HIS
3	DI	30	GLN
3	DI	61	ASN
3	DI	317	HIS
3	DI	320	GLN
3	DI	370	GLN
4	DL	125	HIS
5	DM	27	GLN
5	DM	43	GLN
5	DM	76	ASN
5	DM	193	GLN
6	DN	28	HIS
6	DN	79	ASN
6	DN	223	GLN
6	DN	235	ASN
6	DN	238	ASN
6	DN	246	GLN
7	DO	181	HIS
8	DP	28	ASN
8	DP	98	HIS
8	DP	116	HIS
8	DP	186	HIS
8	DP	194	GLN
8	DP	204	ASN
9	DQ	41	GLN
9	DQ	73	HIS
9	DQ	95	HIS
9	DQ	219	GLN
9	DQ	235	HIS
10	DR	108	GLN
10	DR	145	HIS
10	DR	191	GLN
11	DS	47	ASN
11	DS	134	GLN
11	DS	150	GLN
11	DS	201	HIS
12	DU	63	HIS
12	DU	96	GLN
13	DZ	25	HIS

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Mol	Chain	Res	Type
15	CE	85	ASN
15	CE	105	GLN
15	CE	108	HIS
15	CE	132	HIS
15	CE	159	HIS
15	CE	235	ASN
15	CE	260	ASN
15	CE	317	HIS
15	CE	417	ASN
17	CH	80	HIS
17	CH	116	HIS
17	CH	186	HIS
17	CH	260	ASN
17	CH	267	HIS
17	CH	282	HIS
18	CI	84	ASN
18	CI	104	ASN
18	CI	165	ASN
18	CI	174	GLN
18	CI	211	ASN
19	CK	73	GLN
19	CK	107	GLN
19	CK	111	ASN
19	CK	244	HIS
20	CL	87	ASN
21	CO	82	ASN
21	CO	111	GLN
21	CO	129	GLN
21	CO	214	HIS
21	CO	359	HIS
21	CO	426	HIS
22	CP	84	GLN
22	CP	87	HIS
22	CP	169	ASN
23	CQ	13	ASN
23	CQ	69	GLN
24	CR	24	ASN
24	CR	214	GLN
25	CU	16	HIS
25	CU	72	HIS
25	CU	123	GLN
25	CU	148	ASN

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Mol	Chain	Res	Type
25	CU	174	HIS
27	Ca	14	ASN
27	Ca	76	GLN
27	Ca	177	GLN
27	Ca	227	ASN
27	Ca	423	GLN
27	Ca	441	ASN
27	Ca	506	GLN
27	Ca	519	GLN
27	Ca	585	GLN
28	Cb	64	ASN
28	Cb	67	GLN
28	Cb	191	HIS
28	Cb	280	ASN
29	Cd	48	ASN
29	Cd	72	ASN
29	Cd	87	GLN
29	Cd	155	GLN
29	Cd	159	HIS
29	Cd	182	GLN
30	Cj	34	HIS
30	Cj	153	HIS
31	Cm	56	ASN
31	Cm	73	HIS
31	Cm	155	HIS
31	Cm	168	HIS
31	Cm	182	ASN
31	Cm	184	HIS
32	Cn	149	GLN
32	Cn	192	ASN
33	Cp	91	GLN
33	Cp	154	GLN
34	Cq	20	GLN
34	Cq	29	ASN
34	Cq	93	ASN
34	Cq	104	HIS
34	Cq	129	HIS
34	Cq	155	GLN
34	Cq	196	HIS
35	Cr	58	ASN
35	Cr	80	HIS
35	Cr	125	GLN

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Mol	Chain	Res	Type
35	Cr	157	GLN
35	Cr	287	HIS
36	Cv	147	HIS
36	Cv	166	HIS
36	Cv	198	HIS
36	Cv	245	ASN
36	Cv	312	ASN
36	Cv	321	HIS
36	Cv	392	HIS
36	Cv	411	ASN
36	Cv	511	HIS
36	Cv	523	HIS
36	Cv	559	GLN
36	Cv	678	HIS
36	Cv	739	ASN
36	Cv	755	HIS
36	Cv	830	ASN
36	Cv	878	ASN
36	Cv	948	HIS
36	Cv	960	GLN
36	Cv	1066	GLN
36	Cv	1108	GLN
36	Cv	1129	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	CA	476/621 (76%)	212 (44%)	2 (0%)

All (212) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
37	CA	2	A
37	CA	3	A
37	CA	4	A
37	CA	5	U
37	CA	6	U
37	CA	8	U
37	CA	10	G
37	CA	11	U
37	CA	14	A

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Mol	Chain	Res	Type
37	CA	16	U
37	CA	19	U
37	CA	20	A
37	CA	25	U
37	CA	26	C
37	CA	27	A
37	CA	33	A
37	CA	36	U
37	CA	37	U
37	CA	38	U
37	CA	39	U
37	CA	42	A
37	CA	44	U
37	CA	45	G
37	CA	46	U
37	CA	50	A
37	CA	52	C
37	CA	53	A
37	CA	56	U
37	CA	57	U
37	CA	58	A
37	CA	59	U
37	CA	60	A
37	CA	61	A
37	CA	64	G
37	CA	67	U
37	CA	68	A
37	CA	70	U
37	CA	74	G
37	CA	78	G
37	CA	79	A
37	CA	80	U
37	CA	84	U
37	CA	85	U
37	CA	86	G
37	CA	87	U
37	CA	88	A
37	CA	89	U
37	CA	91	A
37	CA	94	U
37	CA	95	U
37	CA	97	U

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Mol	Chain	Res	Type
37	CA	100	G
37	CA	102	A
37	CA	103	U
37	CA	104	A
37	CA	105	G
37	CA	107	U
37	CA	108	A
37	CA	109	A
37	CA	110	U
37	CA	111	A
37	CA	112	A
37	CA	113	U
37	CA	114	A
37	CA	115	A
37	CA	116	U
37	CA	117	U
37	CA	124	U
37	CA	127	G
37	CA	132	G
37	CA	135	U
37	CA	136	G
37	CA	138	U
37	CA	139	U
37	CA	146	U
37	CA	152	U
37	CA	156	U
37	CA	159	G
37	CA	160	U
37	CA	167	A
37	CA	170	U
37	CA	171	A
37	CA	172	A
37	CA	173	A
37	CA	174	A
37	CA	175	A
37	CA	178	A
37	CA	179	U
37	CA	183	U
37	CA	188	U
37	CA	189	A
37	CA	191	A
37	CA	193	C

