Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:49 am GMT

PDB ID	:	6HIW
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)

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

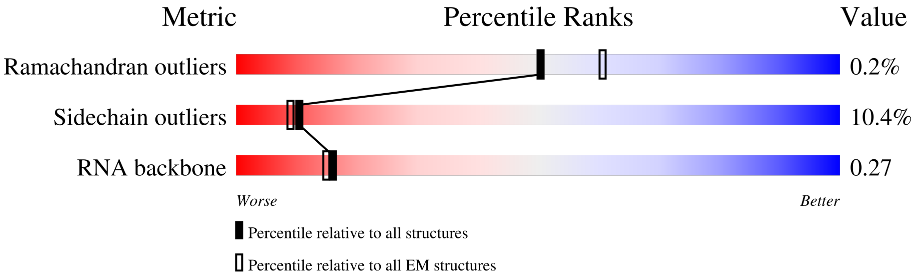
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

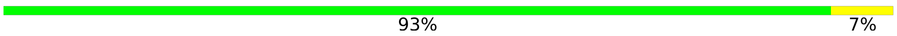
The reported resolution of this entry is 3.37 Å.

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)
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	
2	DD	812	
3	DI	407	
4	DL	307	
5	DM	294	
6	DN	293	
7	DO	282	
8	DP	274	

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Mol	Chain	Length	Quality of chain
9	DQ	268	92% • •
10	DR	270	82% 10% 7%
11	DS	261	84% 7% 9%
12	DU	228	85% 8% 7%
13	DZ	94	83% • 13%
14	Da	64	73% 12% 14%
15	DB	1181	86% 8% 6%
16	DC	1165	86% 8% 6%
17	DE	747	72% 7% 21%
18	DF	666	80% 8% 11%
19	DG	631	80% 9% 10%
20	DH	581	88% 9% •
21	DJ	396	72% 8% 20%
22	DK	324	73% 6% 21%
23	DT	247	86% 11% •
24	DV	183	79% 8% 13%
25	DW	179	82% 8% 10%
26	DX	169	76% 7% 17%
27	DY	163	82% 12% 6%
28	CC	74	88% 12%
29	CE	435	85% 11% •
30	CF	160	• 89% 10% •
31	CH	282	84% 12% •
32	CI	443	89% 7% •
33	CJ	817	88% 10% •

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Mol	Chain	Length	Quality of chain
34	CK	326	80% 10% 10%
35	CL	87	79% 18% •
36	CN	166	84% 11% 5%
37	CO	429	74% 9% 16%
38	CP	188	90% 6% •
39	CQ	307	53% 9% 38%
40	CR	320	89% 8% •
41	CS	244	55% • 42%
42	CU	193	90% 6% 5%
43	CZ	360	38% • 58%
44	Ca	602	89% 9% •
45	Cb	325	70% 7% 22%
46	Cd	440	59% 8% 34%
47	Cg	498	90% 7% •
48	Ci	181	78% 13% 9%
49	Cj	257	80% 8% 12%
50	Ck	874	73% 7% 20%
51	Cm	215	80% 11% 9%
52	Cn	250	39% 5% 56%
53	Cp	187	85% 9% 6%
54	Cq	263	87% 9% •
55	Cr	439	52% 6% 41%
56	Cv	1211	79% 8% 13%
57	CA	621	52% 46% •
58	UO	5	100%

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Mol	Chain	Length	Quality of chain
59	UP	7	100%
60	UQ	32	100%
61	UR	8	100%
62	US	54	100%
63	UT	44	100%

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
			Total	C	N	O	S		
1	DA	1557	12482	7881	2226	2337	38	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	283	2287	1451	423	401	12	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	189	1613	1037	290	277	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 mS49.

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

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
			Total	C	N	O	S		
16	DC	1095	8748	5519	1544	1654	31	0	0

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
			Total	C	N	O	S		
17	DE	590	4831	3075	874	863	19	0	0

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
			Total	C	N	O	S		
18	DF	590	4747	2979	896	847	25	0	0

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
			Total	C	N	O	S		
19	DG	566	4575	2875	835	834	31	0	0

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
			Total	C	N	O	S		
20	DH	564	4578	2872	850	834	22	0	0

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
			Total	C	N	O	S		
21	DJ	315	2572	1646	452	460	14	0	0

- Molecule 22 is a protein called mS58.

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

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 2058	C 1321	N 364	O 362	S 11	0	0

- Molecule 24 is a protein called mS69.

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

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 1359	C 866	N 260	O 228	S 5	0	0

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 1196	C 762	N 226	O 201	S 7	0	0

- Molecule 27 is a protein called mS72.

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

- Molecule 28 is a protein called uS3m.

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

- Molecule 29 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	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 30 is a protein called bS6m.

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

- Molecule 31 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	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 32 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	CI	424	3386	2136	611	622	17	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 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
			Total	C	N	O	S		
37	CO	361	3003	1907	560	520	16	0	0

- Molecule 38 is a protein called bS16m.

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

- Molecule 39 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	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 40 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	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 41 is a protein called uS19m.

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

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
			Total	C	N	O	S		
42	CU	184	1538	965	307	254	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	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 44 is a protein called mS22.

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

- Molecule 45 is a protein called mS23.

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

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
			Total	C	N	O	S		
46	Cd	291	2386	1491	442	443	10	0	0

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
			Total	C	N	O	S		
47	Cg	482	3904	2499	684	701	20	0	0

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
			Total	C	N	O	S		
48	Ci	165	1348	848	247	244	9	0	0

- Molecule 49 is a protein called mS34.

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

- Molecule 50 is a protein called mS35.

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

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
			Total	C	N	O	S		
51	Cm	196	1577	975	304	289	9	0	0

- Molecule 52 is a protein called mS38.

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

- Molecule 53 is a protein called mS41.

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

- Molecule 54 is a protein called mS42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	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 55 is a protein called mS43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	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 56 is a protein called mS47.

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

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
			Total	C	N	O	P		
57	CA	621	13122	5906	2227	4368	621	0	0

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
			Total	C	N	O		
58	UO	5	30	20	5	5	0	0

- Molecule 59 is a protein called Unknown Protein.

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

- Molecule 60 is a protein called Unknown Protein.

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

- Molecule 61 is a protein called Unknown Protein.

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

- Molecule 62 is a protein called Unknown Protein.

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

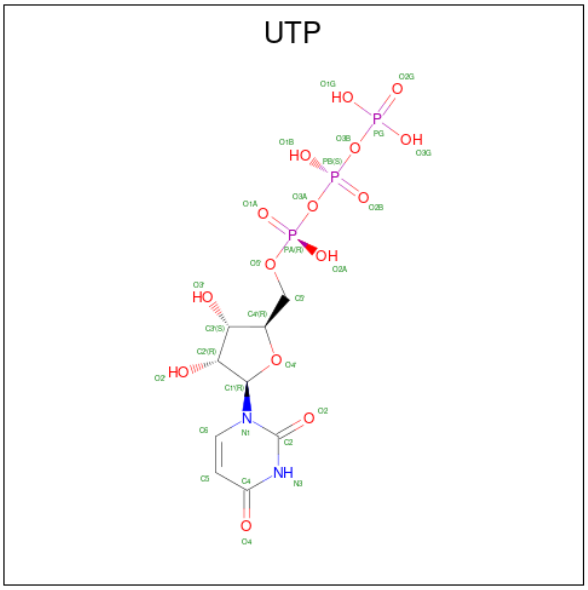
- Molecule 63 is a protein called Unknown Protein.

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

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 65 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).

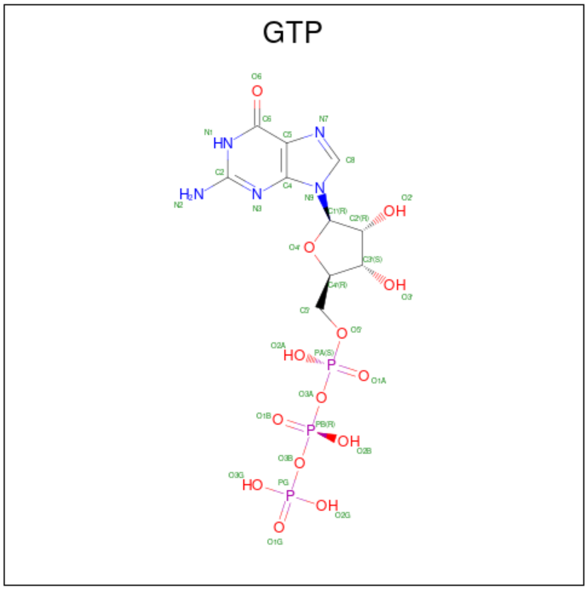


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
65	DJ	1	29	9	2	15	3	0

- Molecule 66 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

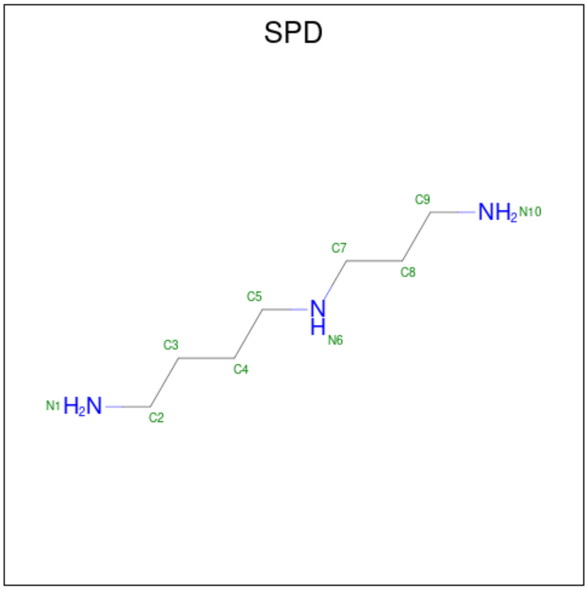
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
66	CQ	1	1	1	0
66	Ca	1	1	1	0
66	Cg	1	1	1	0
66	Cv	1	1	1	0
66	CA	35	35	35	0

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



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

- Molecule 68 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
68	CA	1	40	28	12	0
68	CA	1	40	28	12	0
68	CA	1	40	28	12	0

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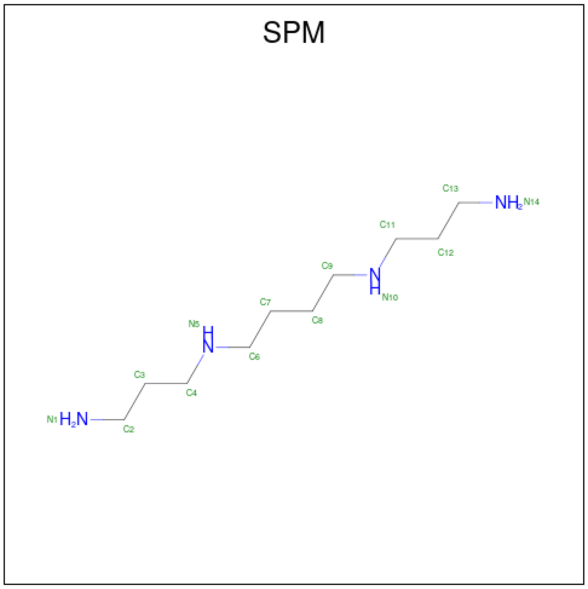
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
68	CA	1	40	28	12	0

- Molecule 69 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



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

- Molecule 70 is water.

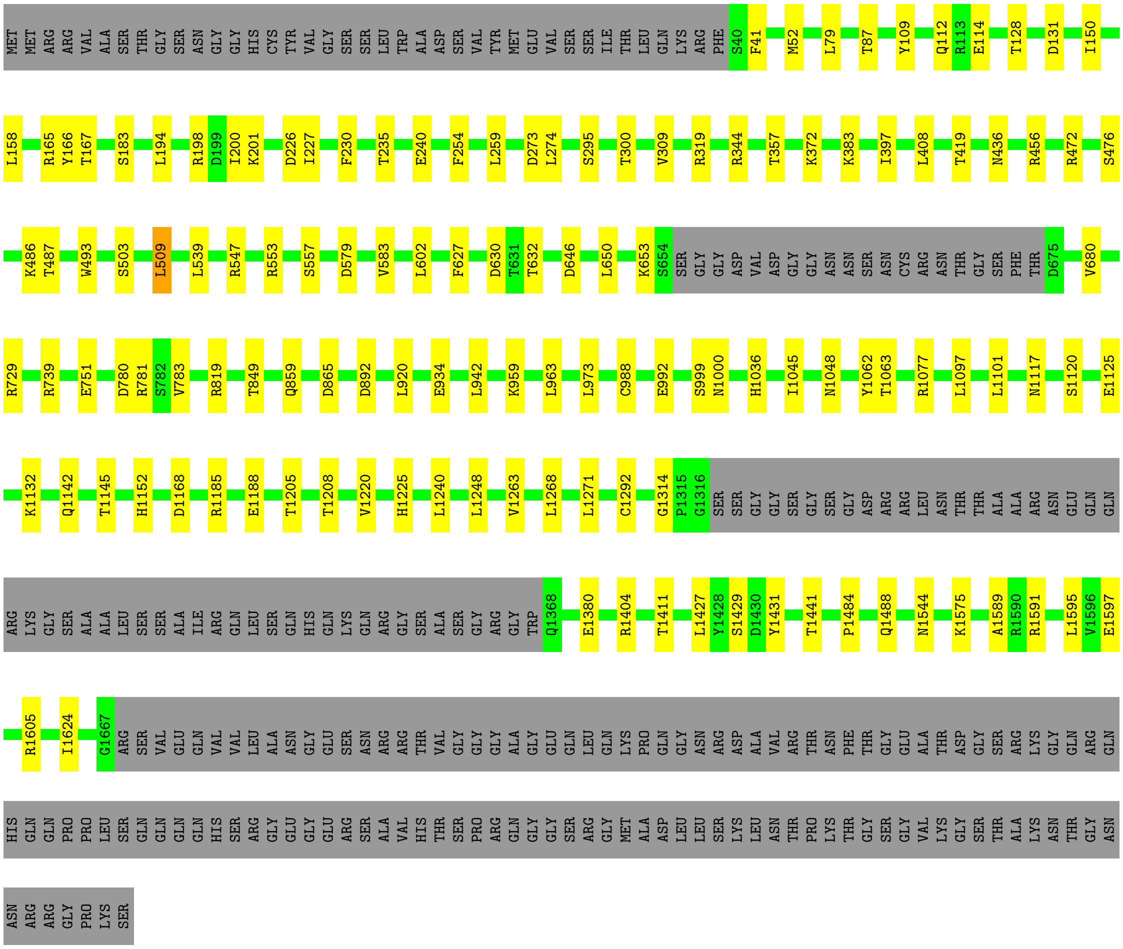
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
70	Cg	3	3	3	0

3 Residue-property plots ⓘ

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

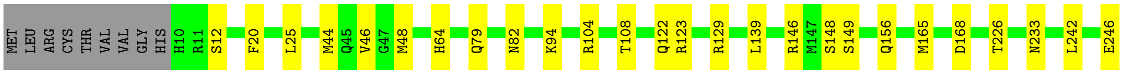
- Molecule 1: mS48

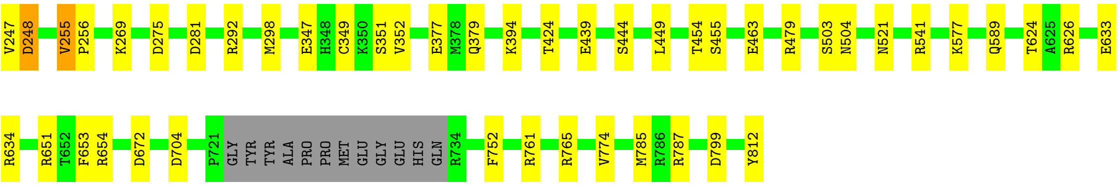
Chain DA:



- Molecule 2: mS51

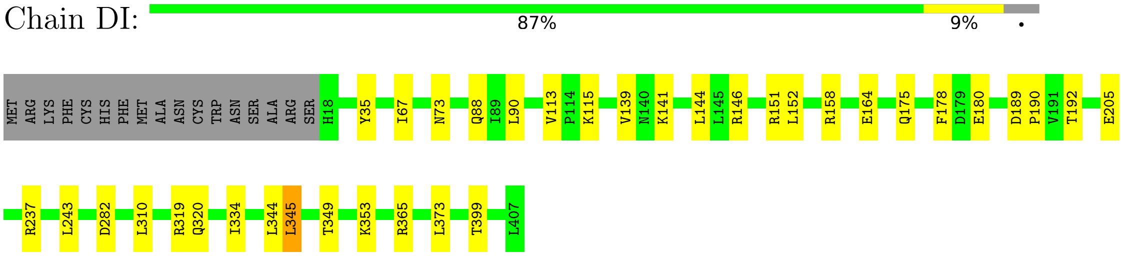
Chain DD:





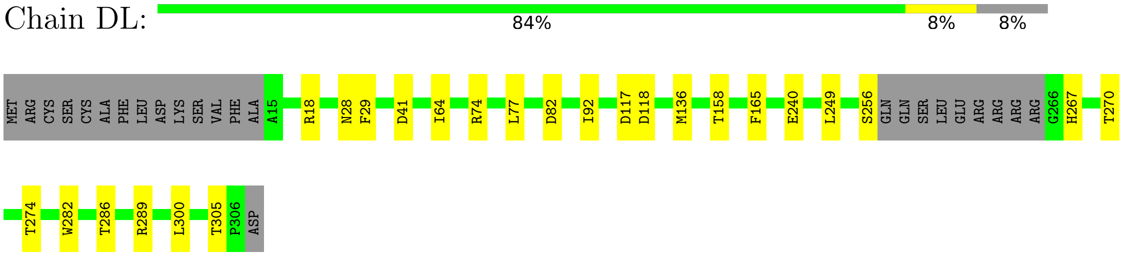
- Molecule 3: mS56

Chain DI:



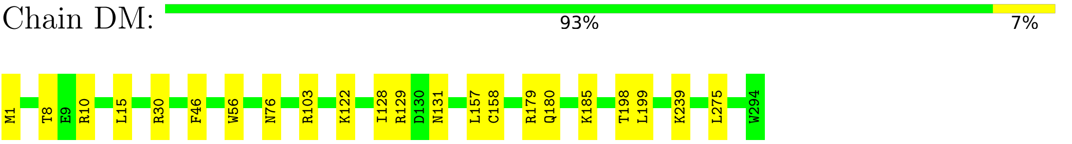
- Molecule 4: mS59

Chain DL:



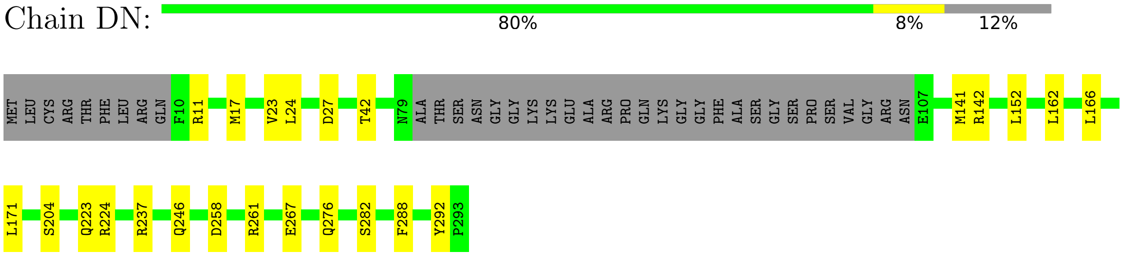
- Molecule 5: mS60

Chain DM:



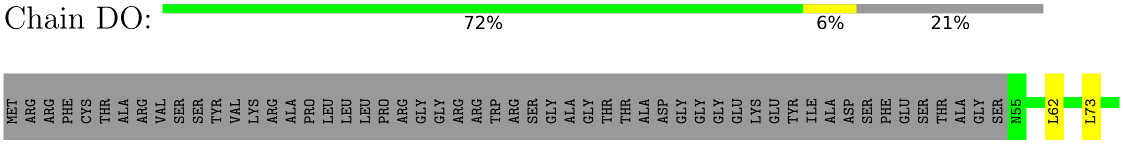
- Molecule 6: mS61

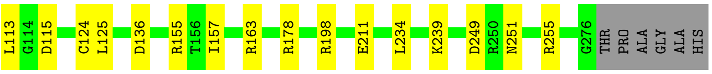
Chain DN:



- Molecule 7: mS62

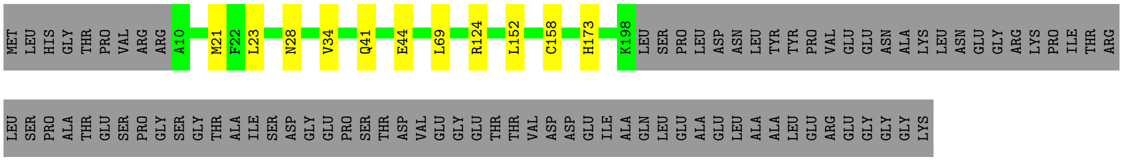
Chain DO:





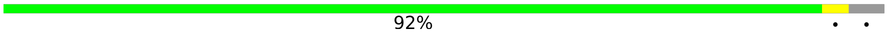
- Molecule 8: mS63

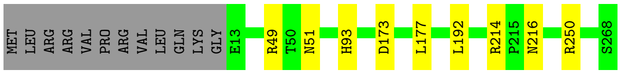
Chain DP:



- Molecule 9: mS64

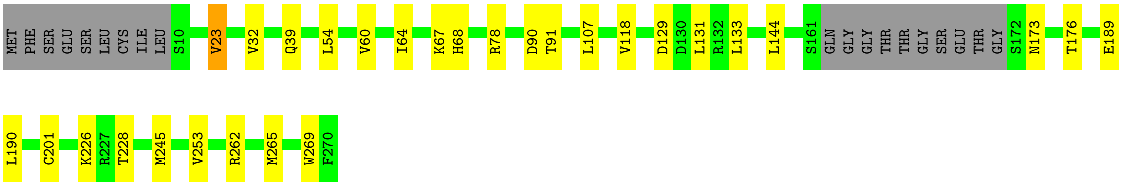
Chain DQ:





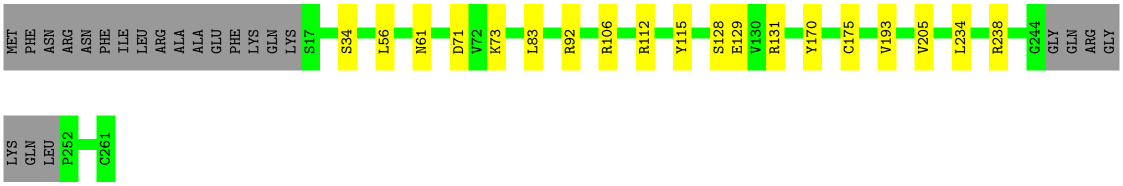
- Molecule 10: mS65

Chain DR:



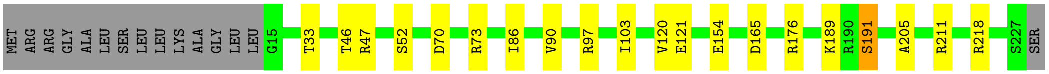
- Molecule 11: mS66

Chain DS:



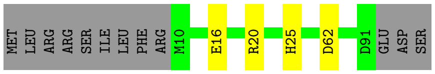
- Molecule 12: mS68

Chain DU:



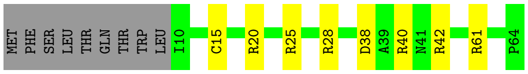
- Molecule 13: mS73

Chain DZ:



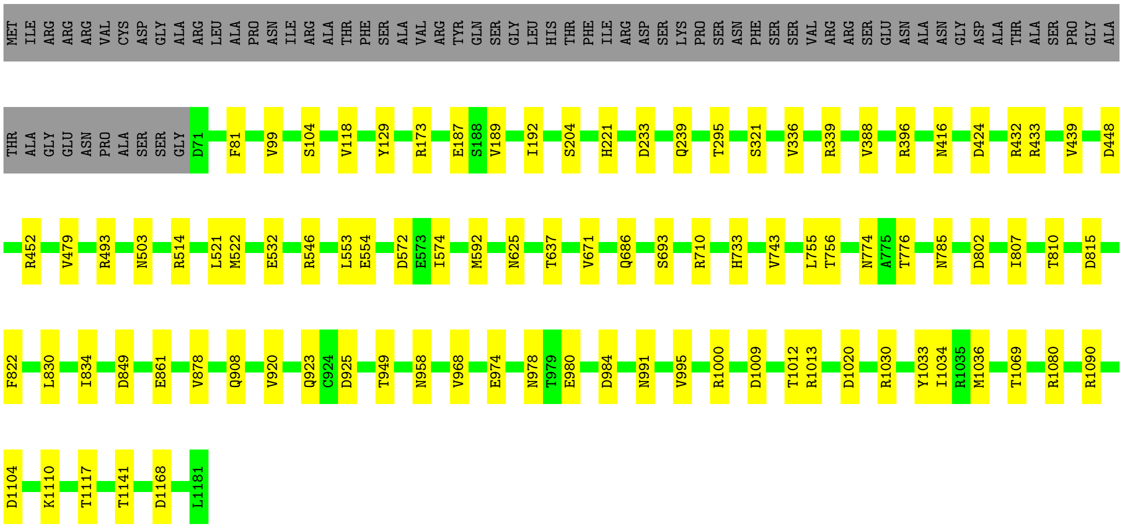
- Molecule 14: mS74

Chain Da:



