Full wwPDB EM Validation Report (i)

Nov 22, 2022 – 04:01 AM EST

PDB ID	:	7N30
EMDB ID	:	EMD-24135
Title	:	Elongating 70S ribosome complex in a hybrid-H2* pre-translocation (PRE-H2*) conformation
Authors	:	Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, K.S.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.
Deposited on	:	2021-05-30
Resolution	:	2.66 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

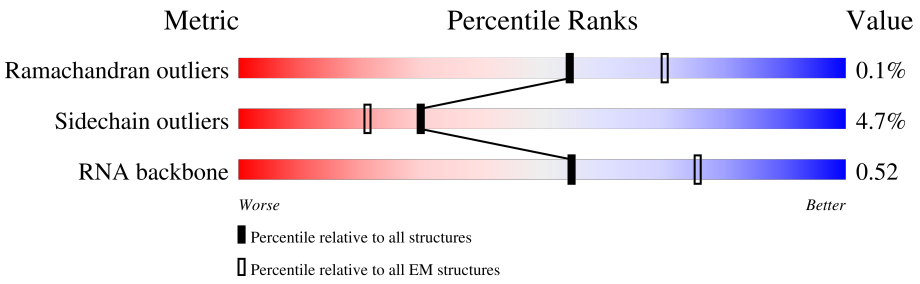
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.66 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	16	1534	17% 82% 17% •
2	SB	241	60% 89% • 7%
3	SC	233	44% 88% • 9%
4	SD	206	71% 96% • •
5	SE	167	17% 89% • 7%
6	SF	135	58% 73% 5% 21%
7	SG	179	78% 78% 6% 16%
8	SH	130	18% 95% • •

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Mol	Chain	Length	Quality of chain
9	SI	130	81% 92% 6%
10	SJ	103	75% 90% 6%
11	SK	129	48% 88% 9%
12	SL	124	14% 94%
13	SM	118	89% 89% 8%
14	SN	101	64% 96%
15	SO	89	38% 97%
16	SP	82	35% 98%
17	SQ	84	40% 92% 5%
18	SR	75	36% 85% 12%
19	SS	92	87% 84% 5% 11%
20	ST	87	59% 95%
21	SU	71	73% 80% 18%
22	mR	60	18% 82%
23	23	2904	12% 81% 18%
24	5	120	12% 87% 13%
25	LB	273	5% 98%
26	LC	209	7% 96%
27	LD	201	18% 98%
28	LE	179	97% 90% 8%
29	LF	177	59% 95%
30	LI	149	93% 93% 7%
31	LM	142	8% 100%
32	LN	123	8% 96%
33	LO	144	8% 94% 6%

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Mol	Chain	Length	Quality of chain
34	LP	136	11% 98%
35	LQ	127	92% 6%
36	LR	117	47% 90% 9%
37	LS	115	17% 93% 6%
38	LT	118	97%
39	LU	103	16% 96%
40	LV	110	9% 97%
41	LW	100	20% 92% 6%
42	LX	104	22% 95%
43	LY	94	24% 98%
44	La	85	6% 87% 12%
45	Lb	78	13% 96%
46	Lc	63	25% 94% 5%
47	Ld	59	10% 95%
48	Le	70	94% 86% 9% 6%
49	Lf	57	11% 96%
50	Lg	55	25% 93% 5%
51	Lh	46	98%
52	Li	65	6% 97%
53	Lj	38	8% 95% 5%
54	Pp	3	100% 100%
55	Pt	76	78% 59% 36% 5%
56	Dt	76	67% 75% 25%