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Mol	Chain	Res	Type
37	CA	194	A
37	CA	197	A
37	CA	199	U
37	CA	200	A
37	CA	202	A
37	CA	203	U
37	CA	204	U
37	CA	205	A
37	CA	206	A
37	CA	208	U
37	CA	209	U
37	CA	210	A
37	CA	211	A
37	CA	214	U
37	CA	216	U
37	CA	217	U
37	CA	218	A
37	CA	219	G
37	CA	221	C
37	CA	223	G
37	CA	230	A
37	CA	236	G
37	CA	242	G
37	CA	246	U
37	CA	247	A
37	CA	250	U
37	CA	256	G
37	CA	258	U
37	CA	259	U
37	CA	261	U
37	CA	262	A
37	CA	263	A
37	CA	272	C
37	CA	275	U
37	CA	276	U
37	CA	279	C
37	CA	280	A
37	CA	281	U
37	CA	282	A
37	CA	283	U
37	CA	286	A
37	CA	296	U

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Mol	Chain	Res	Type
37	CA	297	G
37	CA	299	U
37	CA	300	G
37	CA	301	A
37	CA	305	A
37	CA	311	U
37	CA	315	A
37	CA	316	A
37	CA	321	A
37	CA	323	U
37	CA	325	A
37	CA	326	U
37	CA	327	U
37	CA	328	U
37	CA	330	U
37	CA	334	U
37	CA	335	G
37	CA	337	U
37	CA	338	U
37	CA	340	U
37	CA	341	A
37	CA	342	A
37	CA	343	A
37	CA	350	U
37	CA	351	A
37	CA	352	G
37	CA	356	U
37	CA	357	A
37	CA	358	U
37	CA	359	G
37	CA	360	C
37	CA	361	A
37	CA	364	U
37	CA	367	A
37	CA	368	A
37	CA	369	A
37	CA	371	U
37	CA	374	U
37	CA	378	A
37	CA	380	U
37	CA	384	A
37	CA	385	A

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Mol	Chain	Res	Type
37	CA	386	A
37	CA	389	A
37	CA	394	A
37	CA	539	A
37	CA	540	A
37	CA	544	U
37	CA	546	U
37	CA	547	U
37	CA	548	G
37	CA	555	A
37	CA	556	C
37	CA	558	A
37	CA	560	U
37	CA	564	U
37	CA	565	A
37	CA	566	U
37	CA	567	A
37	CA	570	A
37	CA	576	A
37	CA	581	G
37	CA	586	A
37	CA	587	A
37	CA	588	U
37	CA	590	A
37	CA	602	A
37	CA	603	A
37	CA	611	U
37	CA	613	U
37	CA	614	U
37	CA	615	U
37	CA	616	U
37	CA	617	U
37	CA	618	U
37	CA	619	U
37	CA	620	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
37	CA	38	U
37	CA	39	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 40 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
44	SPD	CA	734	-	9,9,9	0.35	0	8,8,8	0.67	0
44	SPD	CA	733	-	9,9,9	0.49	0	8,8,8	0.49	0
45	SPM	CA	735	-	13,13,13	0.34	0	12,12,12	0.85	0

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
44	SPD	CA	734	-	-	3/7/7/7	-
44	SPD	CA	733	-	-	5/7/7/7	-
45	SPM	CA	735	-	-	8/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	CA	735	SPM	N10-C11-C12-C13
45	CA	735	SPM	C2-C3-C4-N5
44	CA	733	SPD	C3-C4-C5-N6
45	CA	735	SPM	C7-C8-C9-N10
45	CA	735	SPM	C6-C7-C8-C9
44	CA	733	SPD	N1-C2-C3-C4
44	CA	734	SPD	C3-C4-C5-N6
45	CA	735	SPM	C12-C11-N10-C9
44	CA	733	SPD	C7-C8-C9-N10
44	CA	734	SPD	C7-C8-C9-N10
45	CA	735	SPM	C11-C12-C13-N14
45	CA	735	SPM	C7-C6-N5-C4
44	CA	733	SPD	C4-C5-N6-C7
44	CA	733	SPD	C8-C7-N6-C5
45	CA	735	SPM	N1-C2-C3-C4
44	CA	734	SPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

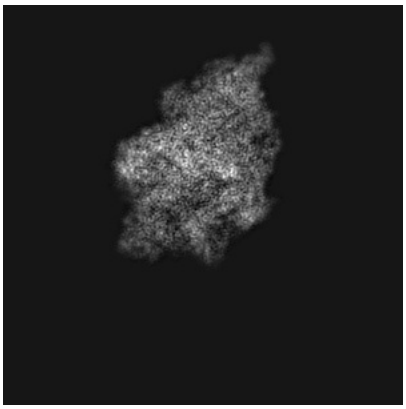
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0232. These allow visual inspection of the internal detail of the map and identification of artifacts.

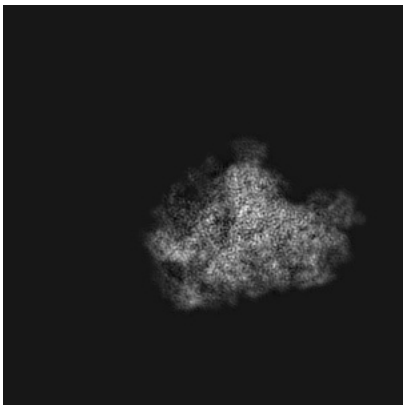
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