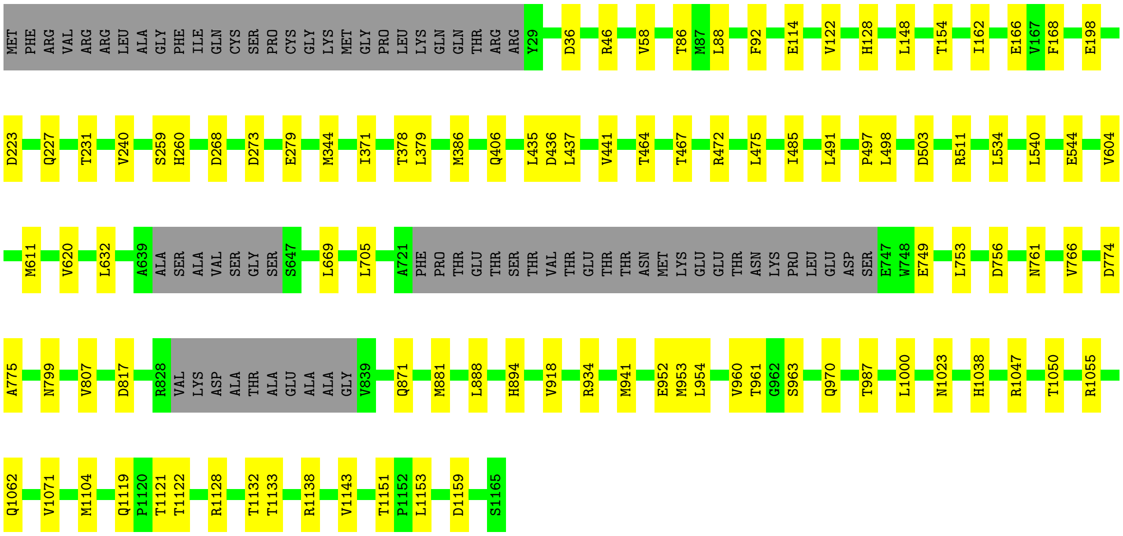
- Molecule 15: mS49

Chain DB:



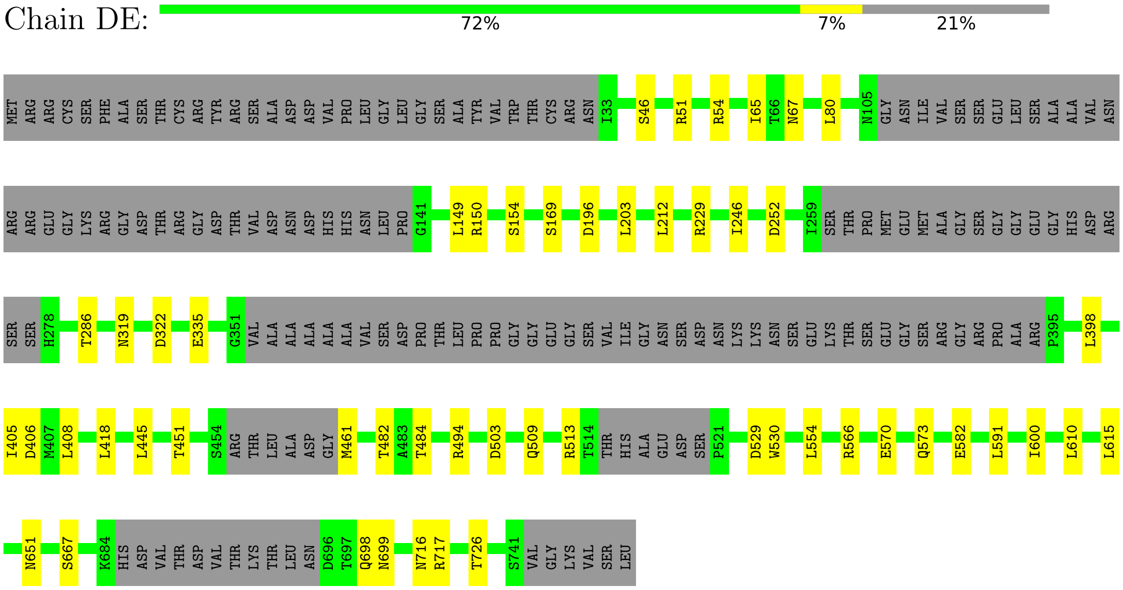
- Molecule 16: mS50

Chain DC:



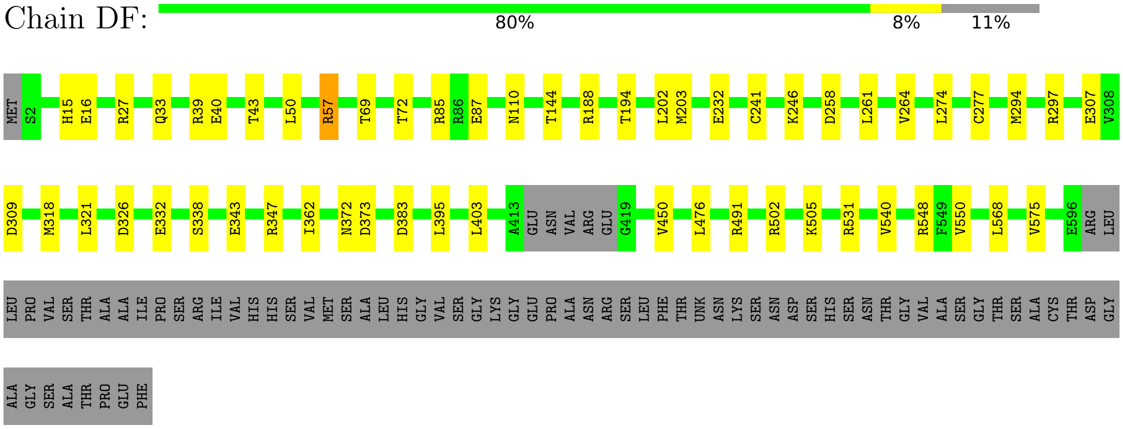
- Molecule 17: mS52

Chain DE:



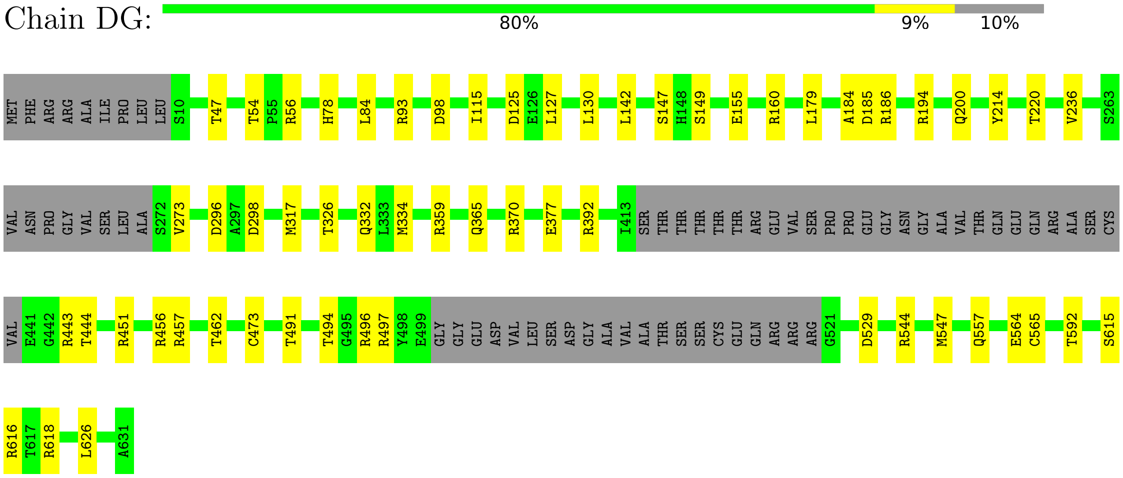
- Molecule 18: mS53

Chain DF:



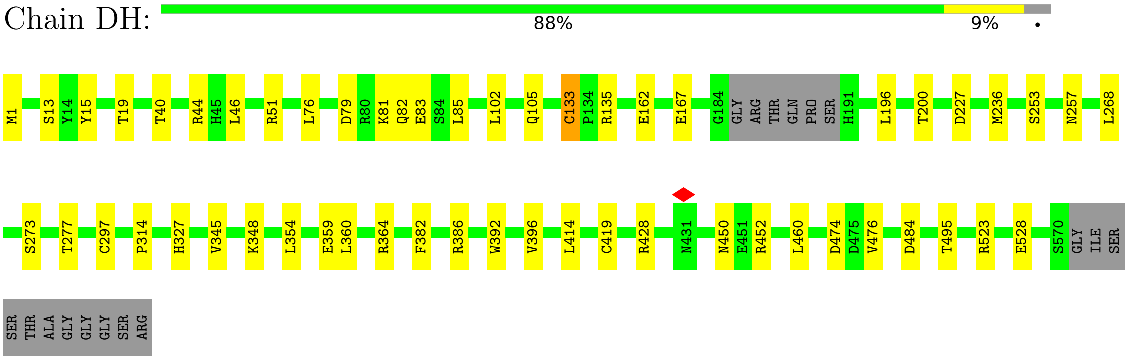
- Molecule 19: mS54

Chain DG:



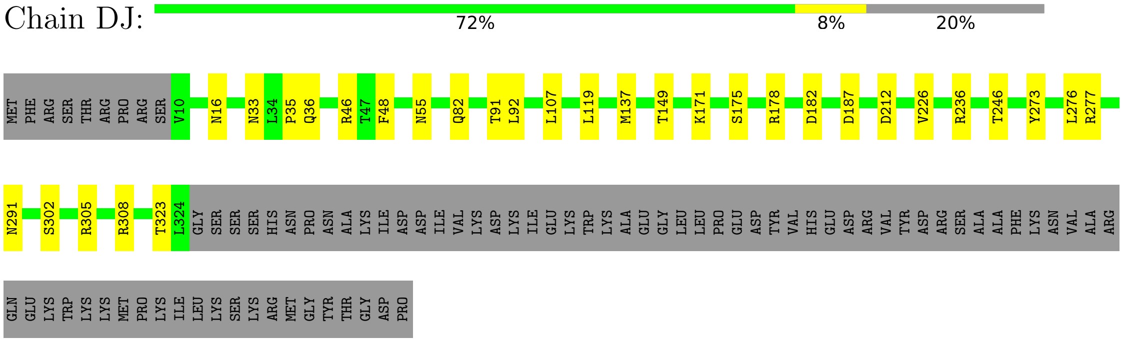
- Molecule 20: mS55

Chain DH:



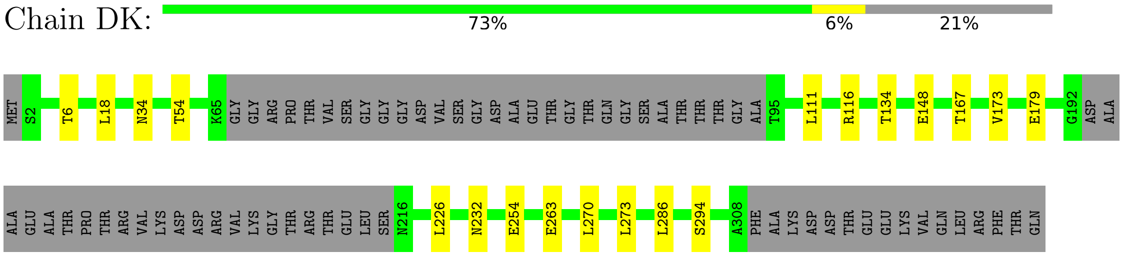
- Molecule 21: mS57

Chain DJ:



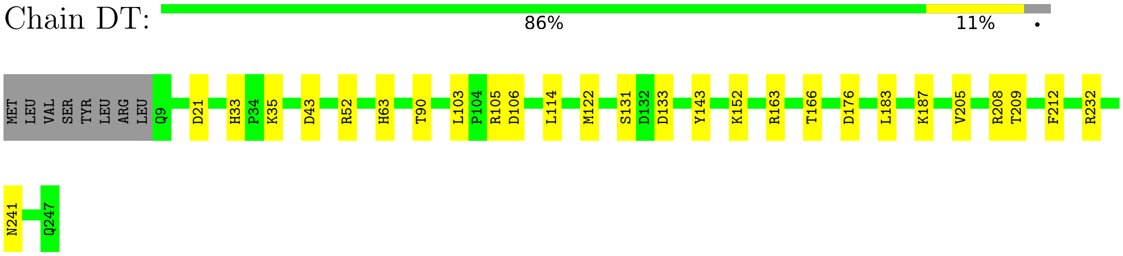
- Molecule 22: mS58

Chain DK:



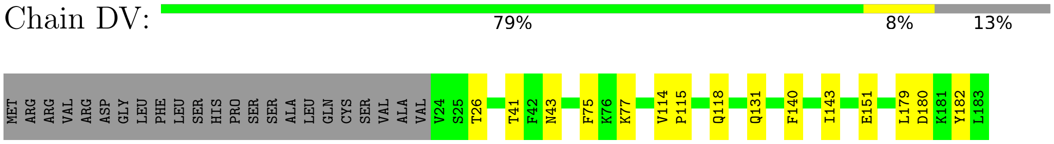
- Molecule 23: mS67

Chain DT:

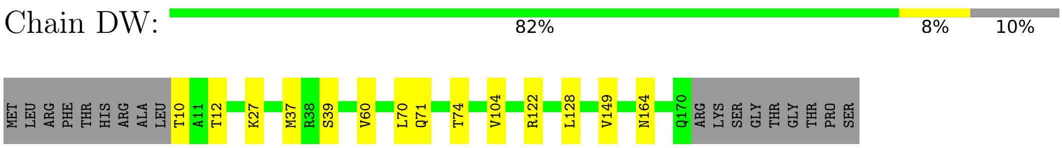


- Molecule 24: mS69

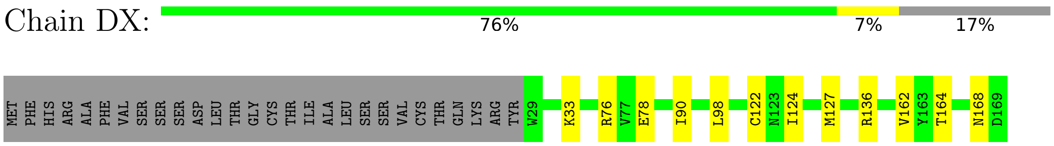
Chain DV:



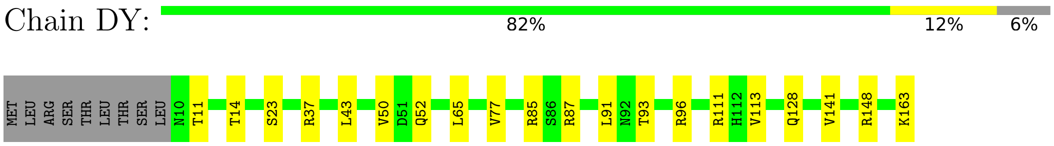
- Molecule 25: mS70



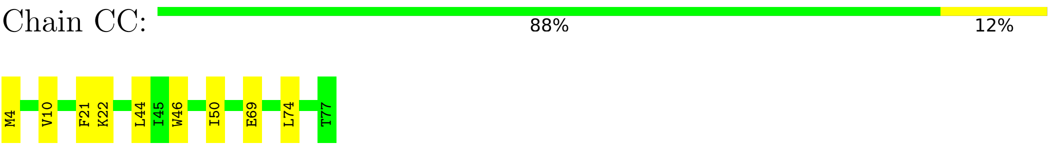
- Molecule 26: mS71



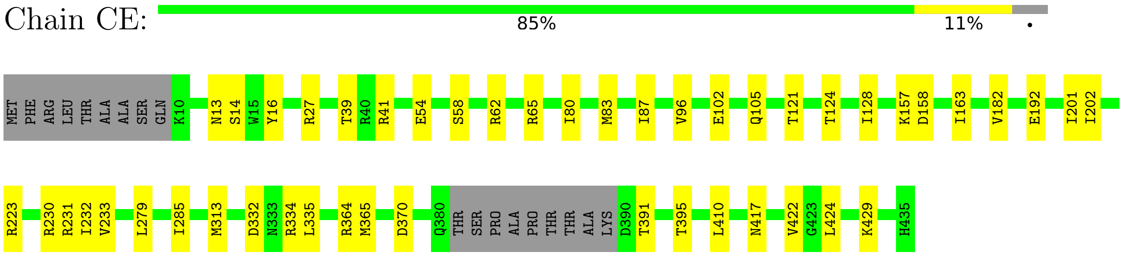
- Molecule 27: mS72



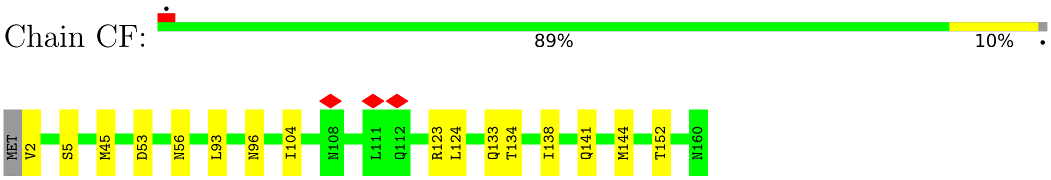
- Molecule 28: uS3m



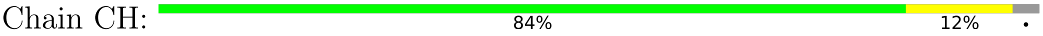
- Molecule 29: uS5m

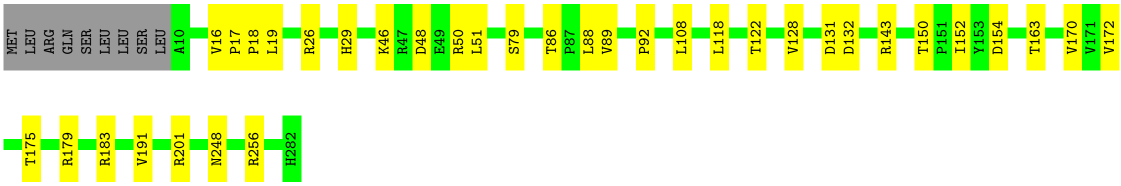


- Molecule 30: bS6m



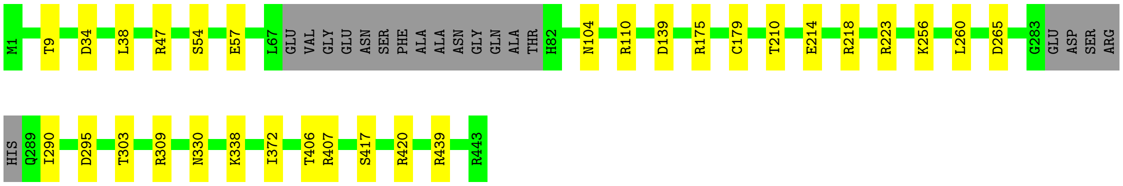
- Molecule 31: uS8m





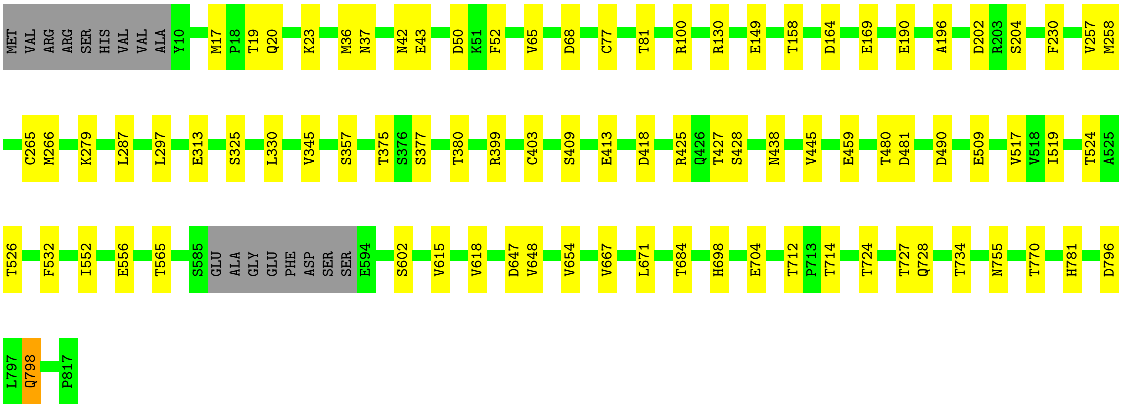
- Molecule 32: uS9m

Chain CI:



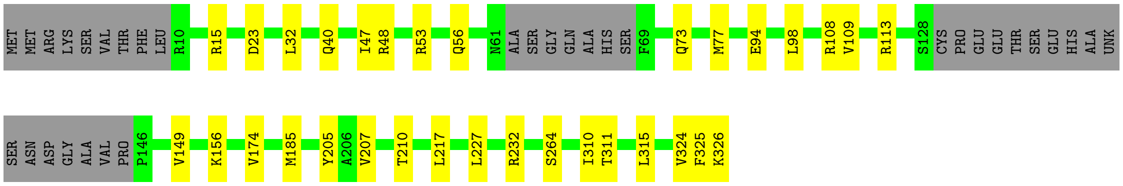
- Molecule 33: uS10m

Chain CJ:



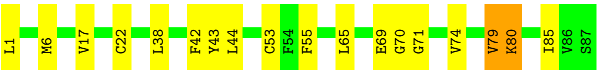
- Molecule 34: uS11m

Chain CK:



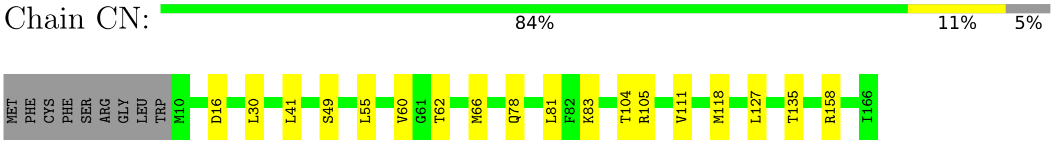
- Molecule 35: uS12m

Chain CL:



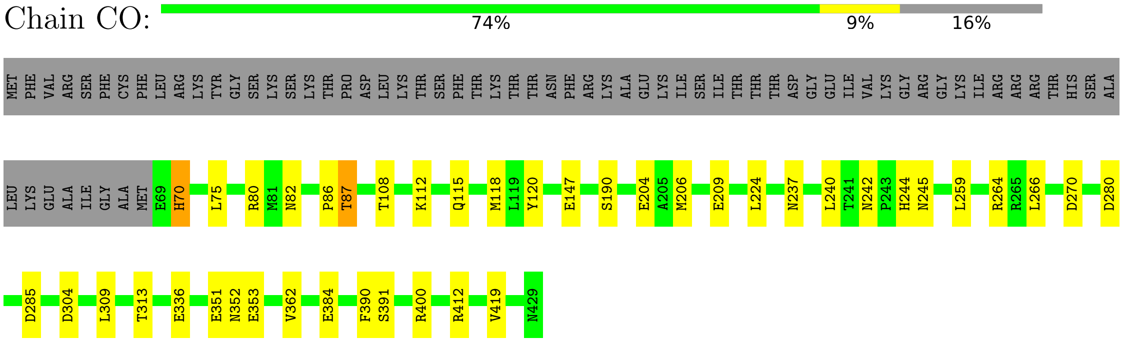
- Molecule 36: uS14m

Chain CN:



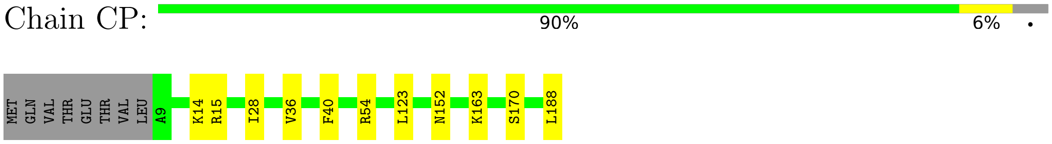
- Molecule 37: uS15m

Chain CO:



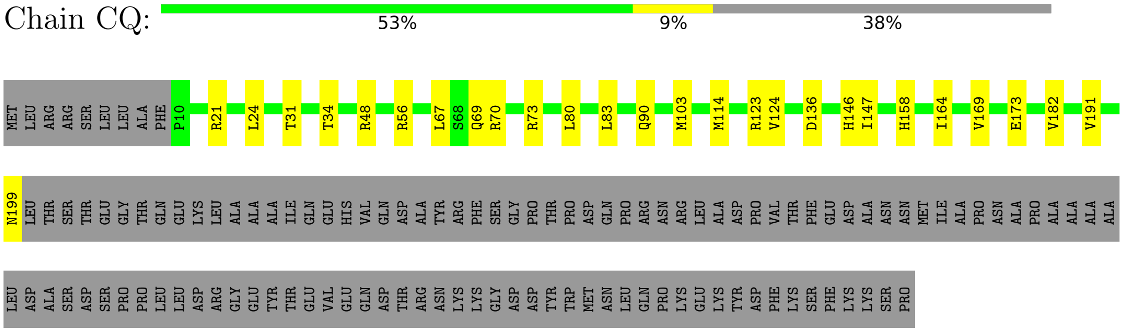
- Molecule 38: bS16m

Chain CP:



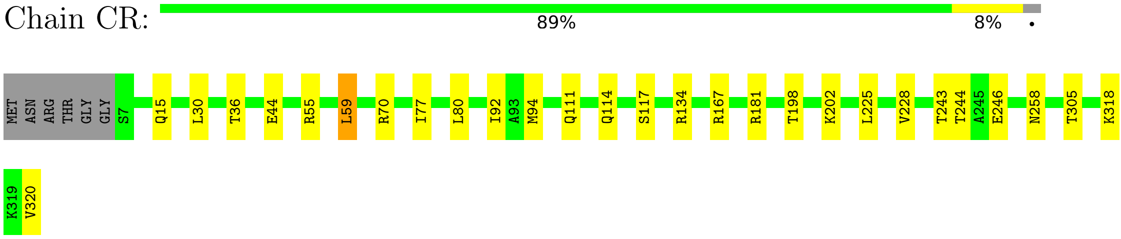
- Molecule 39: uS17m

Chain CQ:



- Molecule 40: bS18m

Chain CR:

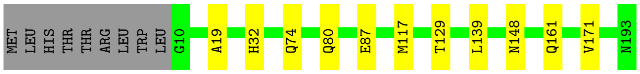


- Molecule 41: uS19m

Chain CS:

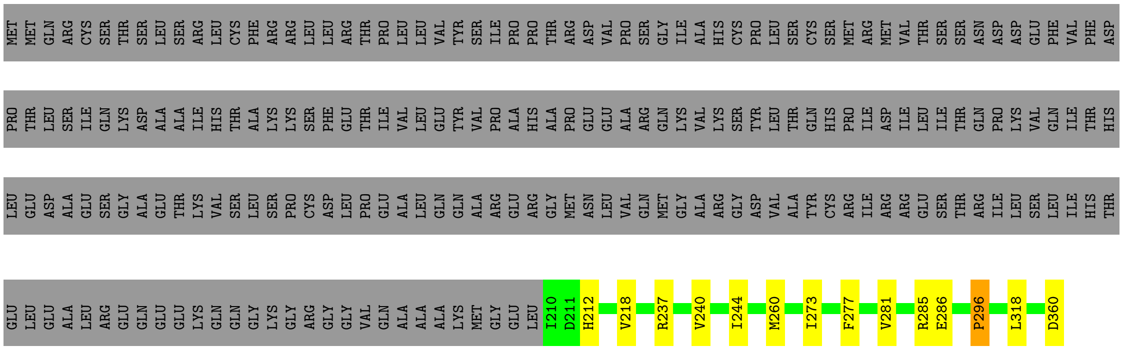
• Molecule 42: bS21m

Chain CU:



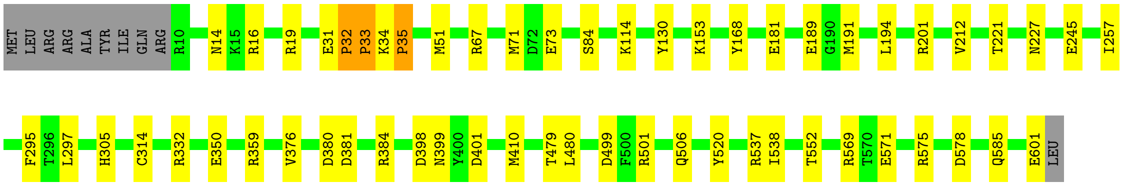
• Molecule 43: mt-IF-3

Chain CZ:



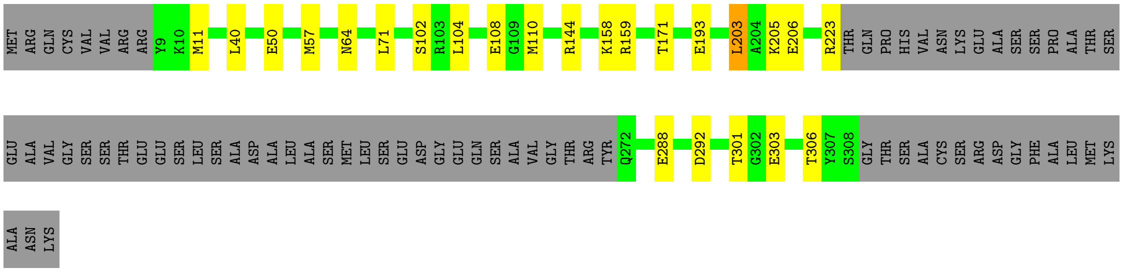
• Molecule 44: mS22

Chain Ca:

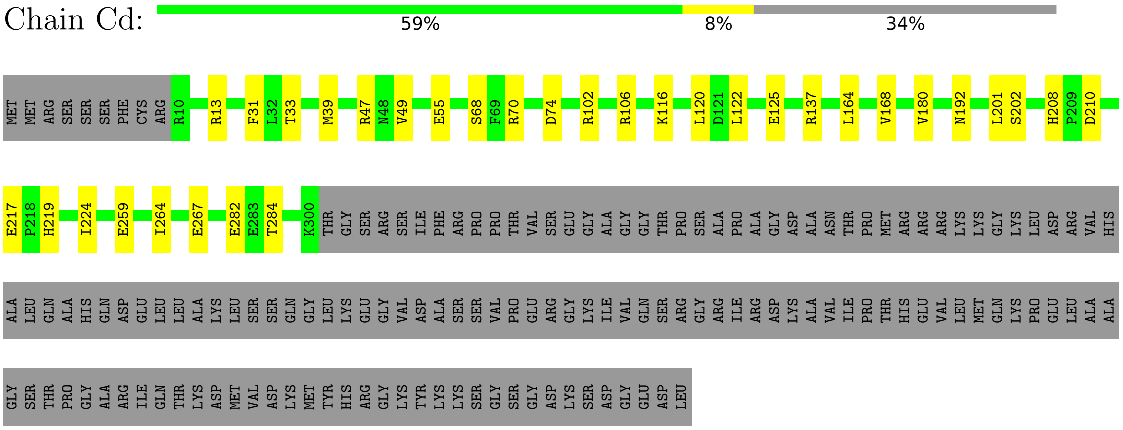


• Molecule 45: mS23

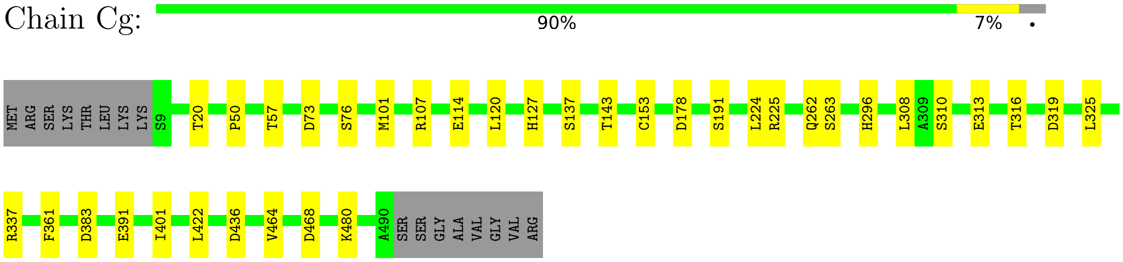
Chain Cb:



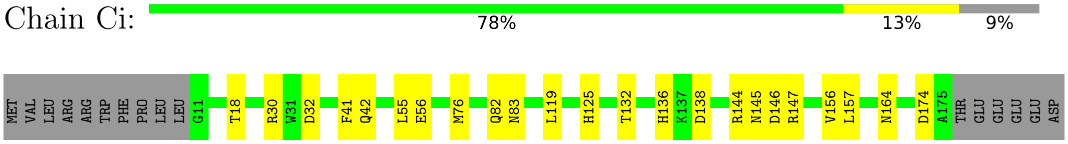
• Molecule 46: mS26



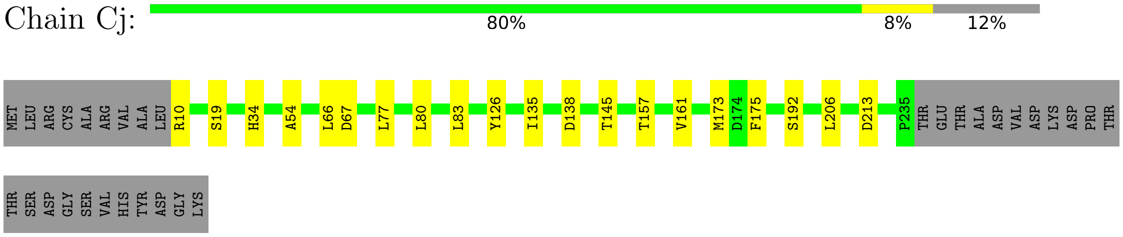
- Molecule 47: mS29



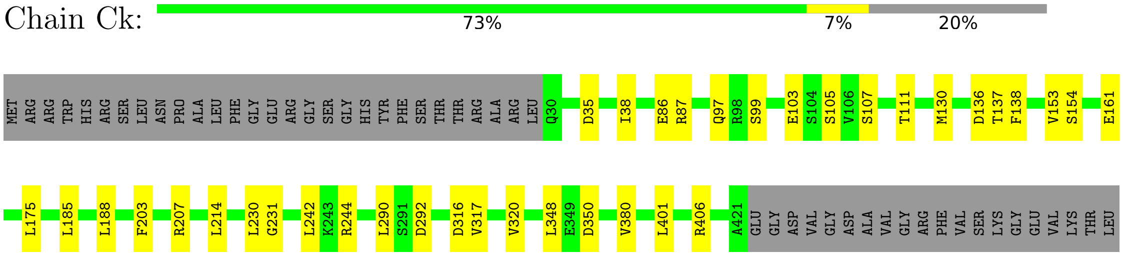
- Molecule 48: mS33

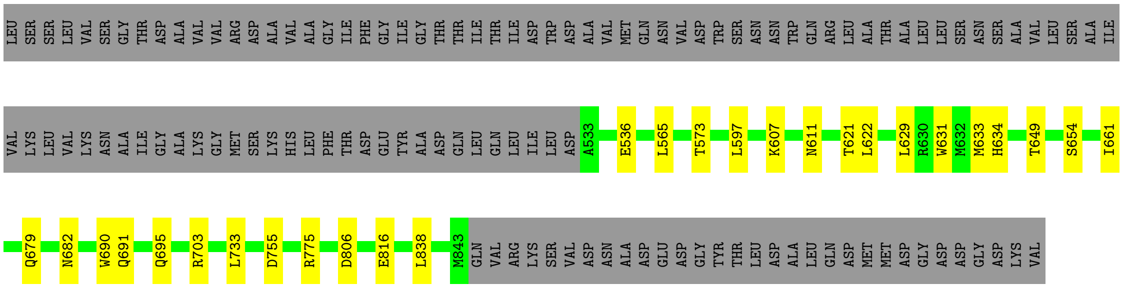


- Molecule 49: mS34



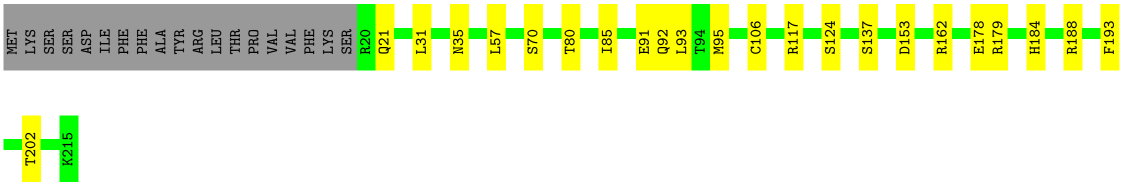
- Molecule 50: mS35





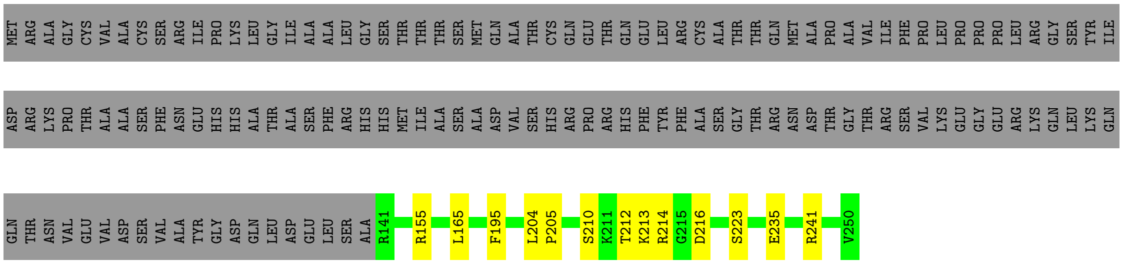
- Molecule 51: mS37

Chain Cm:



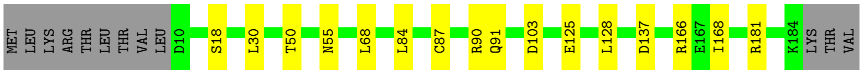
- Molecule 52: mS38

Chain Cn:



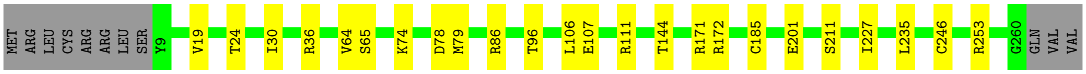
- Molecule 53: mS41

Chain Cp:



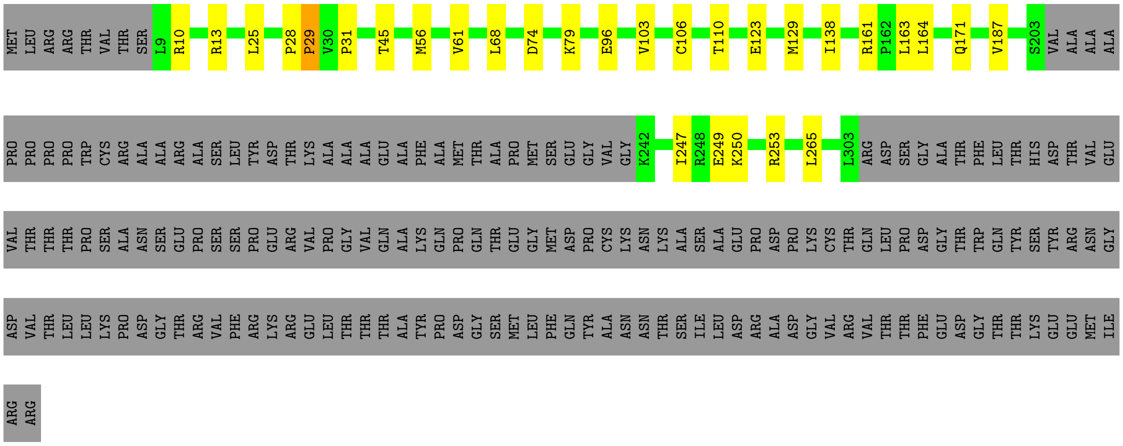
- Molecule 54: mS42

Chain Cq:



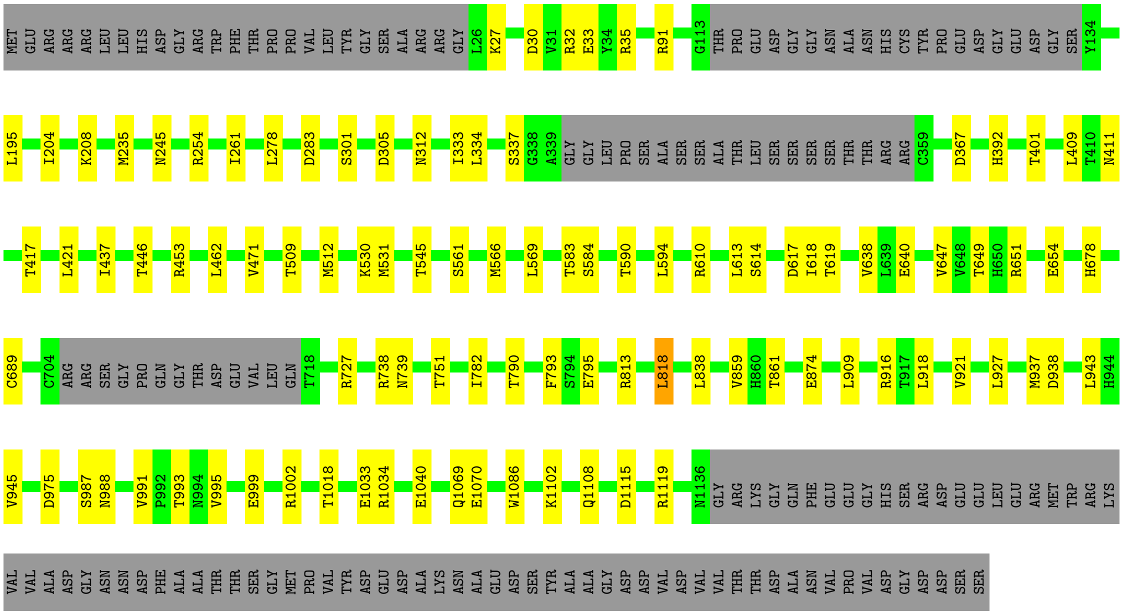
- Molecule 55: mS43

Chain Cr:



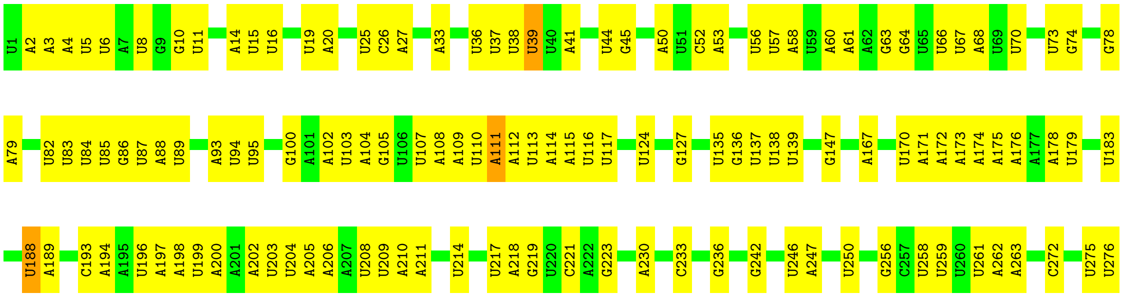
- Molecule 56: mS47

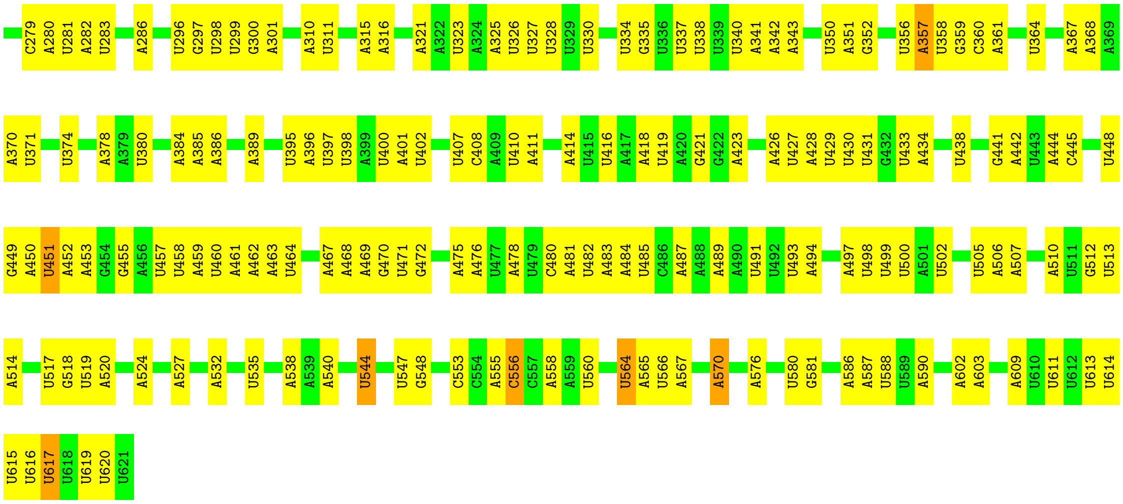
Chain Cv:



- Molecule 57: 9S rRNA

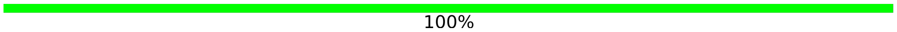
Chain CA:





- Molecule 58: Unknown Protein

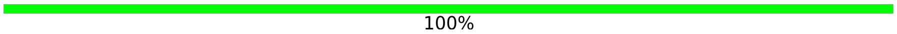
Chain UO:



There are no outlier residues recorded for this chain.

- Molecule 59: Unknown Protein

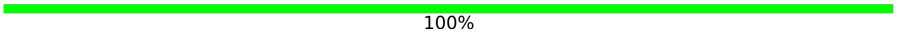
Chain UP:



There are no outlier residues recorded for this chain.

- Molecule 60: Unknown Protein

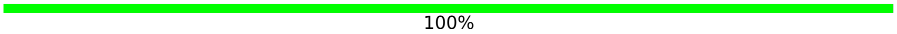
Chain UQ:



There are no outlier residues recorded for this chain.

- Molecule 61: Unknown Protein

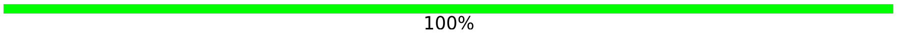
Chain UR:



There are no outlier residues recorded for this chain.

- Molecule 62: Unknown Protein

Chain US:



There are no outlier residues recorded for this chain.

- Molecule 63: Unknown Protein

Chain UT:

There are no outlier residues recorded for this chain.

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 $(e^-/\text{Å}^2)$	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	0.538	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UTP, SPM, SPD, 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	0.37	0/12780	0.55	3/17297 (0.0%)
2	DD	0.38	0/6710	0.57	1/9087 (0.0%)
3	DI	0.37	0/3248	0.57	1/4401 (0.0%)
4	DL	0.42	0/2346	0.60	0/3164
5	DM	0.40	0/2488	0.58	0/3362
6	DN	0.40	0/2148	0.59	0/2916
7	DO	0.38	0/1840	0.60	0/2482
8	DP	0.34	0/1662	0.50	0/2249
9	DQ	0.37	0/2111	0.59	0/2863
10	DR	0.35	0/2090	0.58	0/2849
11	DS	0.35	0/1950	0.54	0/2633
12	DU	0.37	0/1799	0.54	0/2438
13	DZ	0.39	0/725	0.57	0/984
14	Da	0.42	0/520	0.58	0/694
15	DB	0.36	0/9369	0.53	0/12692
16	DC	0.34	0/8952	0.51	0/12145
17	DE	0.32	0/4955	0.51	0/6708
18	DF	0.35	0/4856	0.54	2/6581 (0.0%)
19	DG	0.35	0/4674	0.53	0/6333
20	DH	0.35	0/4684	0.53	1/6347 (0.0%)
21	DJ	0.35	0/2649	0.53	0/3598
22	DK	0.34	0/2045	0.50	0/2759
23	DT	0.35	0/2133	0.53	0/2889
24	DV	0.38	0/1382	0.58	0/1871
25	DW	0.36	0/1407	0.54	0/1916
26	DX	0.36	0/1231	0.54	0/1654
27	DY	0.41	0/1334	0.58	0/1810
28	CC	0.39	0/666	0.59	0/900
29	CE	0.42	0/3484	0.60	0/4708
30	CF	0.39	0/1319	0.57	0/1783
31	CH	0.46	0/2276	0.59	0/3071
32	CI	0.41	0/3453	0.56	0/4655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	CJ	0.42	0/6705	0.58	0/9124
34	CK	0.38	0/2472	0.58	0/3315
35	CL	0.43	0/759	0.63	0/1026
36	CN	0.42	0/1361	0.57	0/1840
37	CO	0.41	0/3085	0.58	0/4165
38	CP	0.43	0/1533	0.61	0/2074
39	CQ	0.48	0/1631	0.66	0/2203
40	CR	0.42	0/2640	0.60	0/3572
41	CS	0.38	0/1209	0.54	0/1626
42	CU	0.38	0/1576	0.55	0/2115
43	CZ	0.35	0/1237	0.55	1/1659 (0.1%)
44	Ca	0.42	0/5159	0.59	3/6980 (0.0%)
45	Cb	0.42	0/2105	0.60	1/2842 (0.0%)
46	Cd	0.41	0/2438	0.56	0/3288
47	Cg	0.38	0/4025	0.57	0/5467
48	Ci	0.39	0/1388	0.64	1/1878 (0.1%)
49	Cj	0.35	0/1842	0.54	0/2511
50	Ck	0.37	0/5696	0.56	0/7705
51	Cm	0.47	0/1616	0.65	0/2175
52	Cn	0.41	0/934	0.58	0/1248
53	Cp	0.36	0/1528	0.55	0/2072
54	Cq	0.42	0/2066	0.58	0/2815
55	Cr	0.34	0/2038	0.56	3/2759 (0.1%)
56	Cv	0.40	0/8780	0.59	1/11901 (0.0%)
57	CA	0.49	1/14679 (0.0%)	1.01	30/22827 (0.1%)
All	All	0.39	1/181788 (0.0%)	0.62	48/249026 (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	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)
57	CA	357	A	N9-C4	-5.86	1.34	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	CA	451	U	N1-C2-O2	7.12	127.78	122.80
57	CA	493	U	C2-N1-C1’	7.02	126.12	117.70
57	CA	188	U	C2-N1-C1’	6.84	125.91	117.70
57	CA	63	G	N3-C4-C5	6.75	131.97	128.60
57	CA	188	U	N3-C2-O2	-6.65	117.55	122.20
57	CA	570	A	N1-C6-N6	6.52	122.51	118.60
57	CA	188	U	N1-C2-O2	6.40	127.28	122.80
44	Ca	32	PRO	N-CA-CB	6.31	110.87	103.30
44	Ca	35	PRO	N-CA-CB	6.26	110.81	103.30
44	Ca	33	PRO	N-CA-CB	6.25	110.80	103.30
2	DD	255	VAL	C-N-CD	-6.24	106.87	120.60
57	CA	451	U	C2-N1-C1’	6.21	125.15	117.70
57	CA	451	U	N3-C2-O2	-6.21	117.86	122.20
1	DA	1484	PRO	N-CA-CB	6.14	110.67	103.30
18	DF	57	ARG	NE-CZ-NH1	6.11	123.36	120.30
55	Cr	28	PRO	N-CA-CB	6.07	110.58	103.30
45	Cb	203	LEU	CA-CB-CG	5.99	129.07	115.30
57	CA	196	U	C2-N1-C1’	5.97	124.86	117.70
57	CA	493	U	C5-C6-N1	5.91	125.65	122.70
57	CA	556	C	C2-N1-C1’	5.89	125.28	118.80
43	CZ	296	PRO	N-CA-CB	5.89	110.37	103.30
57	CA	370	A	O4’-C1’-N9	5.84	112.87	108.20
57	CA	493	U	N1-C2-O2	5.84	126.89	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CA	556	C	C5-C6-N1	5.82	123.91	121.00
57	CA	196	U	N1-C2-O2	5.81	126.87	122.80
57	CA	66	U	C2-N1-C1'	5.80	124.66	117.70
55	Cr	31	PRO	N-CA-CB	5.80	110.26	103.30
57	CA	570	A	C5-C6-N6	-5.62	119.20	123.70
55	Cr	29	PRO	N-CA-CB	5.53	109.94	103.30
1	DA	1314	GLY	N-CA-C	5.53	126.92	113.10
57	CA	310	A	C2-N3-C4	5.53	113.36	110.60
57	CA	39	U	O5'-P-OP2	-5.45	100.80	105.70
57	CA	63	G	N3-C4-N9	-5.43	122.74	126.00
20	DH	133	CYS	C-N-CD	5.42	139.77	128.40
57	CA	499	U	C2-N1-C1'	5.38	124.15	117.70
57	CA	617	U	C2-N1-C1'	5.24	123.99	117.70
3	DI	345	LEU	CA-CB-CG	5.22	127.31	115.30
57	CA	544	U	C5-C6-N1	-5.17	120.11	122.70
57	CA	564	U	C2-N3-C4	5.17	130.10	127.00
1	DA	509	LEU	CA-CB-CG	5.15	127.15	115.30
57	CA	111	A	O4'-C1'-N9	5.14	112.31	108.20
57	CA	564	U	C5-C6-N1	5.13	125.26	122.70
18	DF	261	LEU	CA-CB-CG	-5.08	103.61	115.30
57	CA	564	U	N1-C2-O2	5.06	126.34	122.80
48	Ci	55	LEU	CA-CB-CG	5.03	126.87	115.30
57	CA	66	U	C5-C6-N1	5.02	125.21	122.70
56	Cv	818	LEU	CA-CB-CG	5.01	126.82	115.30
57	CA	233	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	CH	17	PRO	Peptide
31	CH	92	PRO	Peptide
33	CJ	100	ARG	Peptide
33	CJ	798	GLN	Peptide
35	CL	70	GLY	Peptide
35	CL	71	GLY	Peptide
35	CL	79	VAL	Peptide
37	CO	70	HIS	Peptide
37	CO	86	PRO	Peptide
46	Cd	192	ASN	Peptide
47	Cg	50	PRO	Peptide
50	Ck	230	LEU	Peptide