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 146268 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	16	1526	32762	14619	6014	10603	1526	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	224	1753	1109	315	321	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SC	212	1658	1049	311	294	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SD	204	1633	1020	313	296	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SE	155	1143	712	216	209	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SF	106	862	545	156	154	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SG	151	1181	735	227	215	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SH	128	973	613	172	182	6	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SI	127	1022	634	206	179	3	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SJ	99	795	498	152	144	1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SK	117	877	540	174	160	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SL	122	951	588	195	163	5	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SM	114	883	546	178	156	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SN	100	805	499	164	139	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	SO	88	713	439	144	129	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	SP	82	648	406	128	113	1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SQ	80	648	411	121	113	3	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	SR	66	544	345	102	96	1	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	SS	82	656	419	125	110	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	ST	86	670	414	138	115	3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	SU	70	590	366	125	98	1	0	0

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	mR	11	234	105	41	77	11	0	0

- Molecule 23 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	23	2901	62293	27796	11460	20136	2901	0	0

- Molecule 24 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	5	120	2570	1144	468	838	120	0	0

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LB	271	2082	1288	423	364	7	0	0

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LC	209	1565	979	288	294	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LD	201	1552	974	283	290	5	0	0

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LE	177	1410	899	249	256	6	0	0

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LF	176	1323	832	243	246	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	LI	149	1111	699	197	214	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	LM	142	1129	714	212	199	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	LN	122	938	587	180	165	6	0	0

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	LO	144	1053	654	207	190	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LP	136	1075	686	205	178	6	0	0

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	LQ	120	960	593	196	166	5	0	0

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	LR	116	891	552	178	161	0	0

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	LS	114	928	580	183	164	1	1	0

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	LT	117	947	604	192	151	0	0

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LU	103	816	516	153	145	2	0	0

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	LV	110	857	532	166	156	3	0	0

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	LW	94	746	470	140	134	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	LX	102	779	492	146	141	0	0

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	LY	94	752	479	137	133	3	0	0

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	La	75	575	356	116	102	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Lb	77	624	388	129	105	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Lc	62	501	308	98	94	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Ld	58	449	281	87	79	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Le	66	522	323	99	94	6	0	0

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Lf	56	443	269	94	79	1	0	0

- Molecule 50 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	Lg	52	427	275	78	74	0	0

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Lh	46	377	228	90	57	2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Li	64	504	323	105	74	2	0	0

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Lj	38	302	185	65	48	4	0	0

- Molecule 54 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Pp	3	28	20	4	3	1	0	0

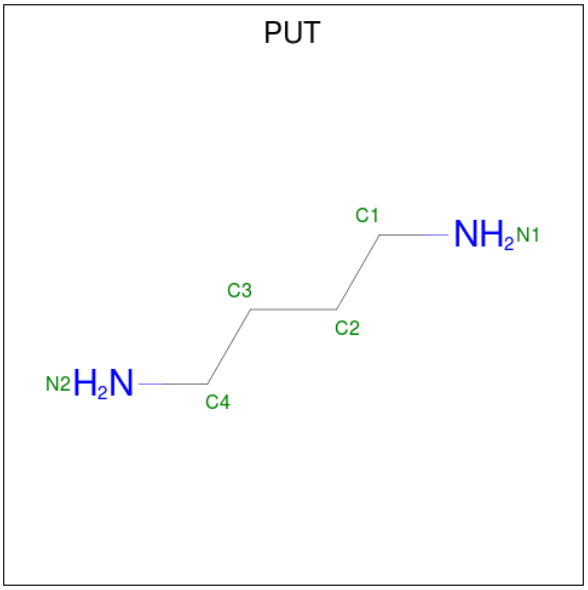
- Molecule 55 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
55	Pt	76	1636	734	284	541	76	1	0	0

- Molecule 56 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
56	Dt	76	1637	735	294	531	75	2	0	0

- Molecule 57 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
57	16	1	6	4	2	0
57	23	1	60	40	20	0
57	23	1	60	40	20	0
57	23	1	60	40	20	0
57	23	1	60	40	20	0
57	23	1	60	40	20	0
57	23	1	60	40	20	0
57	23	1	60	40	20	0
57	23	1	60	40	20	0
57	23	1	60	40	20	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
57	23	1	60	40	20	0