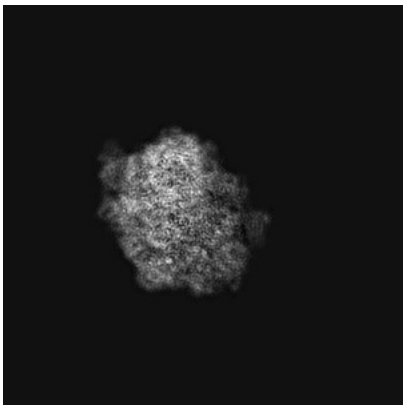
6.1.1 Primary map



X

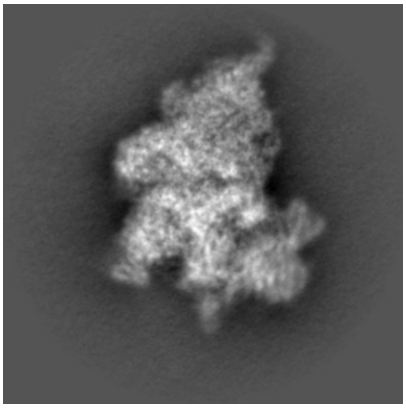


Y

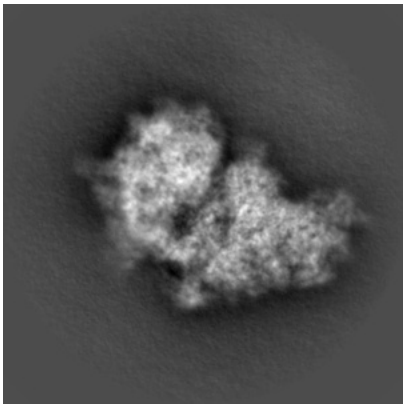


Z

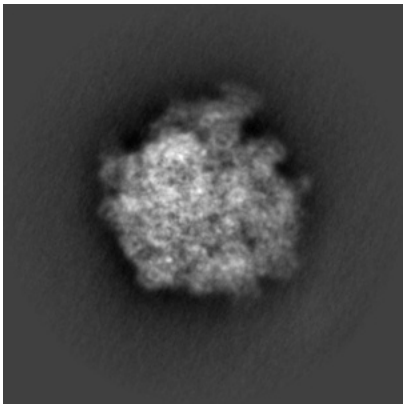
6.1.2 Raw map



X



Y

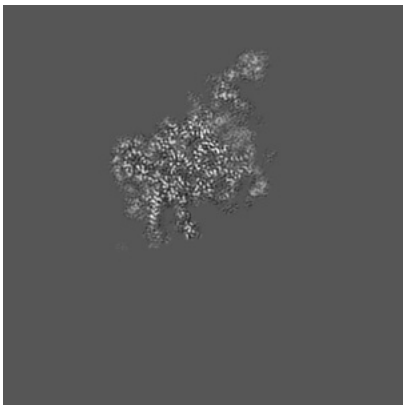


Z

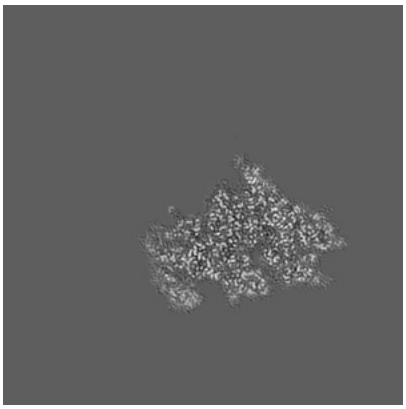
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

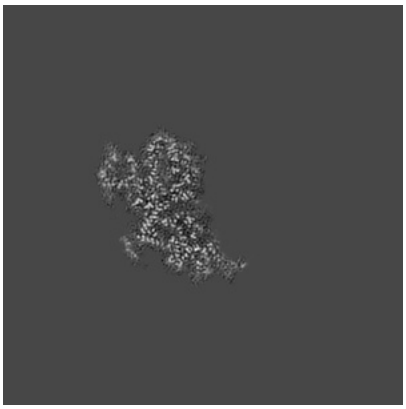
6.2.1 Primary map



X Index: 160

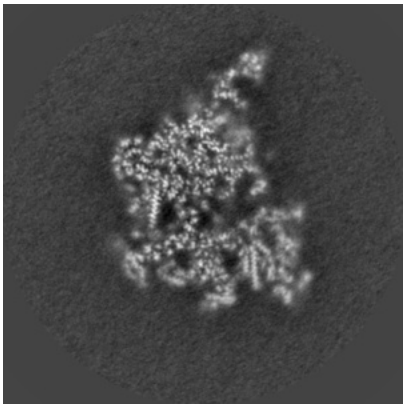


Y Index: 160

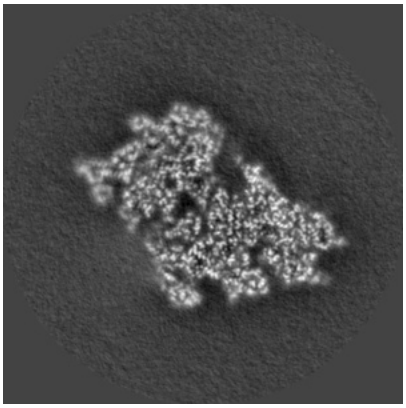


Z Index: 160

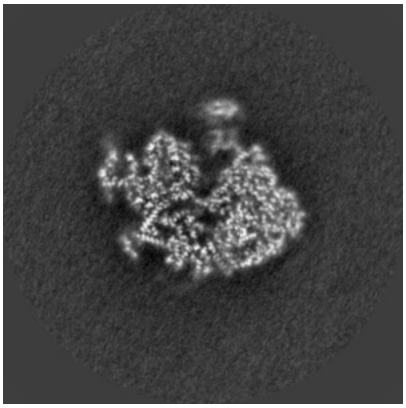
6.2.2 Raw map



X Index: 160



Y Index: 160

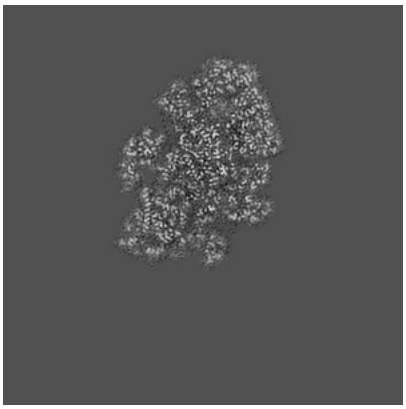


Z Index: 160

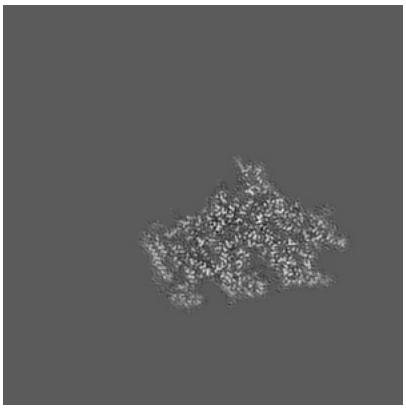
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