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Mol	Chain	Res	Type	Group
56	Cv	545	THR	Peptide
56	Cv	943	LEU	Peptide
1	DA	166	TYR	Peptide
1	DA	273	ASP	Peptide
16	DC	497	PRO	Peptide
16	DC	775	ALA	Peptide
2	DD	247	VAL	Peptide
2	DD	255	VAL	Peptide
2	DD	351	SER	Peptide
19	DG	184	ALA	Peptide
19	DG	592	THR	Peptide
21	DJ	35	PRO	Peptide
6	DN	142	ARG	Peptide
7	DO	124	CYS	Peptide
7	DO	251	ASN	Peptide
10	DR	189	GLU	Peptide
10	DR	23	VAL	Peptide
23	DT	43	ASP	Peptide
26	DX	127	MET	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DA	1551/1788 (87%)	1490 (96%)	59 (4%)	2 (0%)	51	82
2	DD	787/812 (97%)	740 (94%)	44 (6%)	3 (0%)	34	68
3	DI	388/407 (95%)	365 (94%)	22 (6%)	1 (0%)	41	73
4	DL	279/307 (91%)	261 (94%)	18 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	63
8	DP	187/274 (68%)	176 (94%)	11 (6%)	0	100	100
9	DQ	254/268 (95%)	244 (96%)	9 (4%)	1 (0%)	34	68
10	DR	247/270 (92%)	236 (96%)	10 (4%)	1 (0%)	34	68
11	DS	234/261 (90%)	222 (95%)	11 (5%)	1 (0%)	34	68
12	DU	211/228 (92%)	198 (94%)	11 (5%)	2 (1%)	17	51
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%)	51	82
16	DC	1087/1165 (93%)	1053 (97%)	33 (3%)	1 (0%)	51	82
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%)	41	73
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%)	47	78
30	CF	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
31	CH	271/282 (96%)	259 (96%)	11 (4%)	1 (0%)	34	68
32	CI	418/443 (94%)	405 (97%)	13 (3%)	0	100	100
33	CJ	796/817 (97%)	755 (95%)	39 (5%)	2 (0%)	41	73
34	CK	287/326 (88%)	267 (93%)	20 (7%)	0	100	100
35	CL	85/87 (98%)	79 (93%)	5 (6%)	1 (1%)	13	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	CN	155/166 (93%)	148 (96%)	7 (4%)	0	100	100
37	CO	359/429 (84%)	342 (95%)	16 (4%)	1 (0%)	41	73
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%)	41	73
41	CS	140/244 (57%)	132 (94%)	8 (6%)	0	100	100
42	CU	182/193 (94%)	173 (95%)	8 (4%)	1 (0%)	29	63
43	CZ	149/360 (41%)	142 (95%)	6 (4%)	1 (1%)	22	56
44	Ca	590/602 (98%)	551 (93%)	34 (6%)	5 (1%)	19	53
45	Cb	248/325 (76%)	241 (97%)	7 (3%)	0	100	100
46	Cd	288/440 (66%)	277 (96%)	10 (4%)	1 (0%)	41	73
47	Cg	480/498 (96%)	462 (96%)	18 (4%)	0	100	100
48	Ci	163/181 (90%)	154 (94%)	9 (6%)	0	100	100
49	Cj	224/257 (87%)	215 (96%)	8 (4%)	1 (0%)	34	68
50	Ck	699/874 (80%)	676 (97%)	22 (3%)	1 (0%)	51	82
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%)	34	68
56	Cv	1051/1211 (87%)	1010 (96%)	41 (4%)	0	100	100
All	All	19802/22847 (87%)	18951 (96%)	818 (4%)	33 (0%)	50	78

All (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
44	Ca	34	LYS
1	DA	131	ASP
7	DO	115	ASP
15	DB	1033	TYR

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Mol	Chain	Res	Type
21	DJ	36	GLN
29	CE	313	MET
35	CL	80	LYS
40	CR	59	LEU
42	CU	19	ALA
2	DD	256	PRO
49	Cj	54	ALA
2	DD	248	ASP
3	DI	190	PRO
10	DR	269	TRP
12	DU	205	ALA
33	CJ	37	ASN
33	CJ	196	ALA
37	CO	87	THR
46	Cd	224	ILE
1	DA	1589	ALA
9	DQ	173	ASP
11	DS	129	GLU
12	DU	191	SER
50	Ck	231	GLY
16	DC	441	VAL
55	Cr	29	PRO
31	CH	18	PRO
44	Ca	31	GLU

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%)	1199 (91%)	123 (9%)	9	31
2	DD	694/711 (98%)	626 (90%)	68 (10%)	8	29
3	DI	350/365 (96%)	315 (90%)	35 (10%)	7	28
4	DL	241/263 (92%)	216 (90%)	25 (10%)	7	26
5	DM	252/252 (100%)	230 (91%)	22 (9%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	DN	229/256 (90%)	206 (90%)	23 (10%)	7	28
7	DO	186/229 (81%)	171 (92%)	15 (8%)	11	38
8	DP	170/239 (71%)	159 (94%)	11 (6%)	17	48
9	DQ	228/239 (95%)	220 (96%)	8 (4%)	36	65
10	DR	220/235 (94%)	193 (88%)	27 (12%)	4	19
11	DS	209/228 (92%)	191 (91%)	18 (9%)	10	36
12	DU	190/201 (94%)	171 (90%)	19 (10%)	7	28
13	DZ	72/84 (86%)	68 (94%)	4 (6%)	21	52
14	Da	50/59 (85%)	42 (84%)	8 (16%)	2	11
15	DB	976/1030 (95%)	885 (91%)	91 (9%)	9	31
16	DC	927/985 (94%)	832 (90%)	95 (10%)	7	28
17	DE	519/644 (81%)	467 (90%)	52 (10%)	7	28
18	DF	500/560 (89%)	446 (89%)	54 (11%)	6	25
19	DG	490/543 (90%)	433 (88%)	57 (12%)	5	21
20	DH	493/504 (98%)	439 (89%)	54 (11%)	6	24
21	DJ	275/347 (79%)	246 (90%)	29 (10%)	7	26
22	DK	209/261 (80%)	190 (91%)	19 (9%)	9	32
23	DT	220/228 (96%)	194 (88%)	26 (12%)	5	20
24	DV	145/165 (88%)	130 (90%)	15 (10%)	7	27
25	DW	148/163 (91%)	134 (90%)	14 (10%)	8	30
26	DX	124/149 (83%)	113 (91%)	11 (9%)	9	34
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%)	312 (87%)	46 (13%)	4	17
30	CF	136/144 (94%)	120 (88%)	16 (12%)	5	20
31	CH	237/246 (96%)	205 (86%)	32 (14%)	4	16
32	CI	357/371 (96%)	327 (92%)	30 (8%)	11	37
33	CJ	709/723 (98%)	627 (88%)	82 (12%)	5	21
34	CK	257/283 (91%)	225 (88%)	32 (12%)	4	18
35	CL	79/79 (100%)	63 (80%)	16 (20%)	1	4
36	CN	142/150 (95%)	124 (87%)	18 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	CO	318/377 (84%)	277 (87%)	41 (13%)	4	17
38	CP	160/168 (95%)	149 (93%)	11 (7%)	15	46
39	CQ	171/270 (63%)	144 (84%)	27 (16%)	2	11
40	CR	275/279 (99%)	247 (90%)	28 (10%)	7	28
41	CS	126/220 (57%)	118 (94%)	8 (6%)	18	49
42	CU	160/169 (95%)	150 (94%)	10 (6%)	18	49
43	CZ	121/313 (39%)	108 (89%)	13 (11%)	6	25
44	Ca	516/543 (95%)	464 (90%)	52 (10%)	7	28
45	Cb	219/277 (79%)	195 (89%)	24 (11%)	6	24
46	Cd	237/381 (62%)	206 (87%)	31 (13%)	4	17
47	Cg	424/437 (97%)	389 (92%)	35 (8%)	11	37
48	Ci	144/160 (90%)	122 (85%)	22 (15%)	2	12
49	Cj	193/219 (88%)	174 (90%)	19 (10%)	8	29
50	Ck	608/747 (81%)	546 (90%)	62 (10%)	7	28
51	Cm	165/184 (90%)	142 (86%)	23 (14%)	3	15
52	Cn	95/210 (45%)	82 (86%)	13 (14%)	3	15
53	Cp	163/175 (93%)	147 (90%)	16 (10%)	8	29
54	Cq	210/221 (95%)	186 (89%)	24 (11%)	5	22
55	Cr	211/369 (57%)	185 (88%)	26 (12%)	4	19
56	Cv	912/1034 (88%)	813 (89%)	99 (11%)	6	24
All	All	17352/19794 (88%)	15544 (90%)	1808 (10%)	10	26

All (1808) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DA	41	PHE
1	DA	52	MET
1	DA	79	LEU
1	DA	87	THR
1	DA	109	TYR
1	DA	112	GLN
1	DA	114	GLU
1	DA	128	THR
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	183	SER
1	DA	194	LEU
1	DA	198	ARG
1	DA	200	ILE
1	DA	201	LYS
1	DA	226	ASP
1	DA	227	ILE
1	DA	230	PHE
1	DA	235	THR
1	DA	240	GLU
1	DA	254	PHE
1	DA	259	LEU
1	DA	274	LEU
1	DA	295	SER
1	DA	300	THR
1	DA	309	VAL
1	DA	319	ARG
1	DA	344	ARG
1	DA	357	THR
1	DA	372	LYS
1	DA	383	LYS
1	DA	397	ILE
1	DA	408	LEU
1	DA	419	THR
1	DA	436	ASN
1	DA	456	ARG
1	DA	472	ARG
1	DA	476	SER
1	DA	486	LYS
1	DA	487	THR
1	DA	493	TRP
1	DA	503	SER
1	DA	509	LEU
1	DA	539	LEU
1	DA	547	ARG
1	DA	553	ARG
1	DA	557	SER
1	DA	579	ASP
1	DA	583	VAL
1	DA	602	LEU

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Mol	Chain	Res	Type
1	DA	627	PHE
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	729	ARG
1	DA	739	ARG
1	DA	751	GLU
1	DA	780	ASP
1	DA	781	ARG
1	DA	783	VAL
1	DA	819	ARG
1	DA	849	THR
1	DA	859	GLN
1	DA	865	ASP
1	DA	892	ASP
1	DA	920	LEU
1	DA	934	GLU
1	DA	942	LEU
1	DA	959	LYS
1	DA	963	LEU
1	DA	973	LEU
1	DA	988	CYS
1	DA	992	GLU
1	DA	999	SER
1	DA	1000	ASN
1	DA	1036	HIS
1	DA	1045	ILE
1	DA	1048	ASN
1	DA	1062	TYR
1	DA	1063	THR
1	DA	1077	ARG
1	DA	1097	LEU
1	DA	1101	LEU
1	DA	1117	ASN
1	DA	1120	SER
1	DA	1125	GLU
1	DA	1132	LYS
1	DA	1142	GLN
1	DA	1145	THR

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Mol	Chain	Res	Type
1	DA	1152	HIS
1	DA	1168	ASP
1	DA	1185	ARG
1	DA	1188	GLU
1	DA	1205	THR
1	DA	1208	THR
1	DA	1220	VAL
1	DA	1225	HIS
1	DA	1240	LEU
1	DA	1248	LEU
1	DA	1263	VAL
1	DA	1268	LEU
1	DA	1271	LEU
1	DA	1292	CYS
1	DA	1380	GLU
1	DA	1404	ARG
1	DA	1411	THR
1	DA	1427	LEU
1	DA	1429	SER
1	DA	1431	TYR
1	DA	1441	THR
1	DA	1488	GLN
1	DA	1544	ASN
1	DA	1575	LYS
1	DA	1591	ARG
1	DA	1595	LEU
1	DA	1597	GLU
1	DA	1605	ARG
1	DA	1624	ILE
2	DD	12	SER
2	DD	20	PHE
2	DD	25	LEU
2	DD	44	MET
2	DD	46	VAL
2	DD	48	MET
2	DD	64	HIS
2	DD	79	GLN
2	DD	82	ASN
2	DD	94	LYS
2	DD	104	ARG
2	DD	108	THR
2	DD	122	GLN

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Mol	Chain	Res	Type
2	DD	123	ARG
2	DD	129	ARG
2	DD	139	LEU
2	DD	146	ARG
2	DD	148	SER
2	DD	149	SER
2	DD	156	GLN
2	DD	165	MET
2	DD	168	ASP
2	DD	226	THR
2	DD	233	ASN
2	DD	242	LEU
2	DD	246	GLU
2	DD	248	ASP
2	DD	269	LYS
2	DD	275	ASP
2	DD	281	ASP
2	DD	292	ARG
2	DD	298	MET
2	DD	347	GLU
2	DD	349	CYS
2	DD	377	GLU
2	DD	379	GLN
2	DD	394	LYS
2	DD	424	THR
2	DD	439	GLU
2	DD	444	SER
2	DD	449	LEU
2	DD	454	THR
2	DD	455	SER
2	DD	463	GLU
2	DD	479	ARG
2	DD	503	SER
2	DD	504	ASN
2	DD	521	ASN
2	DD	541	ARG
2	DD	577	LYS
2	DD	589	GLN
2	DD	624	THR
2	DD	626	ARG
2	DD	633	GLU
2	DD	634	ARG

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Mol	Chain	Res	Type
2	DD	651	ARG
2	DD	653	PHE
2	DD	654	ARG
2	DD	672	ASP
2	DD	704	ASP
2	DD	752	PHE
2	DD	761	ARG
2	DD	765	ARG
2	DD	774	VAL
2	DD	785	MET
2	DD	787	ARG
2	DD	799	ASP
2	DD	812	TYR
3	DI	35	TYR
3	DI	67	ILE
3	DI	73	ASN
3	DI	88	GLN
3	DI	90	LEU
3	DI	113	VAL
3	DI	115	LYS
3	DI	139	VAL
3	DI	141	LYS
3	DI	144	LEU
3	DI	146	ARG
3	DI	151	ARG
3	DI	152	LEU
3	DI	158	ARG
3	DI	164	GLU
3	DI	175	GLN
3	DI	178	PHE
3	DI	180	GLU
3	DI	189	ASP
3	DI	192	THR
3	DI	205	GLU
3	DI	237	ARG
3	DI	243	LEU
3	DI	282	ASP
3	DI	310	LEU
3	DI	319	ARG
3	DI	320	GLN
3	DI	334	ILE
3	DI	344	LEU

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Mol	Chain	Res	Type
3	DI	345	LEU
3	DI	349	THR
3	DI	353	LYS
3	DI	365	ARG
3	DI	373	LEU
3	DI	399	THR
4	DL	18	ARG
4	DL	28	ASN
4	DL	29	PHE
4	DL	41	ASP
4	DL	64	ILE
4	DL	74	ARG
4	DL	77	LEU
4	DL	82	ASP
4	DL	92	ILE
4	DL	117	ASP
4	DL	118	ASP
4	DL	136	MET
4	DL	158	THR
4	DL	165	PHE
4	DL	240	GLU
4	DL	249	LEU
4	DL	256	SER
4	DL	267	HIS
4	DL	270	THR
4	DL	274	THR
4	DL	282	TRP
4	DL	286	THR
4	DL	289	ARG
4	DL	300	LEU
4	DL	305	THR
5	DM	1	MET
5	DM	8	THR
5	DM	10	ARG
5	DM	15	LEU
5	DM	30	ARG
5	DM	46	PHE
5	DM	56	TRP
5	DM	76	ASN
5	DM	103	ARG
5	DM	122	LYS
5	DM	128	ILE

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Mol	Chain	Res	Type
5	DM	129	ARG
5	DM	131	ASN
5	DM	157	LEU
5	DM	158	CYS
5	DM	179	ARG
5	DM	180	GLN
5	DM	185	LYS
5	DM	198	THR
5	DM	199	LEU
5	DM	239	LYS
5	DM	275	LEU
6	DN	11	ARG
6	DN	17	MET
6	DN	23	VAL
6	DN	24	LEU
6	DN	27	ASP
6	DN	42	THR
6	DN	141	MET
6	DN	152	LEU
6	DN	162	LEU
6	DN	166	LEU
6	DN	171	LEU
6	DN	204	SER
6	DN	223	GLN
6	DN	224	ARG
6	DN	237	ARG
6	DN	246	GLN
6	DN	258	ASP
6	DN	261	ARG
6	DN	267	GLU
6	DN	276	GLN
6	DN	282	SER
6	DN	288	PHE
6	DN	292	TYR
7	DO	62	LEU
7	DO	73	LEU
7	DO	113	LEU
7	DO	125	LEU
7	DO	136	ASP
7	DO	155	ARG
7	DO	157	ILE
7	DO	163	ARG

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Mol	Chain	Res	Type
7	DO	178	ARG
7	DO	198	ARG
7	DO	211	GLU
7	DO	234	LEU
7	DO	239	LYS
7	DO	249	ASP
7	DO	255	ARG
8	DP	21	MET
8	DP	23	LEU
8	DP	28	ASN
8	DP	34	VAL
8	DP	41	GLN
8	DP	44	GLU
8	DP	69	LEU
8	DP	124	ARG
8	DP	152	LEU
8	DP	158	CYS
8	DP	173	HIS
9	DQ	49	ARG
9	DQ	51	ASN
9	DQ	93	HIS
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
10	DR	64	ILE
10	DR	67	LYS
10	DR	68	HIS
10	DR	78	ARG
10	DR	90	ASP
10	DR	91	THR
10	DR	107	LEU
10	DR	118	VAL
10	DR	129	ASP
10	DR	131	LEU
10	DR	133	LEU

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Mol	Chain	Res	Type
10	DR	144	LEU
10	DR	173	ASN
10	DR	176	THR
10	DR	190	LEU
10	DR	201	CYS
10	DR	226	LYS
10	DR	228	THR
10	DR	245	MET
10	DR	253	VAL
10	DR	262	ARG
10	DR	265	MET
11	DS	34	SER
11	DS	56	LEU
11	DS	61	ASN
11	DS	71	ASP
11	DS	73	LYS
11	DS	83	LEU
11	DS	92	ARG
11	DS	106	ARG
11	DS	112	ARG
11	DS	115	TYR
11	DS	128	SER
11	DS	131	ARG
11	DS	170	TYR
11	DS	175	CYS
11	DS	193	VAL
11	DS	205	VAL
11	DS	234	LEU
11	DS	238	ARG
12	DU	33	THR
12	DU	46	THR
12	DU	47	ARG
12	DU	52	SER
12	DU	70	ASP
12	DU	73	ARG
12	DU	86	ILE
12	DU	90	VAL
12	DU	97	ARG
12	DU	103	ILE
12	DU	120	VAL
12	DU	121	GLU
12	DU	154	GLU

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Mol	Chain	Res	Type
12	DU	165	ASP
12	DU	176	ARG
12	DU	189	LYS
12	DU	191	SER
12	DU	211	ARG
12	DU	218	ARG
13	DZ	16	GLU
13	DZ	20	ARG
13	DZ	25	HIS
13	DZ	62	ASP
14	Da	15	CYS
14	Da	20	ARG
14	Da	25	ARG
14	Da	28	ARG
14	Da	38	ASP
14	Da	40	ARG
14	Da	42	ARG
14	Da	61	ARG
15	DB	81	PHE
15	DB	99	VAL
15	DB	104	SER
15	DB	118	VAL
15	DB	129	TYR
15	DB	173	ARG
15	DB	187	GLU
15	DB	189	VAL
15	DB	192	ILE
15	DB	204	SER
15	DB	221	HIS
15	DB	233	ASP
15	DB	239	GLN
15	DB	295	THR
15	DB	321	SER
15	DB	336	VAL
15	DB	339	ARG
15	DB	388	VAL
15	DB	396	ARG
15	DB	416	ASN
15	DB	424	ASP
15	DB	432	ARG
15	DB	433	ARG
15	DB	439	VAL

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Mol	Chain	Res	Type
15	DB	448	ASP
15	DB	452	ARG
15	DB	479	VAL
15	DB	493	ARG
15	DB	503	ASN
15	DB	514	ARG
15	DB	521	LEU
15	DB	522	MET
15	DB	532	GLU
15	DB	546	ARG
15	DB	553	LEU
15	DB	554	GLU
15	DB	572	ASP
15	DB	574	ILE
15	DB	592	MET
15	DB	625	ASN
15	DB	637	THR
15	DB	671	VAL
15	DB	686	GLN
15	DB	693	SER
15	DB	710	ARG
15	DB	733	HIS
15	DB	743	VAL
15	DB	755	LEU
15	DB	756	THR
15	DB	774	ASN
15	DB	776	THR
15	DB	785	ASN
15	DB	802	ASP
15	DB	807	ILE
15	DB	810	THR
15	DB	815	ASP
15	DB	822	PHE
15	DB	830	LEU
15	DB	834	ILE
15	DB	849	ASP
15	DB	861	GLU
15	DB	878	VAL
15	DB	908	GLN
15	DB	920	VAL
15	DB	923	GLN
15	DB	925	ASP

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Mol	Chain	Res	Type
15	DB	949	THR
15	DB	958	ASN
15	DB	968	VAL
15	DB	974	GLU
15	DB	978	ASN
15	DB	980	GLU
15	DB	984	ASP
15	DB	991	ASN
15	DB	995	VAL
15	DB	1000	ARG
15	DB	1009	ASP
15	DB	1012	THR
15	DB	1013	ARG
15	DB	1020	ASP
15	DB	1030	ARG
15	DB	1034	ILE
15	DB	1036	MET
15	DB	1069	THR
15	DB	1080	ARG
15	DB	1090	ARG
15	DB	1104	ASP
15	DB	1110	LYS
15	DB	1117	THR
15	DB	1141	THR
15	DB	1168	ASP
16	DC	36	ASP
16	DC	46	ARG
16	DC	58	VAL
16	DC	86	THR
16	DC	88	LEU
16	DC	92	PHE
16	DC	114	GLU
16	DC	122	VAL
16	DC	128	HIS
16	DC	148	LEU
16	DC	154	THR
16	DC	162	ILE
16	DC	166	GLU
16	DC	168	PHE
16	DC	198	GLU
16	DC	223	ASP
16	DC	227	GLN