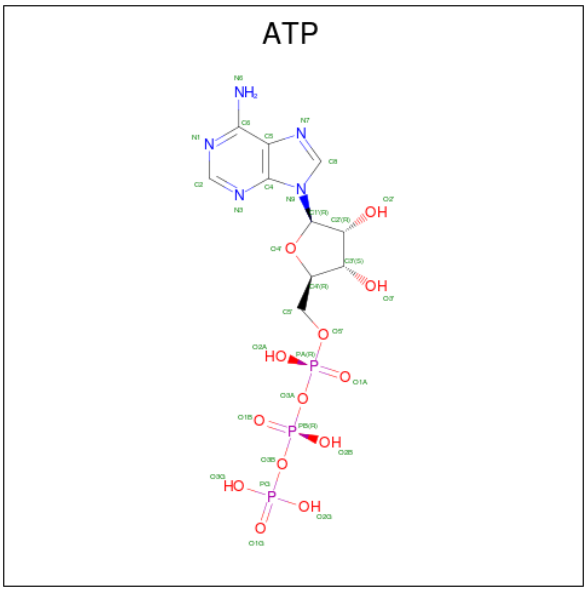
- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	16	76	76	76	0
58	SD	1	1	1	0
58	SS	1	1	1	0
58	23	210	210	210	0
58	5	4	4	4	0
58	LC	1	1	1	0
58	LD	1	1	1	0
58	LX	1	1	1	0
58	Lf	1	1	1	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

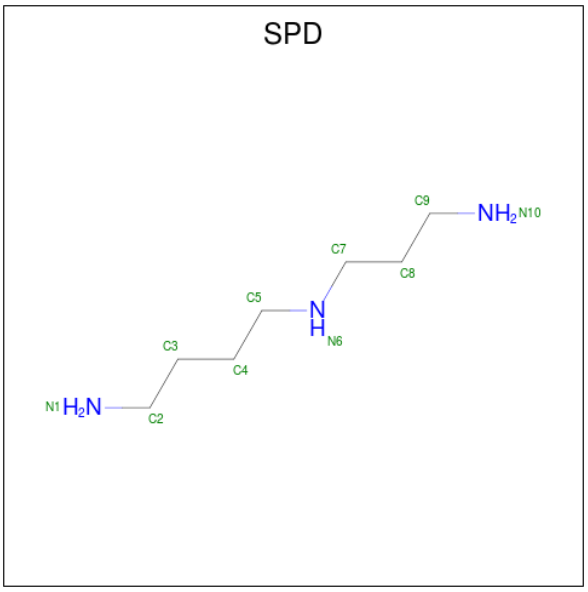
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	SB	1	1	1	0

- Molecule 60 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	23	1	62	20	10	26	6	0
			Total	C	N	O	P	
60	23	1	62	20	10	26	6	0

- Molecule 61 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
61	23	1	40	28	12	0