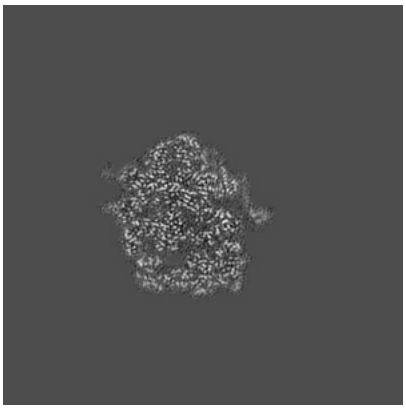
6.3.1 Primary map



X Index: 133

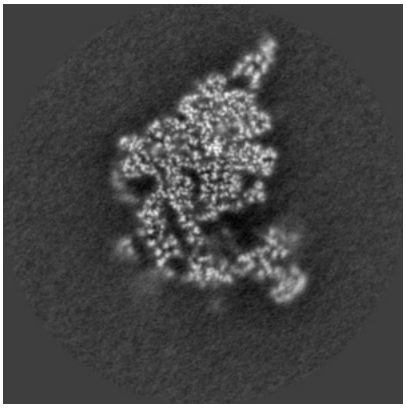


Y Index: 162

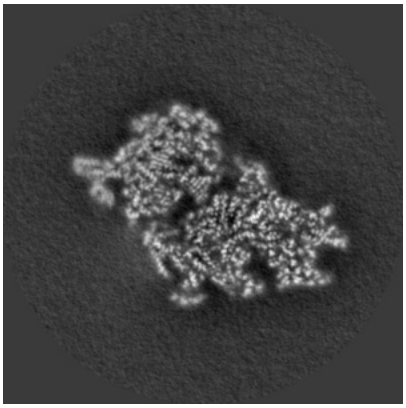


Z Index: 187

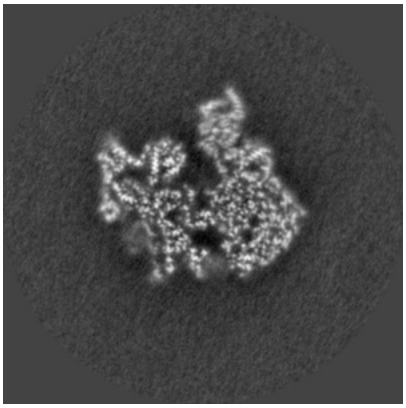
6.3.2 Raw map



X Index: 151



Y Index: 164

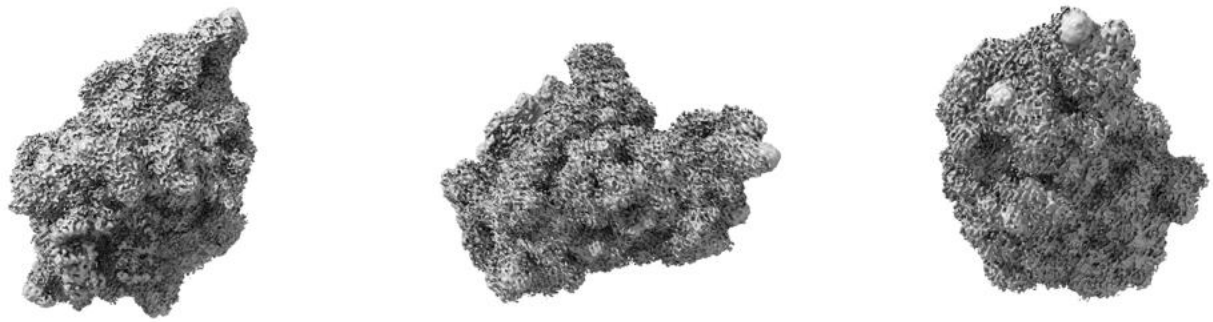


Z Index: 152

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

6.4 Orthogonal surface views (i)

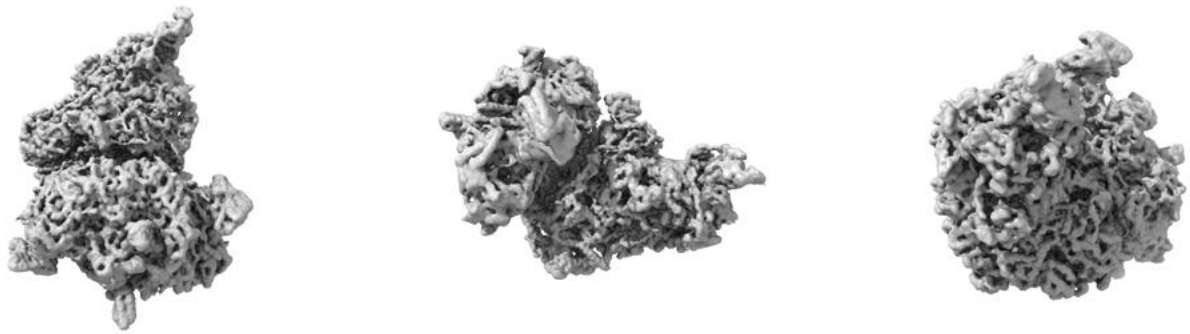
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