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Mol	Chain	Res	Type
16	DC	231	THR
16	DC	240	VAL
16	DC	259	SER
16	DC	260	HIS
16	DC	268	ASP
16	DC	273	ASP
16	DC	279	GLU
16	DC	344	MET
16	DC	371	ILE
16	DC	378	THR
16	DC	379	LEU
16	DC	386	MET
16	DC	406	GLN
16	DC	435	LEU
16	DC	436	ASP
16	DC	437	LEU
16	DC	464	THR
16	DC	467	THR
16	DC	472	ARG
16	DC	475	LEU
16	DC	485	ILE
16	DC	491	LEU
16	DC	498	LEU
16	DC	503	ASP
16	DC	511	ARG
16	DC	534	LEU
16	DC	540	LEU
16	DC	544	GLU
16	DC	604	VAL
16	DC	611	MET
16	DC	620	VAL
16	DC	632	LEU
16	DC	669	LEU
16	DC	705	LEU
16	DC	749	GLU
16	DC	753	LEU
16	DC	756	ASP
16	DC	761	ASN
16	DC	766	VAL
16	DC	774	ASP
16	DC	799	ASN
16	DC	807	VAL

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Mol	Chain	Res	Type
16	DC	817	ASP
16	DC	871	GLN
16	DC	881	MET
16	DC	888	LEU
16	DC	894	HIS
16	DC	918	VAL
16	DC	934	ARG
16	DC	941	MET
16	DC	952	GLU
16	DC	953	MET
16	DC	954	LEU
16	DC	960	VAL
16	DC	961	THR
16	DC	963	SER
16	DC	970	GLN
16	DC	987	THR
16	DC	1000	LEU
16	DC	1023	ASN
16	DC	1038	HIS
16	DC	1047	ARG
16	DC	1050	THR
16	DC	1055	ARG
16	DC	1062	GLN
16	DC	1071	VAL
16	DC	1104	MET
16	DC	1119	GLN
16	DC	1121	THR
16	DC	1122	THR
16	DC	1128	ARG
16	DC	1132	THR
16	DC	1133	THR
16	DC	1138	ARG
16	DC	1143	VAL
16	DC	1151	THR
16	DC	1153	LEU
16	DC	1159	ASP
17	DE	46	SER
17	DE	51	ARG
17	DE	54	ARG
17	DE	65	ILE
17	DE	67	ASN
17	DE	80	LEU

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Mol	Chain	Res	Type
17	DE	149	LEU
17	DE	150	ARG
17	DE	154	SER
17	DE	169	SER
17	DE	196	ASP
17	DE	203	LEU
17	DE	212	LEU
17	DE	229	ARG
17	DE	246	ILE
17	DE	252	ASP
17	DE	286	THR
17	DE	319	ASN
17	DE	322	ASP
17	DE	335	GLU
17	DE	398	LEU
17	DE	405	ILE
17	DE	406	ASP
17	DE	408	LEU
17	DE	418	LEU
17	DE	445	LEU
17	DE	451	THR
17	DE	461	MET
17	DE	482	THR
17	DE	484	THR
17	DE	494	ARG
17	DE	503	ASP
17	DE	509	GLN
17	DE	513	ARG
17	DE	529	ASP
17	DE	530	TRP
17	DE	554	LEU
17	DE	566	ARG
17	DE	570	GLU
17	DE	573	GLN
17	DE	582	GLU
17	DE	591	LEU
17	DE	600	ILE
17	DE	610	LEU
17	DE	615	LEU
17	DE	651	ASN
17	DE	667	SER
17	DE	698	GLN

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Mol	Chain	Res	Type
17	DE	699	ASN
17	DE	716	ASN
17	DE	717	ARG
17	DE	726	THR
18	DF	15	HIS
18	DF	16	GLU
18	DF	27	ARG
18	DF	33	GLN
18	DF	39	ARG
18	DF	40	GLU
18	DF	43	THR
18	DF	50	LEU
18	DF	57	ARG
18	DF	69	THR
18	DF	72	THR
18	DF	85	ARG
18	DF	87	GLU
18	DF	110	ASN
18	DF	144	THR
18	DF	188	ARG
18	DF	194	THR
18	DF	202	LEU
18	DF	203	MET
18	DF	232	GLU
18	DF	241	CYS
18	DF	246	LYS
18	DF	258	ASP
18	DF	264	VAL
18	DF	274	LEU
18	DF	277	CYS
18	DF	294	MET
18	DF	297	ARG
18	DF	307	GLU
18	DF	309	ASP
18	DF	318	MET
18	DF	321	LEU
18	DF	326	ASP
18	DF	332	GLU
18	DF	338	SER
18	DF	343	GLU
18	DF	347	ARG
18	DF	362	ILE

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Mol	Chain	Res	Type
18	DF	372	ASN
18	DF	373	ASP
18	DF	383	ASP
18	DF	395	LEU
18	DF	403	LEU
18	DF	450	VAL
18	DF	476	LEU
18	DF	491	ARG
18	DF	502	ARG
18	DF	505	LYS
18	DF	531	ARG
18	DF	540	VAL
18	DF	548	ARG
18	DF	550	VAL
18	DF	568	LEU
18	DF	575	VAL
19	DG	47	THR
19	DG	54	THR
19	DG	56	ARG
19	DG	78	HIS
19	DG	84	LEU
19	DG	93	ARG
19	DG	98	ASP
19	DG	115	ILE
19	DG	125	ASP
19	DG	127	LEU
19	DG	130	LEU
19	DG	142	LEU
19	DG	147	SER
19	DG	149	SER
19	DG	155	GLU
19	DG	160	ARG
19	DG	179	LEU
19	DG	185	ASP
19	DG	186	ARG
19	DG	194	ARG
19	DG	200	GLN
19	DG	214	TYR
19	DG	220	THR
19	DG	236	VAL
19	DG	273	VAL
19	DG	296	ASP

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Mol	Chain	Res	Type
19	DG	298	ASP
19	DG	317	MET
19	DG	326	THR
19	DG	332	GLN
19	DG	334	MET
19	DG	359	ARG
19	DG	365	GLN
19	DG	370	ARG
19	DG	377	GLU
19	DG	392	ARG
19	DG	443	ARG
19	DG	444	THR
19	DG	451	ARG
19	DG	456	ARG
19	DG	457	ARG
19	DG	462	THR
19	DG	473	CYS
19	DG	491	THR
19	DG	494	THR
19	DG	496	ARG
19	DG	497	ARG
19	DG	529	ASP
19	DG	544	ARG
19	DG	547	MET
19	DG	557	GLN
19	DG	564	GLU
19	DG	565	CYS
19	DG	615	SER
19	DG	616	ARG
19	DG	618	ARG
19	DG	626	LEU
20	DH	1	MET
20	DH	13	SER
20	DH	15	TYR
20	DH	19	THR
20	DH	40	THR
20	DH	44	ARG
20	DH	46	LEU
20	DH	51	ARG
20	DH	76	LEU
20	DH	79	ASP
20	DH	81	LYS

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Mol	Chain	Res	Type
20	DH	82	GLN
20	DH	83	GLU
20	DH	85	LEU
20	DH	102	LEU
20	DH	105	GLN
20	DH	133	CYS
20	DH	135	ARG
20	DH	162	GLU
20	DH	167	GLU
20	DH	196	LEU
20	DH	200	THR
20	DH	227	ASP
20	DH	236	MET
20	DH	253	SER
20	DH	257	ASN
20	DH	268	LEU
20	DH	273	SER
20	DH	277	THR
20	DH	297	CYS
20	DH	314	PRO
20	DH	327	HIS
20	DH	345	VAL
20	DH	348	LYS
20	DH	354	LEU
20	DH	359	GLU
20	DH	360	LEU
20	DH	364	ARG
20	DH	382	PHE
20	DH	386	ARG
20	DH	392	TRP
20	DH	396	VAL
20	DH	414	LEU
20	DH	419	CYS
20	DH	428	ARG
20	DH	450	ASN
20	DH	452	ARG
20	DH	460	LEU
20	DH	474	ASP
20	DH	476	VAL
20	DH	484	ASP
20	DH	495	THR
20	DH	523	ARG

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Mol	Chain	Res	Type
20	DH	528	GLU
21	DJ	16	ASN
21	DJ	33	ASN
21	DJ	46	ARG
21	DJ	48	PHE
21	DJ	55	ASN
21	DJ	82	GLN
21	DJ	91	THR
21	DJ	92	LEU
21	DJ	107	LEU
21	DJ	119	LEU
21	DJ	137	MET
21	DJ	149	THR
21	DJ	171	LYS
21	DJ	175	SER
21	DJ	178	ARG
21	DJ	182	ASP
21	DJ	187	ASP
21	DJ	212	ASP
21	DJ	226	VAL
21	DJ	236	ARG
21	DJ	246	THR
21	DJ	273	TYR
21	DJ	276	LEU
21	DJ	277	ARG
21	DJ	291	ASN
21	DJ	302	SER
21	DJ	305	ARG
21	DJ	308	ARG
21	DJ	323	THR
22	DK	6	THR
22	DK	18	LEU
22	DK	34	ASN
22	DK	54	THR
22	DK	111	LEU
22	DK	116	ARG
22	DK	134	THR
22	DK	148	GLU
22	DK	167	THR
22	DK	173	VAL
22	DK	179	GLU
22	DK	226	LEU

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Mol	Chain	Res	Type
22	DK	232	ASN
22	DK	254	GLU
22	DK	263	GLU
22	DK	270	LEU
22	DK	273	LEU
22	DK	286	LEU
22	DK	294	SER
23	DT	21	ASP
23	DT	33	HIS
23	DT	35	LYS
23	DT	52	ARG
23	DT	63	HIS
23	DT	90	THR
23	DT	103	LEU
23	DT	105	ARG
23	DT	106	ASP
23	DT	114	LEU
23	DT	122	MET
23	DT	131	SER
23	DT	133	ASP
23	DT	143	TYR
23	DT	152	LYS
23	DT	163	ARG
23	DT	166	THR
23	DT	176	ASP
23	DT	183	LEU
23	DT	187	LYS
23	DT	205	VAL
23	DT	208	ARG
23	DT	209	THR
23	DT	212	PHE
23	DT	232	ARG
23	DT	241	ASN
24	DV	26	THR
24	DV	41	THR
24	DV	43	ASN
24	DV	75	PHE
24	DV	77	LYS
24	DV	114	VAL
24	DV	115	PRO
24	DV	118	GLN
24	DV	131	GLN

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Mol	Chain	Res	Type
24	DV	140	PHE
24	DV	143	ILE
24	DV	151	GLU
24	DV	179	LEU
24	DV	180	ASP
24	DV	182	TYR
25	DW	10	THR
25	DW	12	THR
25	DW	27	LYS
25	DW	37	MET
25	DW	39	SER
25	DW	60	VAL
25	DW	70	LEU
25	DW	71	GLN
25	DW	74	THR
25	DW	104	VAL
25	DW	122	ARG
25	DW	128	LEU
25	DW	149	VAL
25	DW	164	ASN
26	DX	33	LYS
26	DX	76	ARG
26	DX	78	GLU
26	DX	90	ILE
26	DX	98	LEU
26	DX	122	CYS
26	DX	124	ILE
26	DX	136	ARG
26	DX	162	VAL
26	DX	164	THR
26	DX	168	ASN
27	DY	11	THR
27	DY	14	THR
27	DY	23	SER
27	DY	37	ARG
27	DY	43	LEU
27	DY	50	VAL
27	DY	52	GLN
27	DY	65	LEU
27	DY	77	VAL
27	DY	85	ARG
27	DY	87	ARG

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Mol	Chain	Res	Type
27	DY	91	LEU
27	DY	93	THR
27	DY	96	ARG
27	DY	111	ARG
27	DY	113	VAL
27	DY	128	GLN
27	DY	141	VAL
27	DY	148	ARG
27	DY	163	LYS
28	CC	4	MET
28	CC	10	VAL
28	CC	21	PHE
28	CC	22	LYS
28	CC	44	LEU
28	CC	46	TRP
28	CC	50	ILE
28	CC	69	GLU
28	CC	74	LEU
29	CE	13	ASN
29	CE	14	SER
29	CE	16	TYR
29	CE	27	ARG
29	CE	39	THR
29	CE	41	ARG
29	CE	54	GLU
29	CE	58	SER
29	CE	62	ARG
29	CE	65	ARG
29	CE	80	ILE
29	CE	83	MET
29	CE	87	ILE
29	CE	96	VAL
29	CE	102	GLU
29	CE	105	GLN
29	CE	121	THR
29	CE	124	THR
29	CE	128	ILE
29	CE	157	LYS
29	CE	158	ASP
29	CE	163	ILE
29	CE	182	VAL
29	CE	192	GLU

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Mol	Chain	Res	Type
29	CE	201	ILE
29	CE	202	ILE
29	CE	223	ARG
29	CE	230	ARG
29	CE	231	ARG
29	CE	232	ILE
29	CE	233	VAL
29	CE	279	LEU
29	CE	285	ILE
29	CE	332	ASP
29	CE	334	ARG
29	CE	335	LEU
29	CE	364	ARG
29	CE	365	MET
29	CE	370	ASP
29	CE	391	THR
29	CE	395	THR
29	CE	410	LEU
29	CE	417	ASN
29	CE	422	VAL
29	CE	424	LEU
29	CE	429	LYS
30	CF	2	VAL
30	CF	5	SER
30	CF	45	MET
30	CF	53	ASP
30	CF	56	ASN
30	CF	93	LEU
30	CF	96	ASN
30	CF	104	ILE
30	CF	123	ARG
30	CF	124	LEU
30	CF	133	GLN
30	CF	134	THR
30	CF	138	ILE
30	CF	141	GLN
30	CF	144	MET
30	CF	152	THR
31	CH	16	VAL
31	CH	19	LEU
31	CH	26	ARG
31	CH	29	HIS

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Mol	Chain	Res	Type
31	CH	46	LYS
31	CH	48	ASP
31	CH	50	ARG
31	CH	51	LEU
31	CH	79	SER
31	CH	86	THR
31	CH	88	LEU
31	CH	89	VAL
31	CH	108	LEU
31	CH	118	LEU
31	CH	122	THR
31	CH	128	VAL
31	CH	131	ASP
31	CH	132	ASP
31	CH	143	ARG
31	CH	150	THR
31	CH	152	ILE
31	CH	154	ASP
31	CH	163	THR
31	CH	170	VAL
31	CH	172	VAL
31	CH	175	THR
31	CH	179	ARG
31	CH	183	ARG
31	CH	191	VAL
31	CH	201	ARG
31	CH	248	ASN
31	CH	256	ARG
32	CI	9	THR
32	CI	34	ASP
32	CI	38	LEU
32	CI	47	ARG
32	CI	54	SER
32	CI	57	GLU
32	CI	104	ASN
32	CI	110	ARG
32	CI	139	ASP
32	CI	175	ARG
32	CI	179	CYS
32	CI	210	THR
32	CI	214	GLU
32	CI	218	ARG

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Mol	Chain	Res	Type
32	CI	223	ARG
32	CI	256	LYS
32	CI	260	LEU
32	CI	265	ASP
32	CI	290	ILE
32	CI	295	ASP
32	CI	303	THR
32	CI	309	ARG
32	CI	330	ASN
32	CI	338	LYS
32	CI	372	ILE
32	CI	406	THR
32	CI	407	ARG
32	CI	417	SER
32	CI	420	ARG
32	CI	439	ARG
33	CJ	17	MET
33	CJ	19	THR
33	CJ	20	GLN
33	CJ	23	LYS
33	CJ	36	MET
33	CJ	42	ASN
33	CJ	43	GLU
33	CJ	50	ASP
33	CJ	52	PHE
33	CJ	65	VAL
33	CJ	68	ASP
33	CJ	77	CYS
33	CJ	81	THR
33	CJ	130	ARG
33	CJ	149	GLU
33	CJ	158	THR
33	CJ	164	ASP
33	CJ	169	GLU
33	CJ	190	GLU
33	CJ	202	ASP
33	CJ	204	SER
33	CJ	230	PHE
33	CJ	257	VAL
33	CJ	258	MET
33	CJ	265	CYS
33	CJ	266	MET

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Mol	Chain	Res	Type
33	CJ	279	LYS
33	CJ	287	LEU
33	CJ	297	LEU
33	CJ	313	GLU
33	CJ	325	SER
33	CJ	330	LEU
33	CJ	345	VAL
33	CJ	357	SER
33	CJ	375	THR
33	CJ	377	SER
33	CJ	380	THR
33	CJ	399	ARG
33	CJ	403	CYS
33	CJ	409	SER
33	CJ	413	GLU
33	CJ	418	ASP
33	CJ	425	ARG
33	CJ	427	THR
33	CJ	428	SER
33	CJ	438	ASN
33	CJ	445	VAL
33	CJ	459	GLU
33	CJ	480	THR
33	CJ	481	ASP
33	CJ	490	ASP
33	CJ	509	GLU
33	CJ	517	VAL
33	CJ	519	ILE
33	CJ	524	THR
33	CJ	526	THR
33	CJ	532	PHE
33	CJ	552	ILE
33	CJ	556	GLU
33	CJ	565	THR
33	CJ	602	SER
33	CJ	615	VAL
33	CJ	618	VAL
33	CJ	647	ASP
33	CJ	648	VAL
33	CJ	654	VAL
33	CJ	667	VAL
33	CJ	671	LEU

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Mol	Chain	Res	Type
33	CJ	684	THR
33	CJ	698	HIS
33	CJ	704	GLU
33	CJ	712	THR
33	CJ	714	THR
33	CJ	724	THR
33	CJ	727	THR
33	CJ	728	GLN
33	CJ	734	THR
33	CJ	755	ASN
33	CJ	770	THR
33	CJ	781	HIS
33	CJ	796	ASP
33	CJ	798	GLN
34	CK	15	ARG
34	CK	23	ASP
34	CK	32	LEU
34	CK	40	GLN
34	CK	47	ILE
34	CK	48	ARG
34	CK	53	ARG
34	CK	56	GLN
34	CK	73	GLN
34	CK	77	MET
34	CK	94	GLU
34	CK	98	LEU
34	CK	108	ARG
34	CK	109	VAL
34	CK	113	ARG
34	CK	149	VAL
34	CK	156	LYS
34	CK	174	VAL
34	CK	185	MET
34	CK	205	TYR
34	CK	207	VAL
34	CK	210	THR
34	CK	217	LEU
34	CK	227	LEU
34	CK	232	ARG
34	CK	264	SER
34	CK	310	ILE
34	CK	311	THR

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Mol	Chain	Res	Type
34	CK	315	LEU
34	CK	324	VAL
34	CK	325	PHE
34	CK	326	LYS
35	CL	1	LEU
35	CL	6	MET
35	CL	17	VAL
35	CL	22	CYS
35	CL	38	LEU
35	CL	42	PHE
35	CL	43	TYR
35	CL	44	LEU
35	CL	53	CYS
35	CL	55	PHE
35	CL	65	LEU
35	CL	69	GLU
35	CL	74	VAL
35	CL	79	VAL
35	CL	80	LYS
35	CL	85	ILE
36	CN	16	ASP
36	CN	30	LEU
36	CN	41	LEU
36	CN	49	SER
36	CN	55	LEU
36	CN	60	VAL
36	CN	62	THR
36	CN	66	MET
36	CN	78	GLN
36	CN	81	LEU
36	CN	83	LYS
36	CN	104	THR
36	CN	105	ARG
36	CN	111	VAL
36	CN	118	MET
36	CN	127	LEU
36	CN	135	THR
36	CN	158	ARG
37	CO	70	HIS
37	CO	75	LEU
37	CO	80	ARG
37	CO	82	ASN

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Mol	Chain	Res	Type
37	CO	87	THR
37	CO	108	THR
37	CO	112	LYS
37	CO	115	GLN
37	CO	118	MET
37	CO	120	TYR
37	CO	147	GLU
37	CO	190	SER
37	CO	204	GLU
37	CO	206	MET
37	CO	209	GLU
37	CO	224	LEU
37	CO	237	ASN
37	CO	240	LEU
37	CO	242	ASN
37	CO	244	HIS
37	CO	245	ASN
37	CO	259	LEU
37	CO	264	ARG
37	CO	266	LEU
37	CO	270	ASP
37	CO	280	ASP
37	CO	285	ASP
37	CO	304	ASP
37	CO	309	LEU
37	CO	313	THR
37	CO	336	GLU
37	CO	351	GLU
37	CO	352	ASN
37	CO	353	GLU
37	CO	362	VAL
37	CO	384	GLU
37	CO	390	PHE
37	CO	391	SER
37	CO	400	ARG
37	CO	412	ARG
37	CO	419	VAL
38	CP	14	LYS
38	CP	15	ARG
38	CP	28	ILE
38	CP	36	VAL
38	CP	40	PHE

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Mol	Chain	Res	Type
38	CP	54	ARG
38	CP	123	LEU
38	CP	152	ASN
38	CP	163	LYS
38	CP	170	SER
38	CP	188	LEU
39	CQ	21	ARG
39	CQ	24	LEU
39	CQ	31	THR
39	CQ	34	THR
39	CQ	48	ARG
39	CQ	56	ARG
39	CQ	67	LEU
39	CQ	69	GLN
39	CQ	70	ARG
39	CQ	73	ARG
39	CQ	80	LEU
39	CQ	83	LEU
39	CQ	90	GLN
39	CQ	103	MET
39	CQ	114	MET
39	CQ	123	ARG
39	CQ	124	VAL
39	CQ	136	ASP
39	CQ	146	HIS
39	CQ	147	ILE
39	CQ	158	HIS
39	CQ	164	ILE
39	CQ	169	VAL
39	CQ	173	GLU
39	CQ	182	VAL
39	CQ	191	VAL
39	CQ	199	ASN
40	CR	15	GLN
40	CR	30	LEU
40	CR	36	THR
40	CR	44	GLU
40	CR	55	ARG
40	CR	59	LEU
40	CR	70	ARG
40	CR	77	ILE
40	CR	80	LEU

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Mol	Chain	Res	Type
40	CR	92	ILE
40	CR	94	MET
40	CR	111	GLN
40	CR	114	GLN
40	CR	117	SER
40	CR	134	ARG
40	CR	167	ARG
40	CR	181	ARG
40	CR	198	THR
40	CR	202	LYS
40	CR	225	LEU
40	CR	228	VAL
40	CR	243	THR
40	CR	244	THR
40	CR	246	GLU
40	CR	258	ASN
40	CR	305	THR
40	CR	318	LYS
40	CR	320	VAL
41	CS	63	SER
41	CS	64	MET
41	CS	75	MET
41	CS	76	THR
41	CS	105	VAL
41	CS	121	SER
41	CS	140	MET
41	CS	149	ASP
42	CU	32	HIS
42	CU	74	GLN
42	CU	80	GLN
42	CU	87	GLU
42	CU	117	MET
42	CU	129	THR
42	CU	139	LEU
42	CU	148	ASN
42	CU	161	GLN
42	CU	171	VAL
43	CZ	212	HIS
43	CZ	218	VAL
43	CZ	237	ARG
43	CZ	240	VAL
43	CZ	244	ILE

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Mol	Chain	Res	Type
43	CZ	260	MET
43	CZ	273	ILE
43	CZ	277	PHE
43	CZ	281	VAL
43	CZ	285	ARG
43	CZ	286	GLU
43	CZ	318	LEU
43	CZ	360	ASP
44	Ca	14	ASN
44	Ca	16	ARG
44	Ca	19	ARG
44	Ca	51	MET
44	Ca	67	ARG
44	Ca	71	MET
44	Ca	73	GLU
44	Ca	84	SER
44	Ca	114	LYS
44	Ca	130	TYR
44	Ca	153	LYS
44	Ca	168	TYR
44	Ca	181	GLU
44	Ca	189	GLU
44	Ca	191	MET
44	Ca	194	LEU
44	Ca	201	ARG
44	Ca	212	VAL
44	Ca	221	THR
44	Ca	227	ASN
44	Ca	245	GLU
44	Ca	257	ILE
44	Ca	295	PHE
44	Ca	297	LEU
44	Ca	305	HIS
44	Ca	314	CYS
44	Ca	332	ARG
44	Ca	350	GLU
44	Ca	359	ARG
44	Ca	376	VAL
44	Ca	380	ASP
44	Ca	381	ASP
44	Ca	384	ARG
44	Ca	398	ASP

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Mol	Chain	Res	Type
44	Ca	399	ASN
44	Ca	401	ASP
44	Ca	410	MET
44	Ca	479	THR
44	Ca	480	LEU
44	Ca	499	ASP
44	Ca	501	ARG
44	Ca	506	GLN
44	Ca	520	TYR
44	Ca	537	ARG
44	Ca	538	ILE
44	Ca	552	THR
44	Ca	569	ARG
44	Ca	571	GLU
44	Ca	575	ARG
44	Ca	578	ASP
44	Ca	585	GLN
44	Ca	601	GLU
45	Cb	11	MET
45	Cb	40	LEU
45	Cb	50	GLU
45	Cb	57	MET
45	Cb	64	ASN
45	Cb	71	LEU
45	Cb	102	SER
45	Cb	104	LEU
45	Cb	108	GLU
45	Cb	110	MET
45	Cb	144	ARG
45	Cb	158	LYS
45	Cb	159	ARG
45	Cb	171	THR
45	Cb	193	GLU
45	Cb	203	LEU
45	Cb	205	LYS
45	Cb	206	GLU
45	Cb	223	ARG
45	Cb	288	GLU
45	Cb	292	ASP
45	Cb	301	THR
45	Cb	303	GLU
45	Cb	306	THR

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Mol	Chain	Res	Type
46	Cd	13	ARG
46	Cd	31	PHE
46	Cd	33	THR
46	Cd	39	MET
46	Cd	47	ARG
46	Cd	49	VAL
46	Cd	55	GLU
46	Cd	68	SER
46	Cd	70	ARG
46	Cd	74	ASP
46	Cd	102	ARG
46	Cd	106	ARG
46	Cd	116	LYS
46	Cd	120	LEU
46	Cd	122	LEU
46	Cd	125	GLU
46	Cd	137	ARG
46	Cd	164	LEU
46	Cd	168	VAL
46	Cd	180	VAL
46	Cd	201	LEU
46	Cd	202	SER
46	Cd	208	HIS
46	Cd	210	ASP
46	Cd	217	GLU
46	Cd	219	HIS
46	Cd	259	GLU
46	Cd	264	ILE
46	Cd	267	GLU
46	Cd	282	GLU
46	Cd	284	THR
47	Cg	20	THR
47	Cg	57	THR
47	Cg	73	ASP
47	Cg	76	SER
47	Cg	101	MET
47	Cg	107	ARG
47	Cg	114	GLU
47	Cg	120	LEU
47	Cg	127	HIS
47	Cg	137	SER
47	Cg	143	THR

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Mol	Chain	Res	Type
47	Cg	153	CYS
47	Cg	178	ASP
47	Cg	191	SER
47	Cg	224	LEU
47	Cg	225	ARG
47	Cg	262	GLN
47	Cg	263	SER
47	Cg	296	HIS
47	Cg	308	LEU
47	Cg	310	SER
47	Cg	313	GLU
47	Cg	316	THR
47	Cg	319	ASP
47	Cg	325	LEU
47	Cg	337	ARG
47	Cg	361	PHE
47	Cg	383	ASP
47	Cg	391	GLU
47	Cg	401	ILE
47	Cg	422	LEU
47	Cg	436	ASP
47	Cg	464	VAL
47	Cg	468	ASP
47	Cg	480	LYS
48	Ci	18	THR
48	Ci	30	ARG
48	Ci	32	ASP
48	Ci	41	PHE
48	Ci	42	GLN
48	Ci	56	GLU
48	Ci	76	MET
48	Ci	82	GLN
48	Ci	83	ASN
48	Ci	119	LEU
48	Ci	125	HIS
48	Ci	132	THR
48	Ci	136	HIS
48	Ci	138	ASP
48	Ci	144	ARG
48	Ci	145	ASN
48	Ci	146	ASP
48	Ci	147	ARG

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Mol	Chain	Res	Type
48	Ci	156	VAL
48	Ci	157	LEU
48	Ci	164	ASN
48	Ci	174	ASP
49	Cj	10	ARG
49	Cj	19	SER
49	Cj	34	HIS
49	Cj	66	LEU
49	Cj	67	ASP
49	Cj	77	LEU
49	Cj	80	LEU
49	Cj	83	LEU
49	Cj	126	TYR
49	Cj	135	ILE
49	Cj	138	ASP
49	Cj	145	THR
49	Cj	157	THR
49	Cj	161	VAL
49	Cj	173	MET
49	Cj	175	PHE
49	Cj	192	SER
49	Cj	206	LEU
49	Cj	213	ASP
50	Ck	35	ASP
50	Ck	38	ILE
50	Ck	86	GLU
50	Ck	87	ARG
50	Ck	97	GLN
50	Ck	99	SER
50	Ck	103	GLU
50	Ck	105	SER
50	Ck	107	SER
50	Ck	111	THR
50	Ck	130	MET
50	Ck	136	ASP
50	Ck	137	THR
50	Ck	138	PHE
50	Ck	153	VAL
50	Ck	154	SER
50	Ck	161	GLU
50	Ck	175	LEU
50	Ck	185	LEU

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Mol	Chain	Res	Type
50	Ck	188	LEU
50	Ck	203	PHE
50	Ck	207	ARG
50	Ck	214	LEU
50	Ck	242	LEU
50	Ck	244	ARG
50	Ck	290	LEU
50	Ck	292	ASP
50	Ck	316	ASP
50	Ck	317	VAL
50	Ck	320	VAL
50	Ck	348	LEU
50	Ck	350	ASP
50	Ck	380	VAL
50	Ck	401	LEU
50	Ck	406	ARG
50	Ck	536	GLU
50	Ck	565	LEU
50	Ck	573	THR
50	Ck	597	LEU
50	Ck	607	LYS
50	Ck	611	ASN
50	Ck	621	THR
50	Ck	622	LEU
50	Ck	629	LEU
50	Ck	631	TRP
50	Ck	633	MET
50	Ck	634	HIS
50	Ck	649	THR
50	Ck	654	SER
50	Ck	661	ILE
50	Ck	679	GLN
50	Ck	682	ASN
50	Ck	690	TRP
50	Ck	691	GLN
50	Ck	695	GLN
50	Ck	703	ARG
50	Ck	733	LEU
50	Ck	755	ASP
50	Ck	775	ARG
50	Ck	806	ASP
50	Ck	816	GLU

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Mol	Chain	Res	Type
50	Ck	838	LEU
51	Cm	21	GLN
51	Cm	31	LEU
51	Cm	35	ASN
51	Cm	57	LEU
51	Cm	70	SER
51	Cm	80	THR
51	Cm	85	ILE
51	Cm	91	GLU
51	Cm	92	GLN
51	Cm	93	LEU
51	Cm	95	MET
51	Cm	106	CYS
51	Cm	117	ARG
51	Cm	124	SER
51	Cm	137	SER
51	Cm	153	ASP
51	Cm	162	ARG
51	Cm	178	GLU
51	Cm	179	ARG
51	Cm	184	HIS
51	Cm	188	ARG
51	Cm	193	PHE
51	Cm	202	THR
52	Cn	155	ARG
52	Cn	165	LEU
52	Cn	195	PHE
52	Cn	204	LEU
52	Cn	205	PRO
52	Cn	210	SER
52	Cn	212	THR
52	Cn	213	LYS
52	Cn	214	ARG
52	Cn	216	ASP
52	Cn	223	SER
52	Cn	235	GLU
52	Cn	241	ARG
53	Cp	18	SER
53	Cp	30	LEU
53	Cp	50	THR
53	Cp	55	ASN
53	Cp	68	LEU

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Mol	Chain	Res	Type
53	Cp	84	LEU
53	Cp	87	CYS
53	Cp	90	ARG
53	Cp	91	GLN
53	Cp	103	ASP
53	Cp	125	GLU
53	Cp	128	LEU
53	Cp	137	ASP
53	Cp	166	ARG
53	Cp	168	ILE
53	Cp	181	ARG
54	Cq	19	VAL
54	Cq	24	THR
54	Cq	30	ILE
54	Cq	36	ARG
54	Cq	64	VAL
54	Cq	65	SER
54	Cq	74	LYS
54	Cq	78	ASP
54	Cq	79	MET
54	Cq	86	ARG
54	Cq	96	THR
54	Cq	106	LEU
54	Cq	107	GLU
54	Cq	111	ARG
54	Cq	144	THR
54	Cq	171	ARG
54	Cq	172	ARG
54	Cq	185	CYS
54	Cq	201	GLU
54	Cq	211	SER
54	Cq	227	ILE
54	Cq	235	LEU
54	Cq	246	CYS
54	Cq	253	ARG
55	Cr	10	ARG
55	Cr	13	ARG
55	Cr	25	LEU
55	Cr	45	THR
55	Cr	56	MET
55	Cr	61	VAL
55	Cr	68	LEU

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Mol	Chain	Res	Type
55	Cr	74	ASP
55	Cr	79	LYS
55	Cr	96	GLU
55	Cr	103	VAL
55	Cr	106	CYS
55	Cr	110	THR
55	Cr	123	GLU
55	Cr	129	MET
55	Cr	138	ILE
55	Cr	161	ARG
55	Cr	163	LEU
55	Cr	164	LEU
55	Cr	171	GLN
55	Cr	187	VAL
55	Cr	247	ILE
55	Cr	249	GLU
55	Cr	250	LYS
55	Cr	253	ARG
55	Cr	265	LEU
56	Cv	27	LYS
56	Cv	30	ASP
56	Cv	32	ARG
56	Cv	33	GLU
56	Cv	35	ARG
56	Cv	91	ARG
56	Cv	195	LEU
56	Cv	204	ILE
56	Cv	208	LYS
56	Cv	235	MET
56	Cv	245	ASN
56	Cv	254	ARG
56	Cv	261	ILE
56	Cv	278	LEU
56	Cv	283	ASP
56	Cv	301	SER
56	Cv	305	ASP
56	Cv	312	ASN
56	Cv	333	ILE
56	Cv	334	LEU
56	Cv	337	SER
56	Cv	367	ASP
56	Cv	392	HIS

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Mol	Chain	Res	Type
56	Cv	401	THR
56	Cv	409	LEU
56	Cv	411	ASN
56	Cv	417	THR
56	Cv	421	LEU
56	Cv	437	ILE
56	Cv	446	THR
56	Cv	453	ARG
56	Cv	462	LEU
56	Cv	471	VAL
56	Cv	509	THR
56	Cv	512	MET
56	Cv	530	LYS
56	Cv	531	MET
56	Cv	561	SER
56	Cv	566	MET
56	Cv	569	LEU
56	Cv	583	THR
56	Cv	584	SER
56	Cv	590	THR
56	Cv	594	LEU
56	Cv	610	ARG
56	Cv	613	LEU
56	Cv	614	SER
56	Cv	617	ASP
56	Cv	618	ILE
56	Cv	619	THR
56	Cv	638	VAL
56	Cv	640	GLU
56	Cv	647	VAL
56	Cv	649	THR
56	Cv	651	ARG
56	Cv	654	GLU
56	Cv	678	HIS
56	Cv	689	CYS
56	Cv	727	ARG
56	Cv	738	ARG
56	Cv	739	ASN
56	Cv	751	THR
56	Cv	782	ILE
56	Cv	790	THR
56	Cv	793	PHE

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Mol	Chain	Res	Type
56	Cv	795	GLU
56	Cv	813	ARG
56	Cv	818	LEU
56	Cv	838	LEU
56	Cv	859	VAL
56	Cv	861	THR
56	Cv	874	GLU
56	Cv	909	LEU
56	Cv	916	ARG
56	Cv	918	LEU
56	Cv	921	VAL
56	Cv	927	LEU
56	Cv	937	MET
56	Cv	938	ASP
56	Cv	945	VAL
56	Cv	975	ASP
56	Cv	987	SER
56	Cv	988	ASN
56	Cv	991	VAL
56	Cv	993	THR
56	Cv	995	VAL
56	Cv	999	GLU
56	Cv	1002	ARG
56	Cv	1018	THR
56	Cv	1033	GLU
56	Cv	1034	ARG
56	Cv	1040	GLU
56	Cv	1069	GLN
56	Cv	1070	GLU
56	Cv	1086	TRP
56	Cv	1102	LYS
56	Cv	1108	GLN
56	Cv	1115	ASP
56	Cv	1119	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (379) such sidechains are listed below:

Mol	Chain	Res	Type
1	DA	49	HIS
1	DA	59	HIS
1	DA	112	GLN
1	DA	117	GLN

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Mol	Chain	Res	Type
1	DA	123	HIS
1	DA	205	HIS
1	DA	237	HIS
1	DA	287	HIS
1	DA	414	HIS
1	DA	626	GLN
1	DA	644	HIS
1	DA	746	GLN
1	DA	882	GLN
1	DA	907	GLN
1	DA	910	HIS
1	DA	979	GLN
1	DA	980	HIS
1	DA	984	GLN
1	DA	1042	HIS
1	DA	1048	ASN
1	DA	1117	ASN
1	DA	1152	HIS
1	DA	1258	ASN
1	DA	1385	ASN
1	DA	1399	ASN
1	DA	1488	GLN
1	DA	1513	GLN
1	DA	1562	GLN
1	DA	1570	ASN
2	DD	10	HIS
2	DD	63	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	233	ASN
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	408	HIS

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Mol	Chain	Res	Type
2	DD	453	ASN
2	DD	507	GLN
2	DD	521	ASN
2	DD	542	HIS
2	DD	687	HIS
3	DI	30	GLN
3	DI	127	GLN
3	DI	193	ASN
3	DI	294	ASN
3	DI	296	ASN
3	DI	320	GLN
3	DI	370	GLN
3	DI	372	ASN
4	DL	238	GLN
5	DM	27	GLN
5	DM	76	ASN
5	DM	292	ASN
6	DN	28	HIS
6	DN	223	GLN
6	DN	234	HIS
6	DN	238	ASN
6	DN	246	GLN
7	DO	181	HIS
8	DP	98	HIS
8	DP	143	ASN
8	DP	186	HIS
9	DQ	41	GLN
9	DQ	51	ASN
9	DQ	73	HIS
9	DQ	95	HIS
9	DQ	207	HIS
9	DQ	235	HIS
10	DR	75	HIS
10	DR	108	GLN
10	DR	191	GLN
10	DR	198	HIS
10	DR	223	GLN
11	DS	47	ASN
11	DS	134	GLN
11	DS	150	GLN
11	DS	201	HIS
12	DU	63	HIS

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Mol	Chain	Res	Type
14	Da	30	HIS
15	DB	92	HIS
15	DB	111	ASN
15	DB	122	HIS
15	DB	153	HIS
15	DB	194	GLN
15	DB	315	GLN
15	DB	414	GLN
15	DB	445	ASN
15	DB	461	GLN
15	DB	486	HIS
15	DB	551	HIS
15	DB	562	GLN
15	DB	569	HIS
15	DB	703	HIS
15	DB	733	HIS
15	DB	748	HIS
15	DB	848	GLN
15	DB	898	GLN
15	DB	923	GLN
15	DB	958	ASN
15	DB	973	ASN
15	DB	981	HIS
15	DB	1029	HIS
15	DB	1051	GLN
15	DB	1055	GLN
15	DB	1124	HIS
16	DC	81	HIS
16	DC	242	HIS
16	DC	445	HIS
16	DC	530	GLN
16	DC	574	GLN
16	DC	916	HIS
16	DC	920	HIS
16	DC	943	HIS
16	DC	970	GLN
16	DC	1134	HIS
16	DC	1141	GLN
16	DC	1160	GLN
17	DE	105	ASN
17	DE	202	HIS
17	DE	414	ASN

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Mol	Chain	Res	Type
17	DE	442	HIS
17	DE	501	HIS
17	DE	567	HIS
17	DE	578	GLN
17	DE	651	ASN
17	DE	671	ASN
17	DE	698	GLN
18	DF	15	HIS
18	DF	41	ASN
18	DF	115	HIS
18	DF	154	ASN
18	DF	175	GLN
18	DF	187	ASN
18	DF	198	HIS
18	DF	214	HIS
18	DF	283	HIS
18	DF	351	HIS
18	DF	474	GLN
18	DF	543	HIS
18	DF	569	GLN
18	DF	572	HIS
19	DG	65	ASN
19	DG	71	ASN
19	DG	92	GLN
19	DG	143	HIS
19	DG	200	GLN
19	DG	230	ASN
19	DG	365	GLN
19	DG	405	GLN
19	DG	476	GLN
19	DG	477	GLN
20	DH	4	GLN
20	DH	45	HIS
20	DH	100	HIS
20	DH	123	HIS
20	DH	146	GLN
20	DH	257	ASN
20	DH	302	GLN
20	DH	490	HIS
20	DH	526	ASN
21	DJ	31	HIS
21	DJ	33	ASN

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Mol	Chain	Res	Type
21	DJ	42	HIS
21	DJ	82	GLN
21	DJ	227	GLN
21	DJ	247	ASN
21	DJ	291	ASN
21	DJ	301	HIS
21	DJ	309	GLN
21	DJ	314	GLN
22	DK	163	HIS
22	DK	171	GLN
23	DT	45	HIS
23	DT	58	HIS
23	DT	72	HIS
23	DT	82	HIS
23	DT	139	HIS
23	DT	161	ASN
23	DT	219	GLN
24	DV	31	HIS
24	DV	48	HIS
24	DV	71	GLN
24	DV	83	GLN
24	DV	131	GLN
25	DW	71	GLN
25	DW	99	HIS
25	DW	121	HIS
25	DW	154	HIS
26	DX	43	HIS
26	DX	58	HIS
26	DX	111	ASN
26	DX	168	ASN
27	DY	101	GLN
27	DY	106	GLN
27	DY	128	GLN
27	DY	144	HIS
29	CE	85	ASN
29	CE	105	GLN
29	CE	108	HIS
29	CE	132	HIS
29	CE	260	ASN
29	CE	359	HIS
29	CE	417	ASN
30	CF	141	GLN

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Mol	Chain	Res	Type
31	CH	80	HIS
31	CH	129	GLN
31	CH	135	GLN
31	CH	186	HIS
31	CH	247	HIS
31	CH	248	ASN
31	CH	260	ASN
31	CH	267	HIS
32	CI	2	GLN
32	CI	104	ASN
32	CI	318	HIS
32	CI	329	HIS
33	CJ	82	HIS
33	CJ	83	HIS
33	CJ	105	ASN
33	CJ	134	GLN
33	CJ	151	ASN
33	CJ	170	HIS
33	CJ	232	ASN
33	CJ	274	GLN
33	CJ	441	HIS
33	CJ	450	HIS
33	CJ	460	HIS
33	CJ	476	ASN
33	CJ	494	GLN
33	CJ	619	HIS
33	CJ	621	ASN
33	CJ	711	HIS
33	CJ	728	GLN
33	CJ	755	ASN
33	CJ	761	GLN
33	CJ	769	GLN
33	CJ	781	HIS
33	CJ	792	HIS
33	CJ	815	ASN
34	CK	73	GLN
34	CK	111	ASN
34	CK	203	ASN
34	CK	244	HIS
34	CK	289	GLN
34	CK	300	ASN
35	CL	34	ASN

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Mol	Chain	Res	Type
36	CN	63	HIS
36	CN	150	HIS
36	CN	153	ASN
37	CO	82	ASN
37	CO	111	GLN
37	CO	129	GLN
37	CO	214	HIS
37	CO	314	ASN
37	CO	359	HIS
37	CO	426	HIS
38	CP	49	HIS
38	CP	70	HIS
38	CP	87	HIS
38	CP	169	ASN
39	CQ	13	ASN
39	CQ	199	ASN
40	CR	24	ASN
40	CR	125	ASN
40	CR	128	ASN
40	CR	252	GLN
40	CR	266	ASN
41	CS	88	ASN
41	CS	104	GLN
41	CS	110	HIS
42	CU	16	HIS
42	CU	67	HIS
42	CU	72	HIS
42	CU	74	GLN
42	CU	148	ASN
42	CU	174	HIS
42	CU	180	GLN
43	CZ	238	HIS
44	Ca	177	GLN
44	Ca	227	ASN
44	Ca	423	GLN
44	Ca	440	HIS
44	Ca	506	GLN
44	Ca	519	GLN
44	Ca	561	GLN
45	Cb	62	ASN
45	Cb	67	GLN
45	Cb	74	HIS

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Mol	Chain	Res	Type
45	Cb	191	HIS
46	Cd	11	GLN
46	Cd	37	HIS
46	Cd	72	ASN
46	Cd	87	GLN
46	Cd	159	HIS
46	Cd	182	GLN
47	Cg	87	GLN
47	Cg	184	HIS
47	Cg	241	GLN
47	Cg	262	GLN
47	Cg	289	ASN
47	Cg	301	HIS
47	Cg	418	ASN
48	Ci	19	HIS
48	Ci	29	GLN
48	Ci	42	GLN
48	Ci	96	ASN
48	Ci	112	ASN
48	Ci	125	HIS
48	Ci	136	HIS
48	Ci	143	GLN
48	Ci	145	ASN
49	Cj	34	HIS
49	Cj	142	ASN
49	Cj	153	HIS
50	Ck	95	HIS
50	Ck	97	GLN
50	Ck	110	HIS
50	Ck	134	HIS
50	Ck	135	ASN
50	Ck	264	ASN
50	Ck	394	ASN
50	Ck	547	ASN
50	Ck	589	GLN
50	Ck	611	ASN
50	Ck	644	HIS
50	Ck	679	GLN
50	Ck	682	ASN
50	Ck	691	GLN
50	Ck	695	GLN
50	Ck	728	GLN

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Mol	Chain	Res	Type
51	Cm	73	HIS
51	Cm	92	GLN
51	Cm	155	HIS
51	Cm	168	HIS
51	Cm	184	HIS
52	Cn	192	ASN
53	Cp	91	GLN
53	Cp	154	GLN
54	Cq	20	GLN
54	Cq	29	ASN
54	Cq	93	ASN
54	Cq	104	HIS
54	Cq	129	HIS
54	Cq	155	GLN
54	Cq	196	HIS
55	Cr	125	GLN
55	Cr	142	ASN
55	Cr	157	GLN
55	Cr	267	GLN
56	Cv	108	HIS
56	Cv	147	HIS
56	Cv	166	HIS
56	Cv	245	ASN
56	Cv	312	ASN
56	Cv	321	HIS
56	Cv	392	HIS
56	Cv	411	ASN
56	Cv	535	HIS
56	Cv	578	GLN
56	Cv	739	ASN
56	Cv	755	HIS
56	Cv	830	ASN
56	Cv	860	HIS
56	Cv	881	HIS
56	Cv	944	HIS
56	Cv	948	HIS
56	Cv	1066	GLN
56	Cv	1069	GLN
56	Cv	1108	GLN

5.3.3 RNA ⓘ

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

All (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
57	CA	8	U
57	CA	10	G
57	CA	11	U
57	CA	15	U
57	CA	16	U
57	CA	19	U
57	CA	20	A
57	CA	25	U
57	CA	26	C
57	CA	27	A
57	CA	33	A
57	CA	36	U
57	CA	37	U
57	CA	38	U
57	CA	39	U
57	CA	41	A
57	CA	44	U
57	CA	45	G
57	CA	50	A
57	CA	52	C
57	CA	53	A
57	CA	56	U
57	CA	57	U
57	CA	58	A
57	CA	60	A
57	CA	61	A
57	CA	64	G
57	CA	67	U
57	CA	68	A
57	CA	70	U
57	CA	73	U
57	CA	74	G
57	CA	78	G

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Mol	Chain	Res	Type
57	CA	79	A
57	CA	82	U
57	CA	83	U
57	CA	84	U
57	CA	85	U
57	CA	86	G
57	CA	87	U
57	CA	88	A
57	CA	89	U
57	CA	93	A
57	CA	94	U
57	CA	95	U
57	CA	100	G
57	CA	102	A
57	CA	103	U
57	CA	104	A
57	CA	105	G
57	CA	107	U
57	CA	108	A
57	CA	109	A
57	CA	110	U
57	CA	111	A
57	CA	112	A
57	CA	113	U
57	CA	114	A
57	CA	115	A
57	CA	116	U
57	CA	117	U
57	CA	124	U
57	CA	127	G
57	CA	135	U
57	CA	136	G
57	CA	137	U
57	CA	138	U
57	CA	139	U
57	CA	147	G
57	CA	167	A
57	CA	170	U
57	CA	171	A
57	CA	172	A
57	CA	173	A
57	CA	174	A

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Mol	Chain	Res	Type
57	CA	175	A
57	CA	176	A
57	CA	178	A
57	CA	179	U
57	CA	183	U
57	CA	188	U
57	CA	189	A
57	CA	193	C
57	CA	194	A
57	CA	197	A
57	CA	198	A
57	CA	199	U
57	CA	200	A
57	CA	202	A
57	CA	203	U
57	CA	204	U
57	CA	205	A
57	CA	206	A
57	CA	208	U
57	CA	209	U
57	CA	210	A
57	CA	211	A
57	CA	214	U
57	CA	217	U
57	CA	218	A
57	CA	219	G
57	CA	221	C
57	CA	223	G
57	CA	230	A
57	CA	236	G
57	CA	242	G
57	CA	246	U
57	CA	247	A
57	CA	250	U
57	CA	256	G
57	CA	258	U
57	CA	259	U
57	CA	261	U
57	CA	262	A
57	CA	263	A
57	CA	272	C
57	CA	275	U

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Mol	Chain	Res	Type
57	CA	276	U
57	CA	279	C
57	CA	280	A
57	CA	281	U
57	CA	282	A
57	CA	283	U
57	CA	286	A
57	CA	296	U
57	CA	297	G
57	CA	298	U
57	CA	299	U
57	CA	300	G
57	CA	301	A
57	CA	311	U
57	CA	315	A
57	CA	316	A
57	CA	321	A
57	CA	323	U
57	CA	325	A
57	CA	326	U
57	CA	327	U
57	CA	328	U
57	CA	330	U
57	CA	334	U
57	CA	335	G
57	CA	337	U
57	CA	338	U
57	CA	340	U
57	CA	341	A
57	CA	342	A
57	CA	343	A
57	CA	350	U
57	CA	351	A
57	CA	352	G
57	CA	356	U
57	CA	357	A
57	CA	358	U
57	CA	359	G
57	CA	360	C
57	CA	361	A
57	CA	364	U
57	CA	367	A