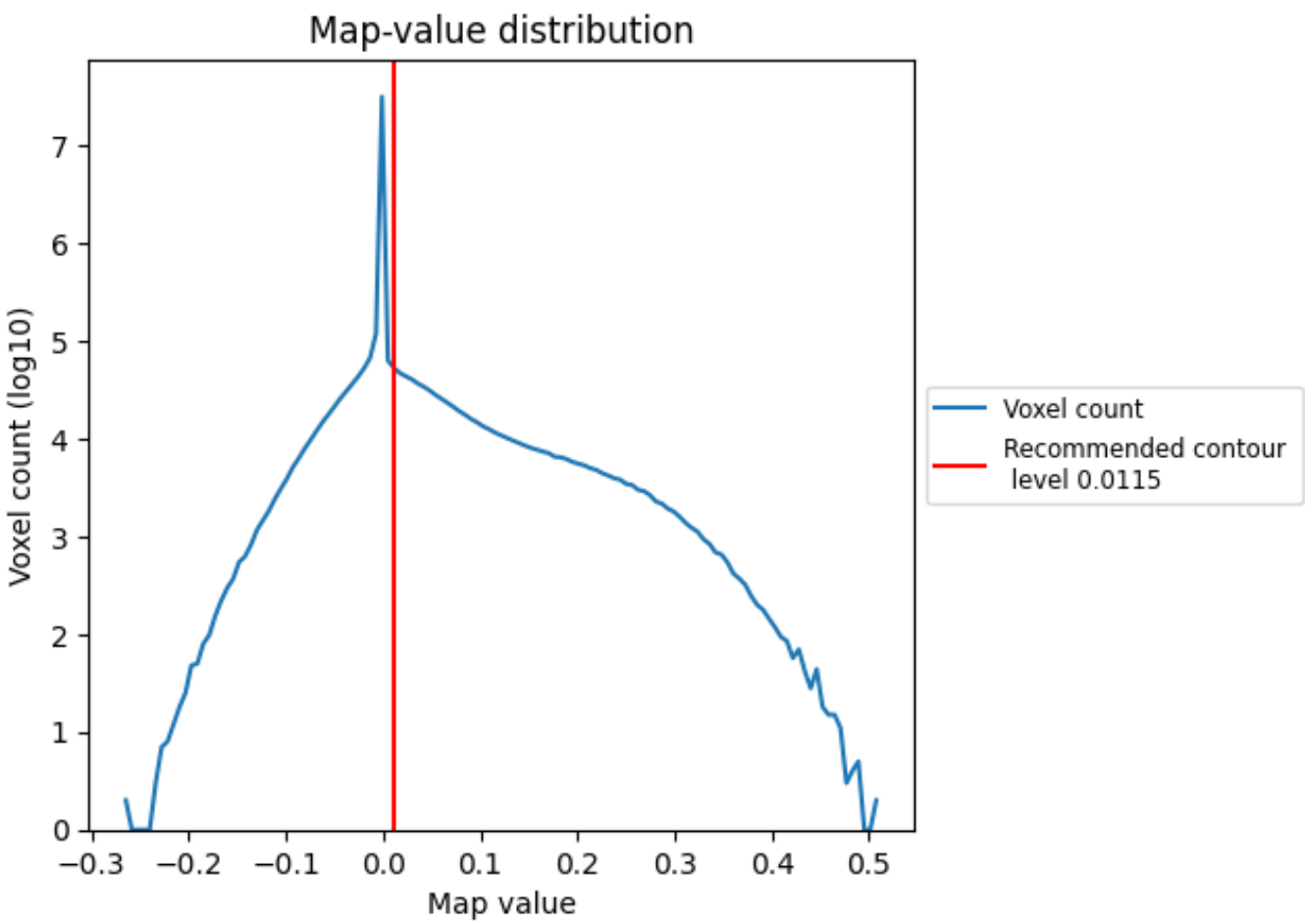
6.5 Mask visualisation (i)

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

7 Map analysis (i)

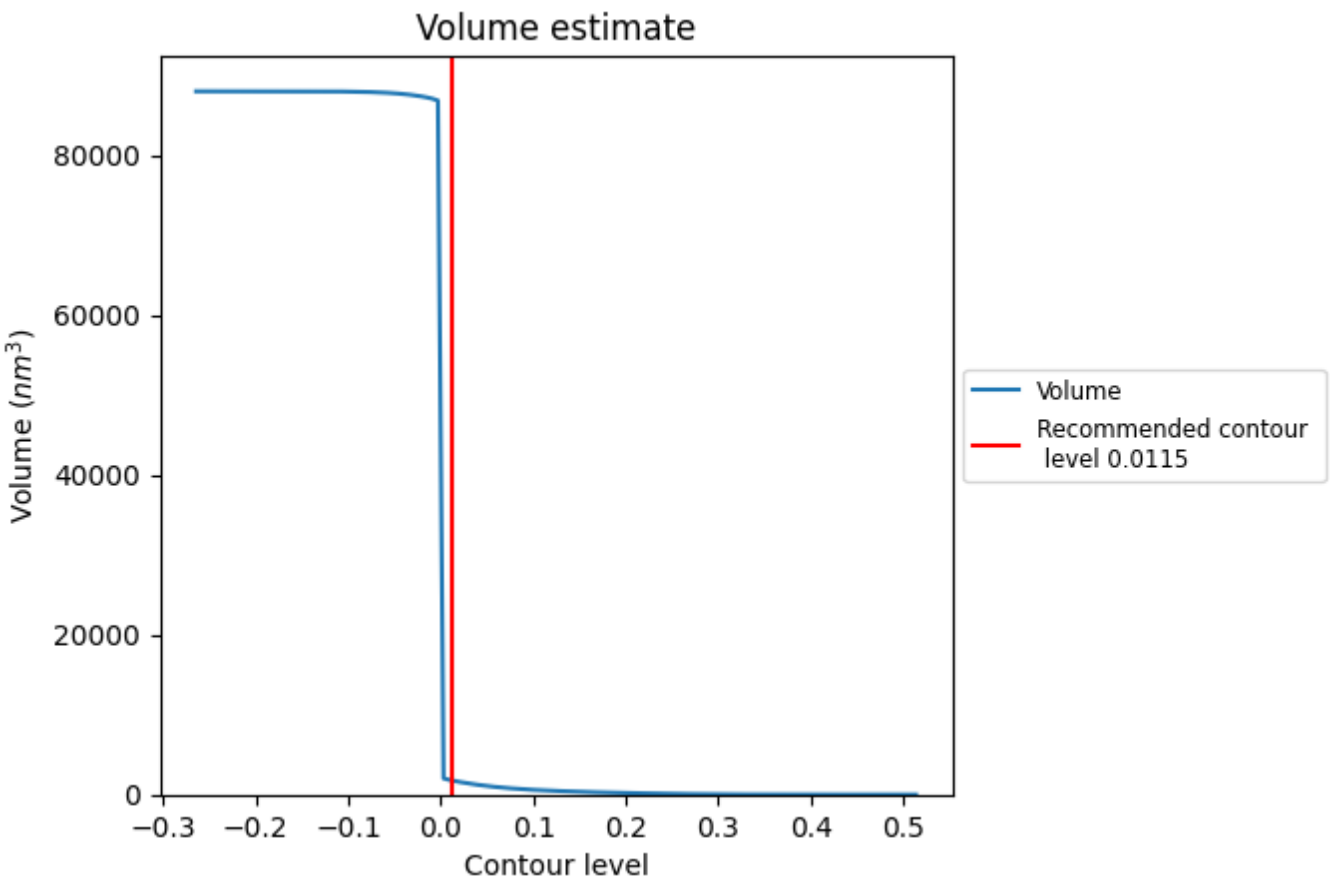
This section contains the results of statistical analysis of the map.