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Mol	Chain	Res	Type
57	CA	368	A
57	CA	371	U
57	CA	374	U
57	CA	378	A
57	CA	380	U
57	CA	384	A
57	CA	385	A
57	CA	386	A
57	CA	389	A
57	CA	395	U
57	CA	396	A
57	CA	397	U
57	CA	398	U
57	CA	400	U
57	CA	401	A
57	CA	402	U
57	CA	407	U
57	CA	408	C
57	CA	410	U
57	CA	411	A
57	CA	414	A
57	CA	416	U
57	CA	418	A
57	CA	419	U
57	CA	421	G
57	CA	423	A
57	CA	426	A
57	CA	427	U
57	CA	428	A
57	CA	429	U
57	CA	430	U
57	CA	431	U
57	CA	433	U
57	CA	434	A
57	CA	438	U
57	CA	441	G
57	CA	442	A
57	CA	444	A
57	CA	445	C
57	CA	448	U
57	CA	449	G
57	CA	450	A

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Mol	Chain	Res	Type
57	CA	451	U
57	CA	452	A
57	CA	453	A
57	CA	455	G
57	CA	457	U
57	CA	458	U
57	CA	459	A
57	CA	460	U
57	CA	461	A
57	CA	462	A
57	CA	463	A
57	CA	464	U
57	CA	467	A
57	CA	468	A
57	CA	469	A
57	CA	470	G
57	CA	471	U
57	CA	472	G
57	CA	475	A
57	CA	476	A
57	CA	478	A
57	CA	480	C
57	CA	481	A
57	CA	482	U
57	CA	483	A
57	CA	484	A
57	CA	485	U
57	CA	487	A
57	CA	489	A
57	CA	491	U
57	CA	494	A
57	CA	497	A
57	CA	498	U
57	CA	500	U
57	CA	502	U
57	CA	505	U
57	CA	506	A
57	CA	507	A
57	CA	510	A
57	CA	513	U
57	CA	514	A
57	CA	517	U

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Mol	Chain	Res	Type
57	CA	518	G
57	CA	519	U
57	CA	520	A
57	CA	524	A
57	CA	532	A
57	CA	535	U
57	CA	538	A
57	CA	540	A
57	CA	544	U
57	CA	547	U
57	CA	548	G
57	CA	553	C
57	CA	555	A
57	CA	556	C
57	CA	558	A
57	CA	560	U
57	CA	564	U
57	CA	565	A
57	CA	566	U
57	CA	567	A
57	CA	570	A
57	CA	576	A
57	CA	580	U
57	CA	581	G
57	CA	586	A
57	CA	587	A
57	CA	588	U
57	CA	590	A
57	CA	602	A
57	CA	603	A
57	CA	609	A
57	CA	611	U
57	CA	613	U
57	CA	614	U
57	CA	615	U
57	CA	616	U
57	CA	617	U
57	CA	619	U
57	CA	620	U

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	CA	14	A
57	CA	38	U
57	CA	84	U
57	CA	275	U
57	CA	350	U
57	CA	361	A
57	CA	512	G
57	CA	527	A
57	CA	547	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	$\#\|Z\| > 2$
67	GTP	Cg	501	66	26,34,34	1.23	1 (3%)	32,54,54	1.56	8 (25%)
68	SPD	CA	736	-	9,9,9	0.34	0	8,8,8	0.73	0
68	SPD	CA	738	-	9,9,9	0.53	0	8,8,8	0.48	0
68	SPD	CA	739	-	9,9,9	0.41	0	8,8,8	0.59	0
68	SPD	CA	737	-	9,9,9	0.35	0	8,8,8	0.71	0
69	SPM	CA	740	-	13,13,13	0.35	0	12,12,12	0.81	0
65	UTP	DJ	401	-	22,30,30	2.04	3 (13%)	27,47,47	1.50	7 (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
67	GTP	Cg	501	66	-	4/18/38/38	0/3/3/3
68	SPD	CA	736	-	-	4/7/7/7	-
68	SPD	CA	738	-	-	3/7/7/7	-
68	SPD	CA	739	-	-	2/7/7/7	-
68	SPD	CA	737	-	-	0/7/7/7	-
69	SPM	CA	740	-	-	4/11/11/11	-
65	UTP	DJ	401	-	-	9/20/38/38	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	DJ	401	UTP	O4'-C1'	5.40	1.48	1.41
65	DJ	401	UTP	C6-N1	4.86	1.41	1.35
67	Cg	501	GTP	C5-C6	-4.32	1.38	1.47
65	DJ	401	UTP	C4-N3	3.86	1.39	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
65	DJ	401	UTP	PB-O3B-PG	-3.46	120.96	132.83
67	Cg	501	GTP	PB-O3B-PG	-3.34	121.38	132.83
67	Cg	501	GTP	C2-N1-C6	-3.17	119.25	125.10
67	Cg	501	GTP	C8-N7-C5	3.08	108.85	102.99
67	Cg	501	GTP	N2-C2-N1	2.90	122.89	116.71
67	Cg	501	GTP	O3G-PG-O3B	2.57	113.27	104.64
65	DJ	401	UTP	PB-O3A-PA	-2.46	124.40	132.83
67	Cg	501	GTP	C5-C6-N1	2.43	118.24	113.95
65	DJ	401	UTP	O3G-PG-O1G	2.37	116.68	107.64
67	Cg	501	GTP	N2-C2-N3	-2.29	115.27	119.74
65	DJ	401	UTP	C6-N1-C2	-2.20	117.70	121.20
65	DJ	401	UTP	C2'-C3'-C4'	-2.19	98.39	102.64
67	Cg	501	GTP	O6-C6-C5	-2.16	120.15	124.37
65	DJ	401	UTP	O4'-C1'-C2'	-2.09	103.87	106.93
65	DJ	401	UTP	C5-C4-N3	-2.05	118.81	123.31

There are no chirality outliers.

All (26) torsion outliers are listed below:

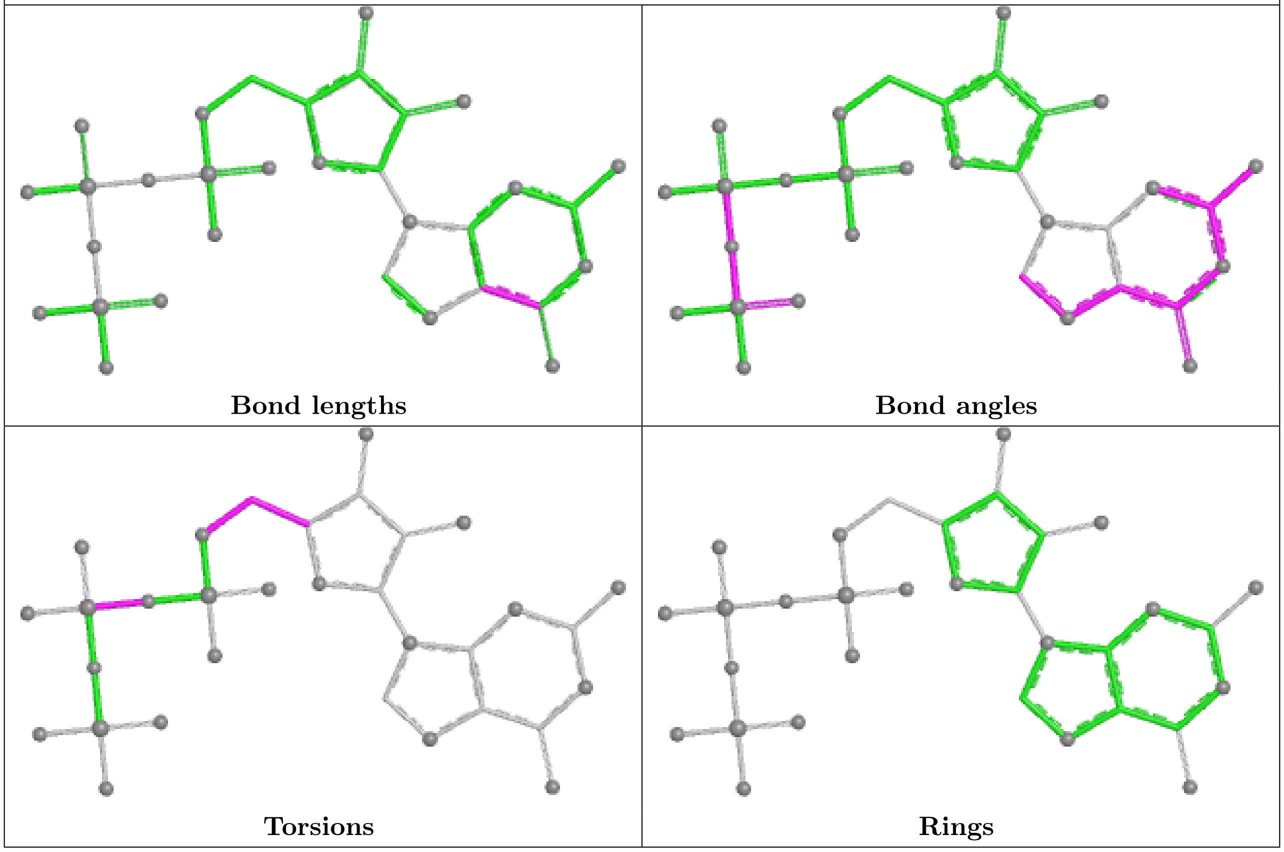
Mol	Chain	Res	Type	Atoms
65	DJ	401	UTP	C5’-O5’-PA-O1A
65	DJ	401	UTP	C5’-O5’-PA-O2A
65	DJ	401	UTP	C5’-O5’-PA-O3A
65	DJ	401	UTP	O4’-C4’-C5’-O5’
65	DJ	401	UTP	O4’-C1’-N1-C6
65	DJ	401	UTP	C2’-C1’-N1-C6
68	CA	738	SPD	C3-C4-C5-N6
67	Cg	501	GTP	O4’-C4’-C5’-O5’
68	CA	736	SPD	C3-C4-C5-N6
69	CA	740	SPM	C3-C4-N5-C6
65	DJ	401	UTP	C3’-C4’-C5’-O5’
68	CA	736	SPD	N6-C7-C8-C9
68	CA	739	SPD	C7-C8-C9-N10
68	CA	739	SPD	C3-C4-C5-N6
69	CA	740	SPM	C6-C7-C8-C9
68	CA	736	SPD	C2-C3-C4-C5
68	CA	736	SPD	C4-C5-N6-C7
68	CA	738	SPD	C7-C8-C9-N10
65	DJ	401	UTP	PA-O3A-PB-O2B
67	Cg	501	GTP	PA-O3A-PB-O2B
69	CA	740	SPM	C8-C9-N10-C11
65	DJ	401	UTP	PA-O3A-PB-O1B
67	Cg	501	GTP	PA-O3A-PB-O1B
69	CA	740	SPM	C7-C6-N5-C4
68	CA	738	SPD	C8-C7-N6-C5
67	Cg	501	GTP	C4’-C5’-O5’-PA

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand GTP Cg 501



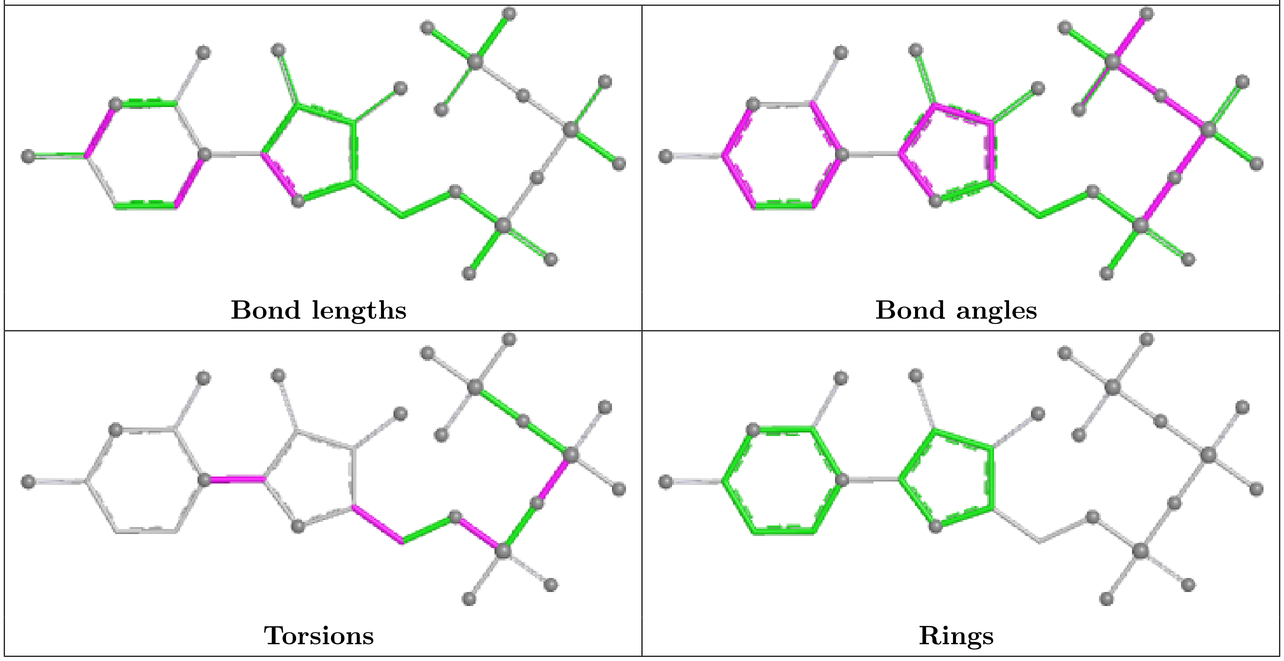
Bond lengths

Bond angles

Torsions

Rings

Ligand UTP DJ 401



Bond lengths

Bond angles

Torsions

Rings

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

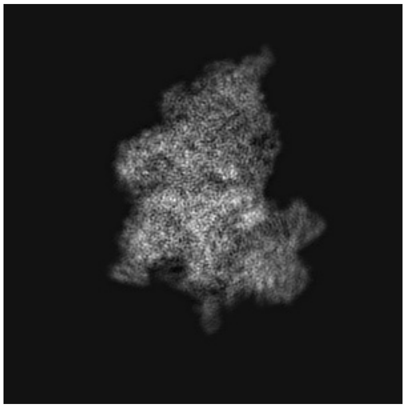
6 Map visualisation ⓘ

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.

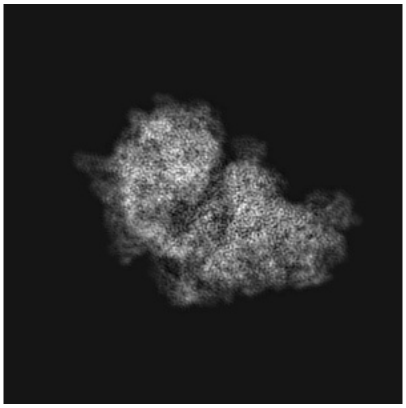
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

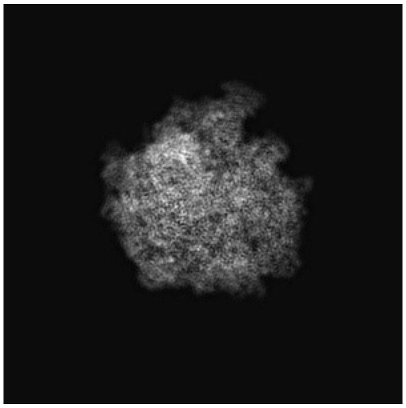
6.1.1 Primary map



X

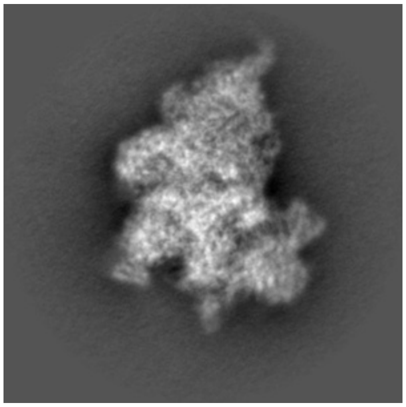


Y

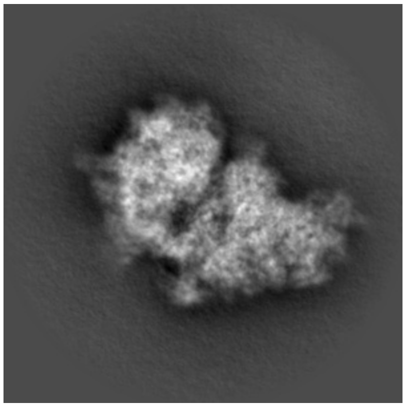


Z

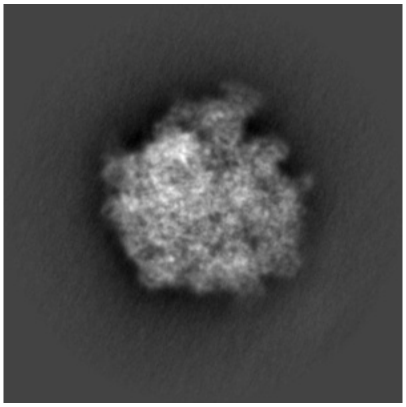
6.1.2 Raw map



X



Y

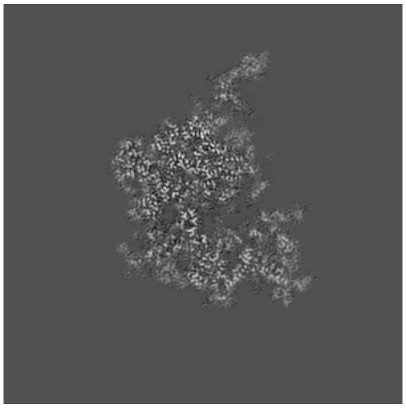


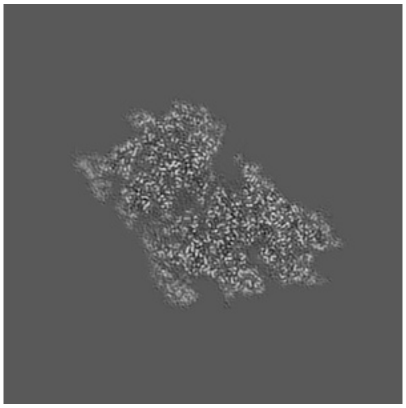
Z

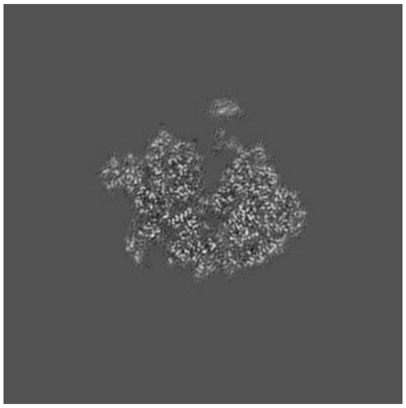
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

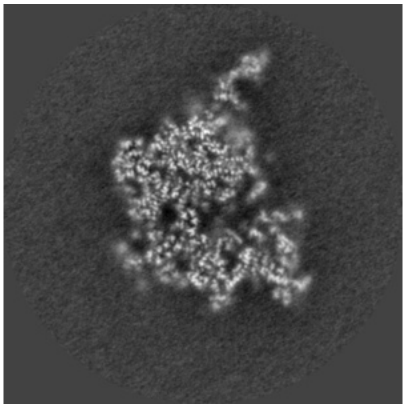
6.2.1 Primary map

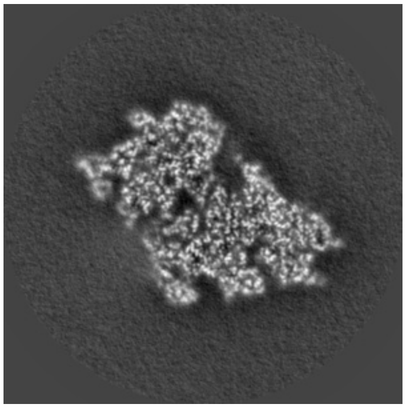

X Index: 160

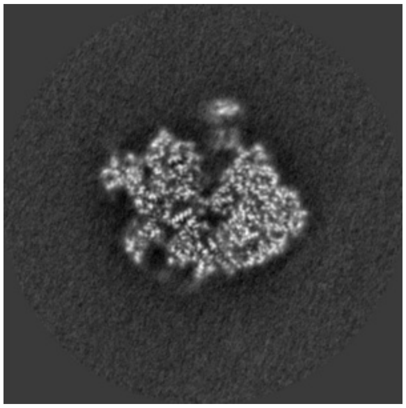

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

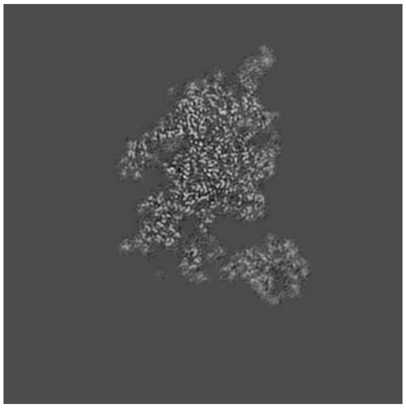

Y Index: 160


Z Index: 160

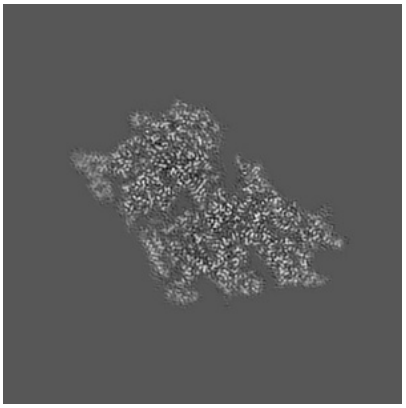
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

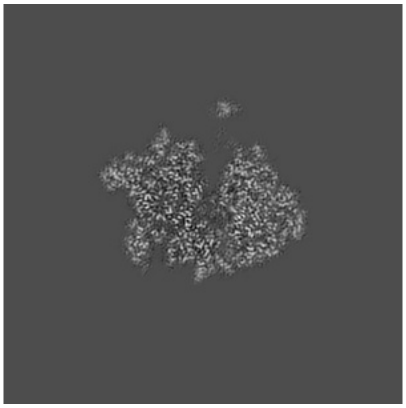
6.3.1 Primary map



X Index: 143

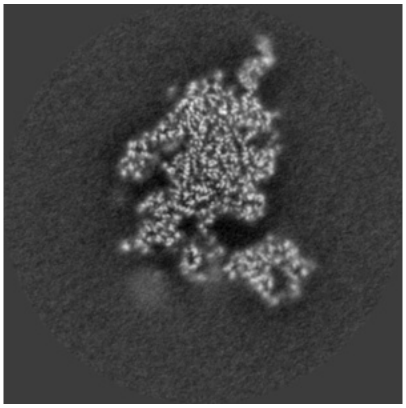


Y Index: 162

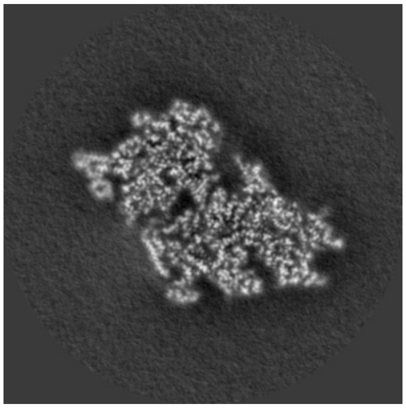


Z Index: 162

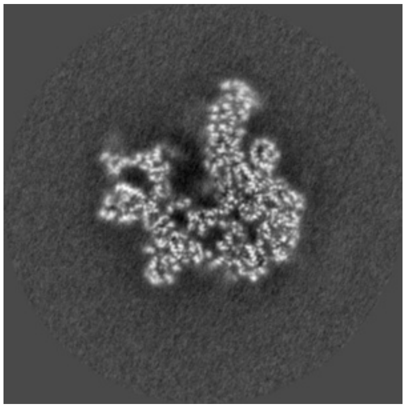
6.3.2 Raw map



X Index: 143



Y Index: 162

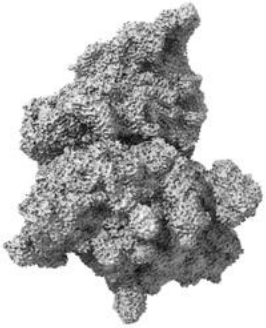


Z Index: 143

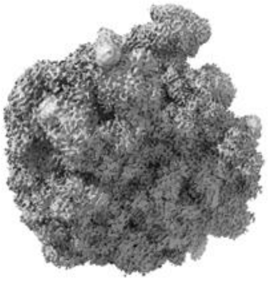
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map