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.

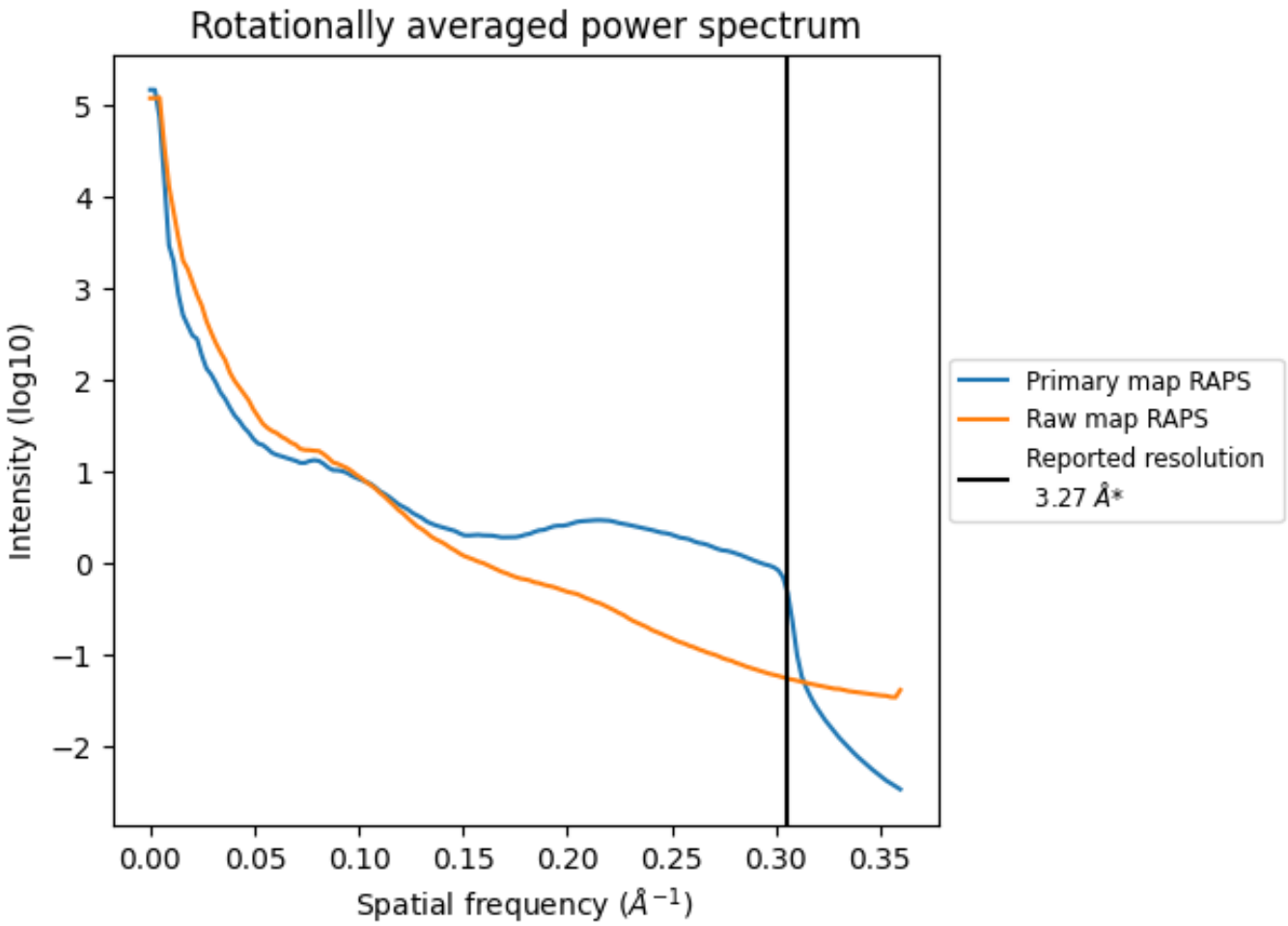
7.2 Volume estimate (i)



The volume at the recommended contour level is 1779 nm^3; this corresponds to an approximate mass of 1607 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