X


Y

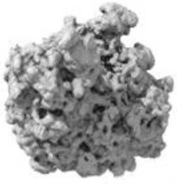

Z

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

6.4.2 Raw map


X


Y


Z

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

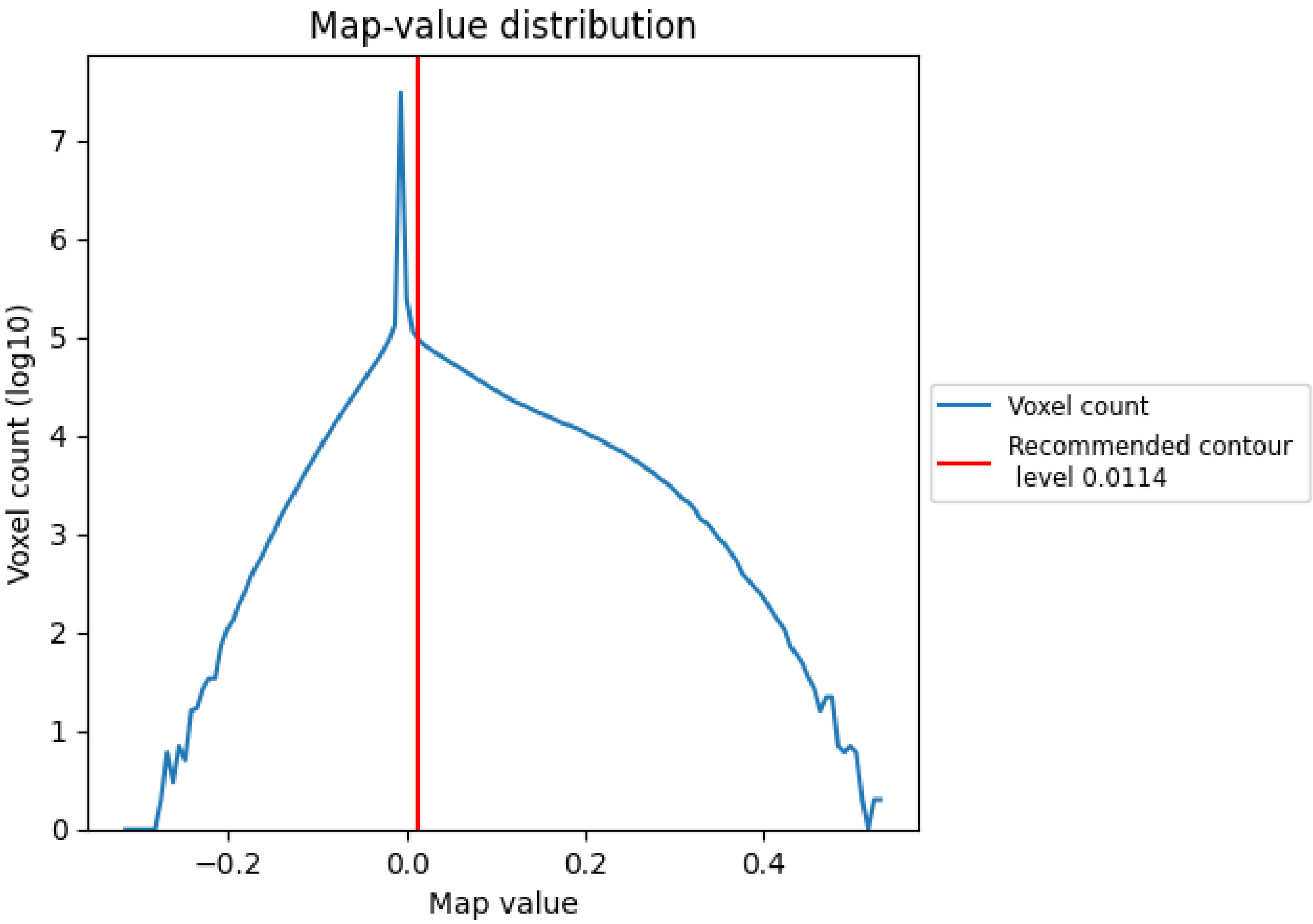
6.5 Mask visualisation ⓘ

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

7 Map analysis (i)

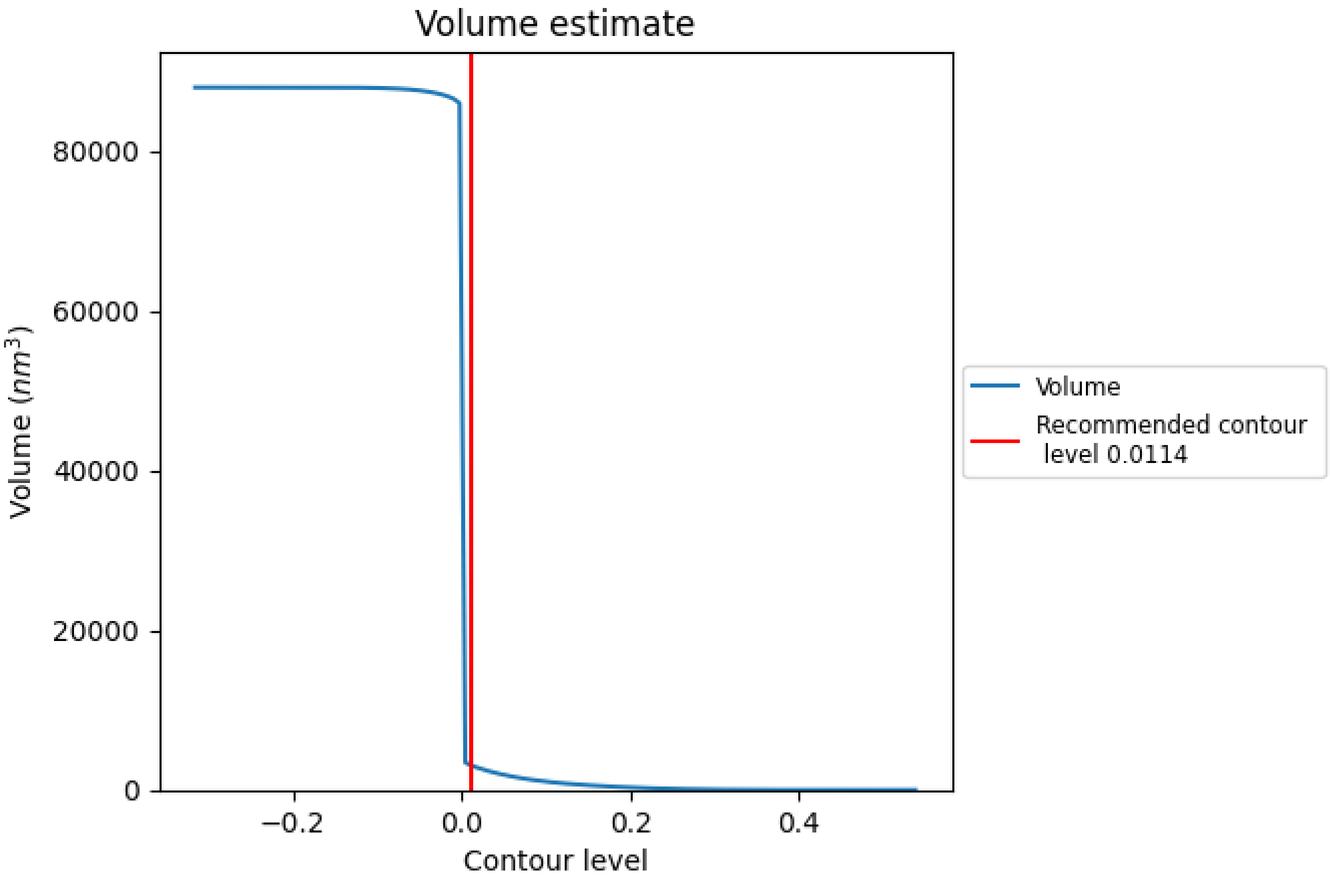
This section contains the results of statistical analysis of the map.

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.

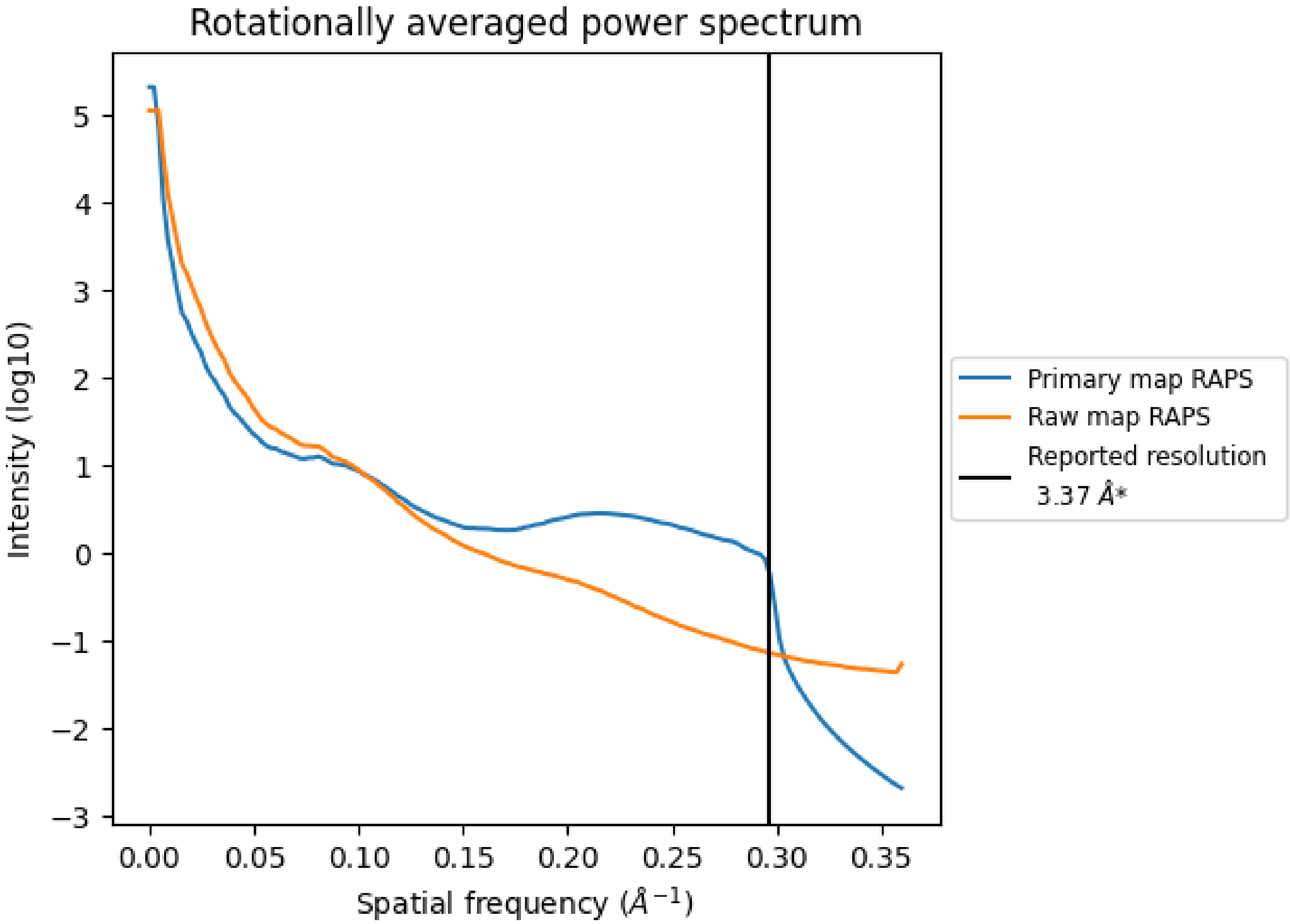
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 3069 nm^3; 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 ⓘ

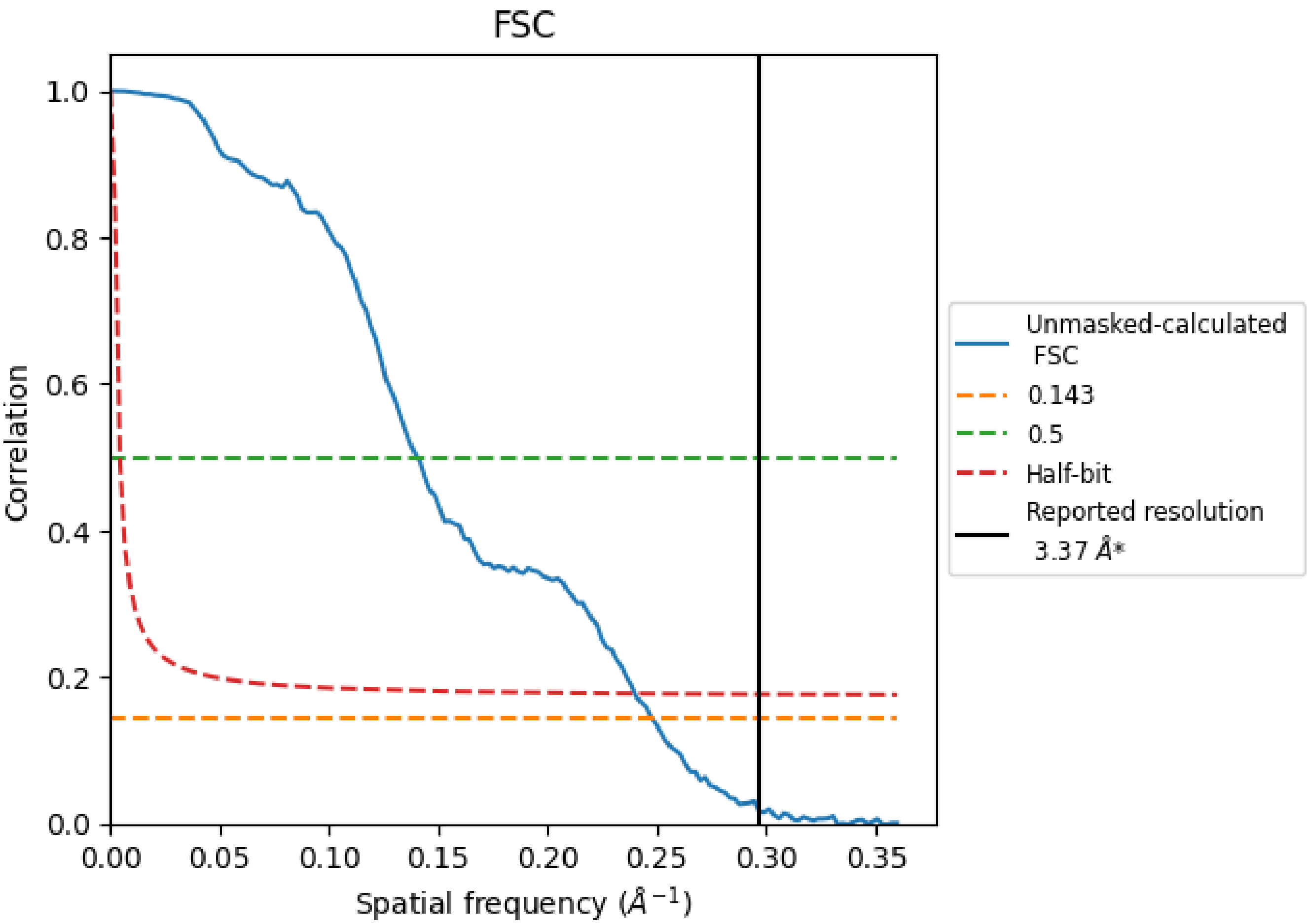


*Reported resolution corresponds to spatial frequency of 0.297 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.297 Å^{-1}

8.2 Resolution estimates

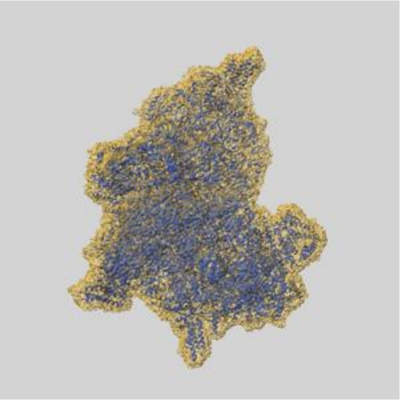
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	7.13	4.17

*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 %

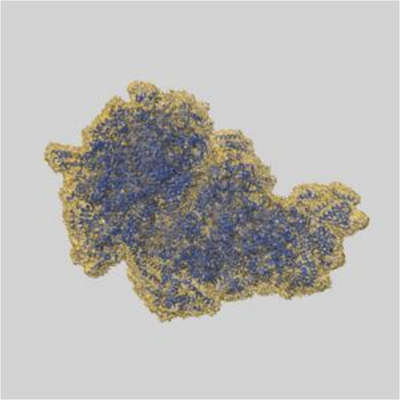
9 Map-model fit ⓘ

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.

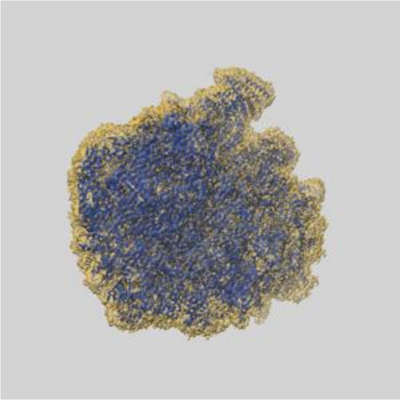
9.1 Map-model overlay ⓘ



X



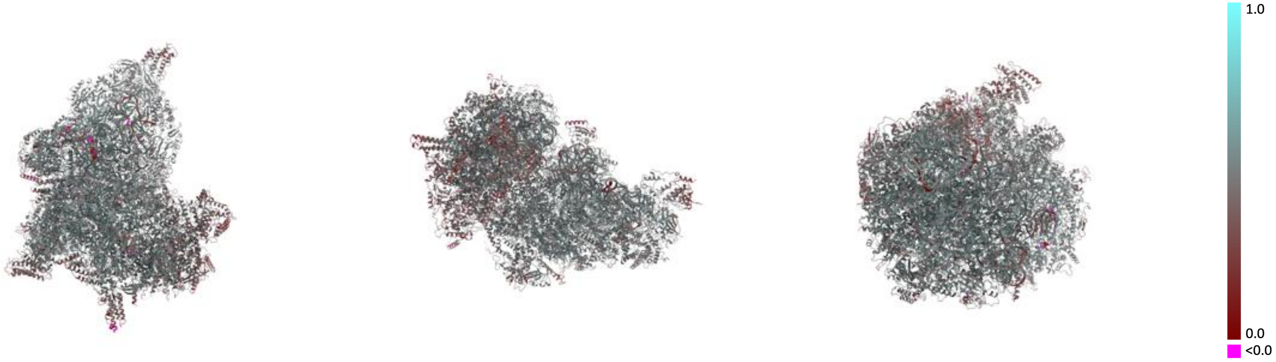
Y



Z

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.

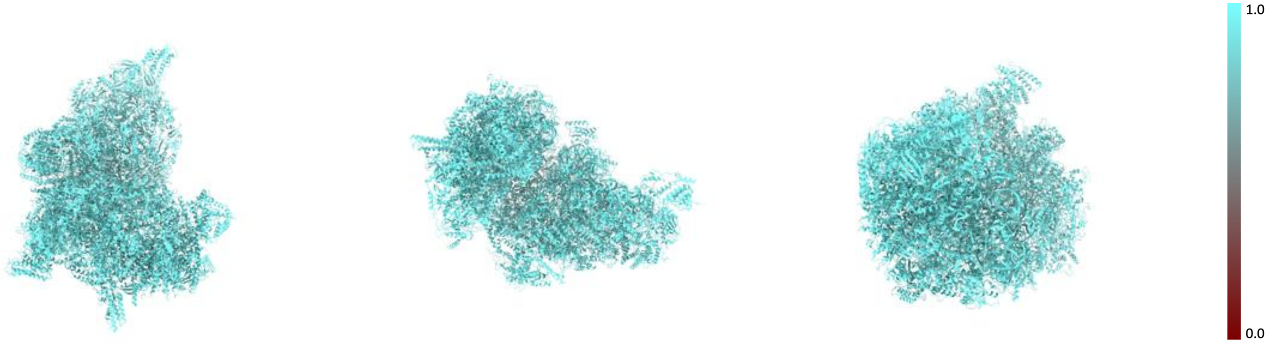
9.2 Q-score mapped to coordinate model (i)



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.

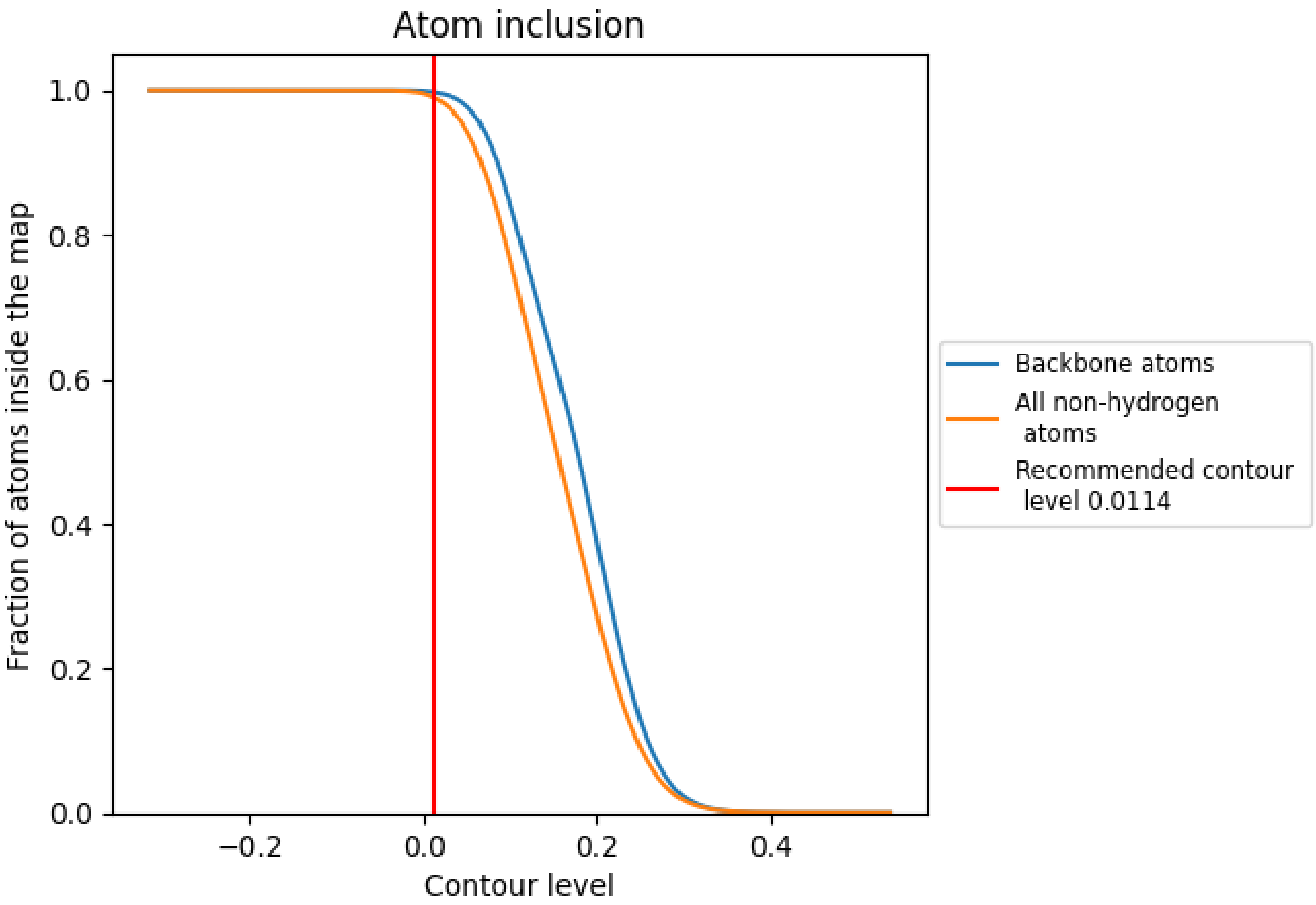
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0114).

9.4 Atom inclusion ⓘ



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	0.9904	0.4880
CA	0.9935	0.5000
CC	0.9734	0.5070
CE	0.9918	0.5330
CF	0.9840	0.4870
CH	0.9828	0.5160
CI	0.9872	0.5190
CJ	0.9861	0.5010
CK	0.9944	0.4860
CL	0.9944	0.5200
CN	0.9914	0.5310
CO	0.9959	0.5210
CP	0.9958	0.5250
CQ	0.9974	0.5500
CR	0.9860	0.5100
CS	0.9948	0.5120
CU	0.9939	0.5090
CZ	0.9855	0.3940
Ca	0.9899	0.5130
Cb	0.9930	0.4990
Cd	0.9896	0.4760
Cg	0.9917	0.5000
Ci	0.9877	0.5170
Cj	0.9989	0.4810
Ck	0.9798	0.4500
Cm	0.9817	0.5070
Cn	0.9977	0.5270
Cp	0.9965	0.4630
Cq	0.9939	0.5180
Cr	0.9954	0.4560
Cv	0.9942	0.5120
DA	0.9920	0.4800
DB	0.9845	0.4860
DC	0.9883	0.3980
DD	0.9924	0.5080

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
DE	0.9913	0.4280
DF	0.9937	0.4900
DG	0.9887	0.4560
DH	0.9885	0.4870
DI	0.9958	0.4970
DJ	0.9917	0.4820
DK	0.9888	0.4680
DL	0.9751	0.5140
DM	0.9940	0.5260
DN	0.9901	0.5130
DO	0.9937	0.4740
DP	0.9974	0.4270
DQ	0.9960	0.4900
DR	0.9975	0.4740
DS	0.9989	0.4800
DT	0.9920	0.4960
DU	0.9918	0.5000
DV	0.9869	0.5200
DW	0.9909	0.5100
DX	0.9887	0.5040
DY	0.9887	0.5170
DZ	0.9883	0.5220
Da	1.0000	0.5490
UO	1.0000	0.4330
UP	1.0000	0.3640
UQ	0.9896	0.4000
UR	1.0000	0.3800
US	0.9938	0.4110
UT	0.9659	0.3610