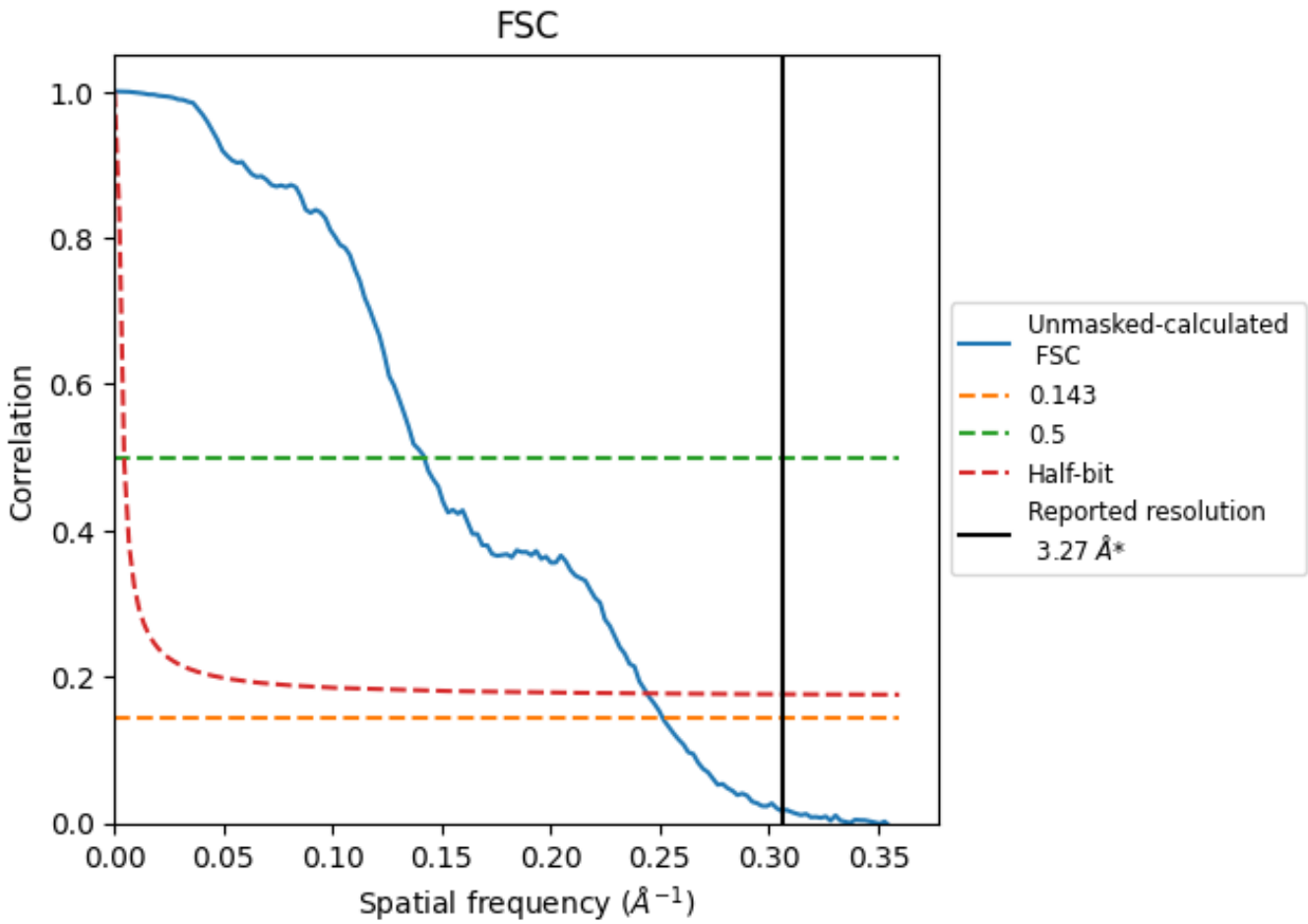


*Reported resolution corresponds to spatial frequency of 0.306 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.306 Å^{-1}

8.2 Resolution estimates (i)

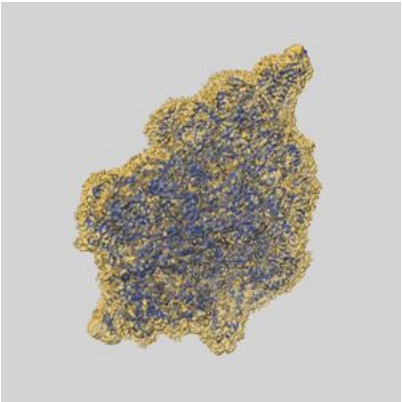
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	7.05	4.10

*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 3.98 differs from the reported value 3.27 by more than 10 %

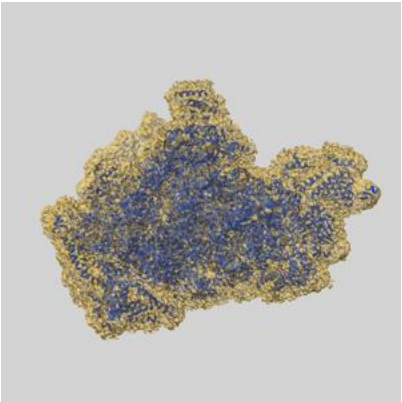
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0232 and PDB model 6HIY. Per-residue inclusion information can be found in section 3 on page 16.

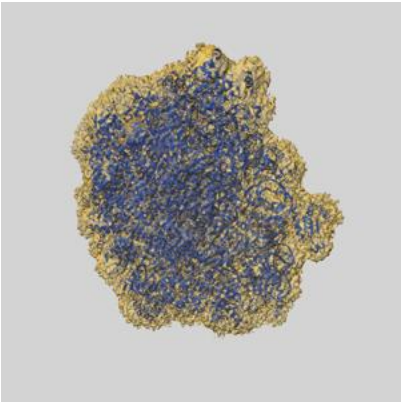
9.1 Map-model overlay (i)



X



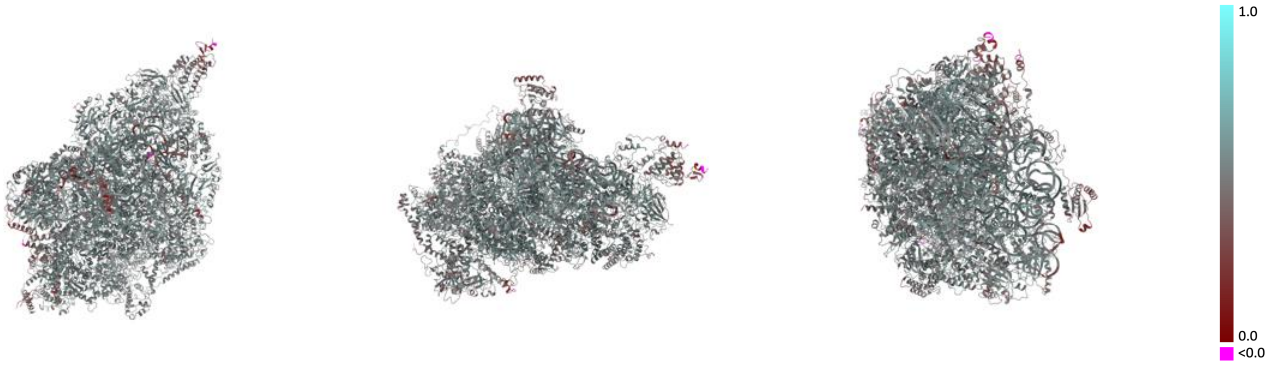
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

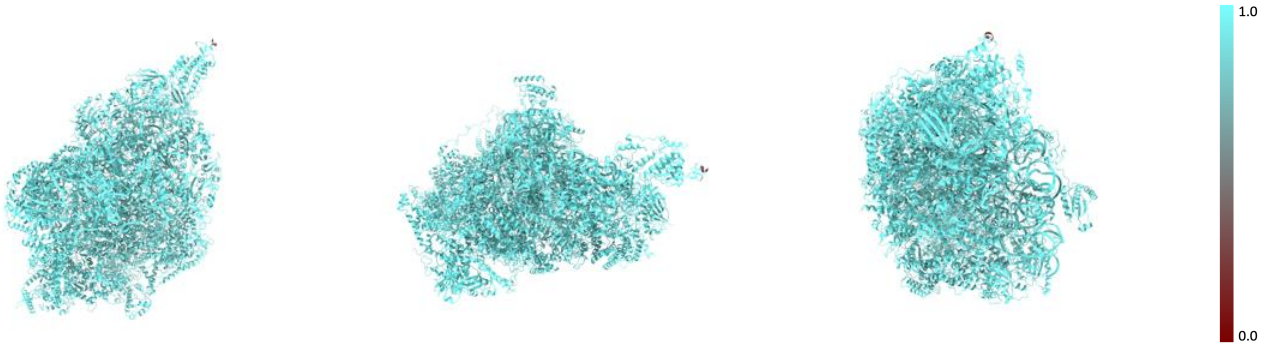
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

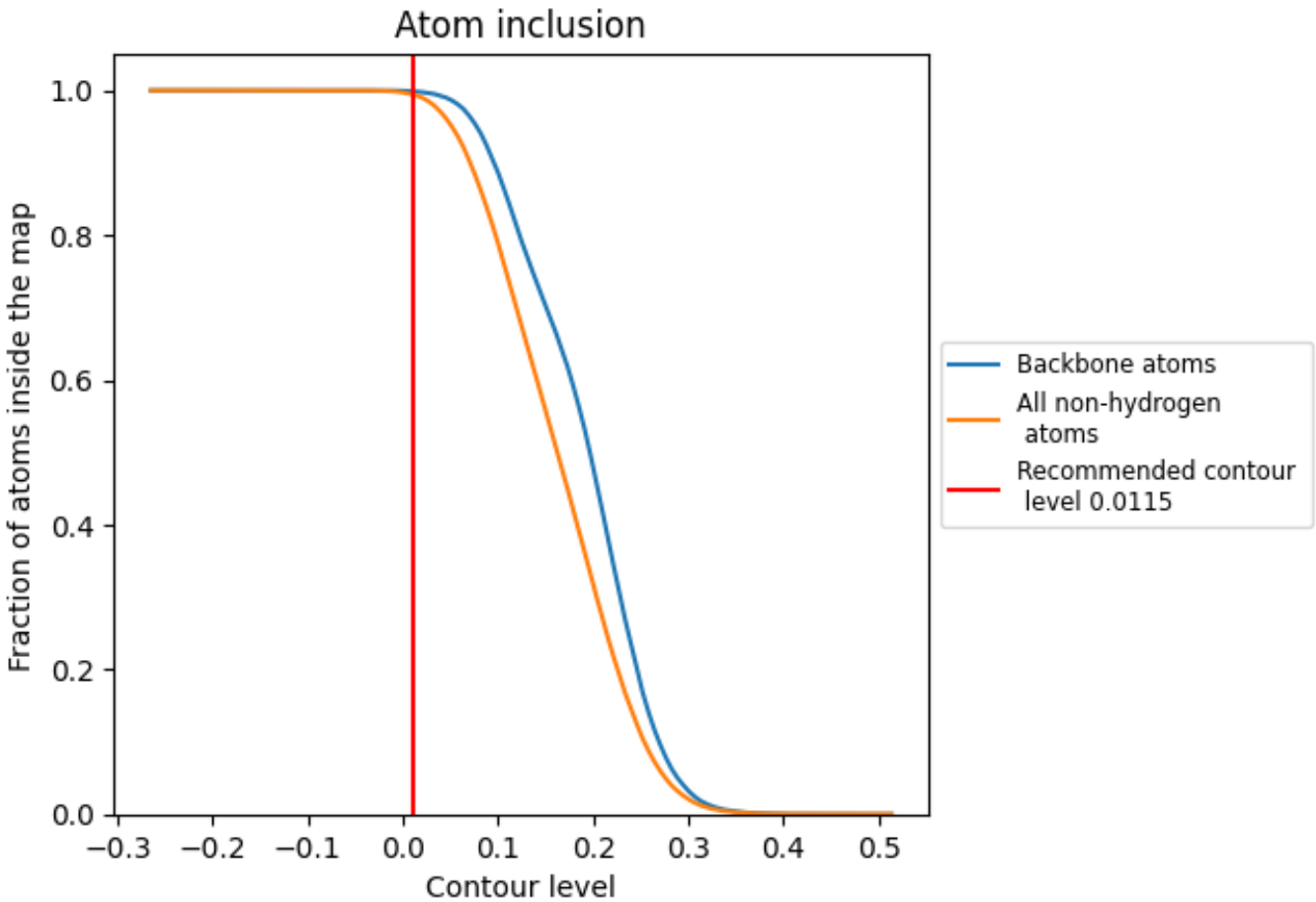
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0115).

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 (i)

The table lists the average atom inclusion at the recommended contour level (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9939	0.5160
CA	0.9956	0.5150
CE	0.9909	0.5410
CF	0.9816	0.5040
CH	0.9907	0.5270
CI	0.9912	0.5300
CK	0.9953	0.5020
CL	0.9972	0.5380
CO	0.9986	0.5330
CP	0.9979	0.5360
CQ	0.9980	0.5640
CR	0.9880	0.5220
CU	0.9966	0.5270
CZ	0.9796	0.4120
Ca	0.9932	0.5320
Cb	0.9925	0.5060
Cd	0.9927	0.5030
Cj	0.9994	0.5140
Cm	0.9836	0.5160
Cn	0.9977	0.5310
Cp	0.9986	0.4980
Cq	0.9908	0.5240
Cr	0.9974	0.4760
Cv	0.9951	0.5290
DA	0.9951	0.5030
DD	0.9929	0.5250
DI	0.9971	0.5100
DL	0.9881	0.5430
DM	0.9957	0.5400
DN	0.9911	0.5360
DO	0.9966	0.4930
DP	0.9836	0.4450
DQ	0.9965	0.5010
DR	0.9995	0.5020
DS	0.9973	0.5160

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Chain	Atom inclusion	Q-score
DU	0.9959	0.5150
DZ	0.9927	0.5400
Da	0.9979	0.5590
UQ	1.0000	0.4100
UR	1.0000	0.4000
US	0.9877	0.4230
UT	0.9659	0.3910