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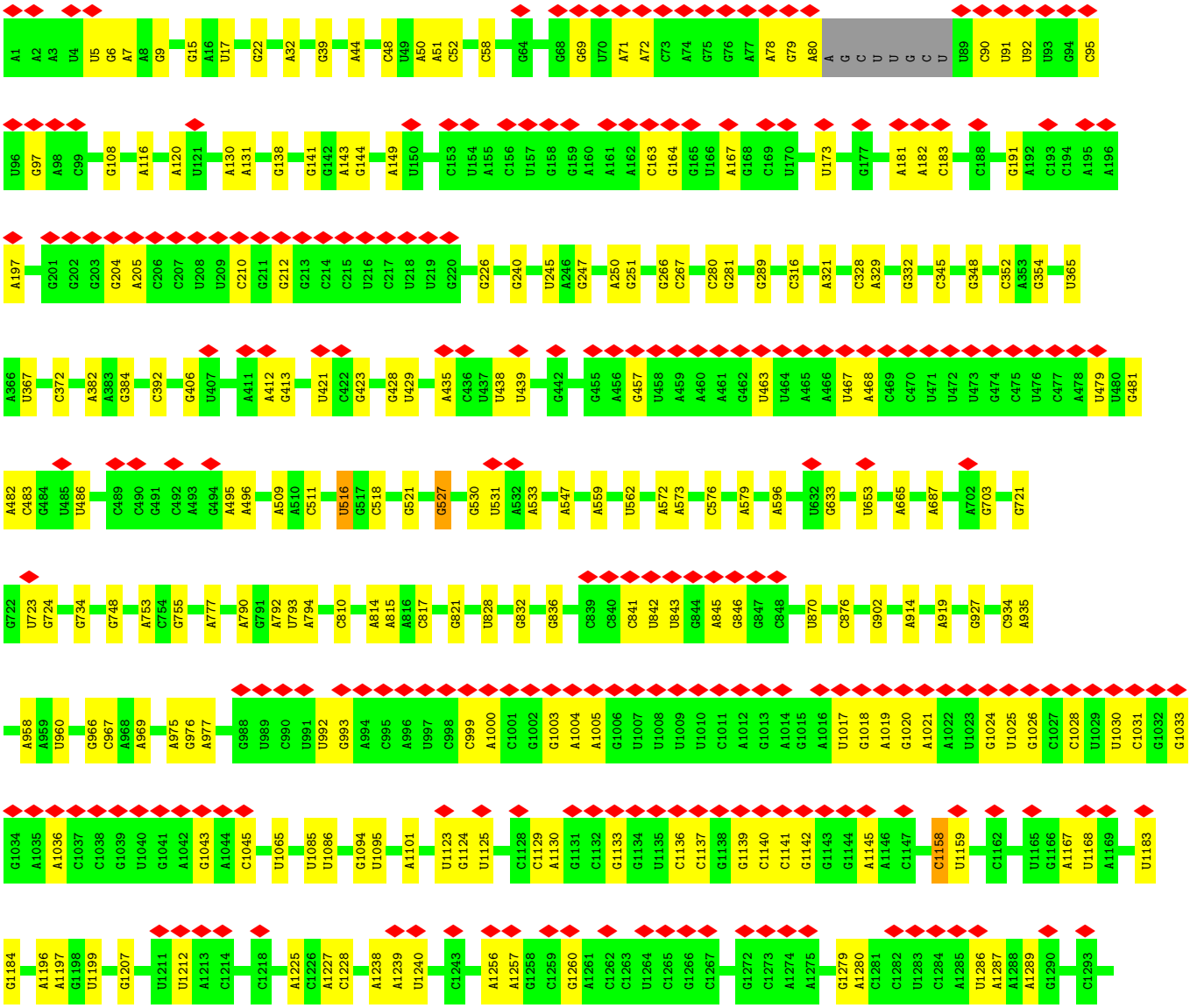
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
61	23	1	40	28	12	0
			Total	C	N	
61	23	1	40	28	12	0
			Total	C	N	
61	23	1	40	28	12	0

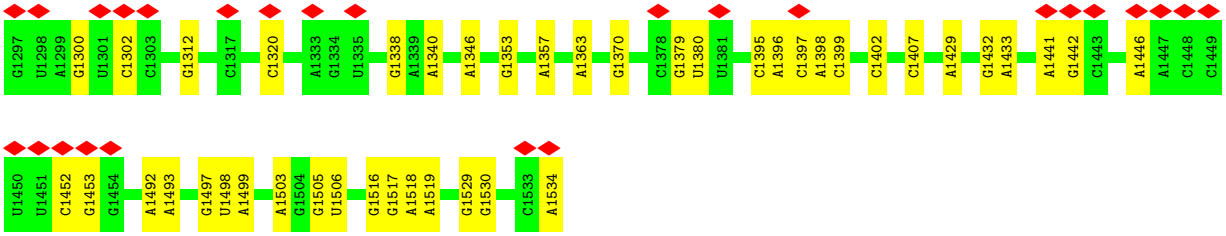
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

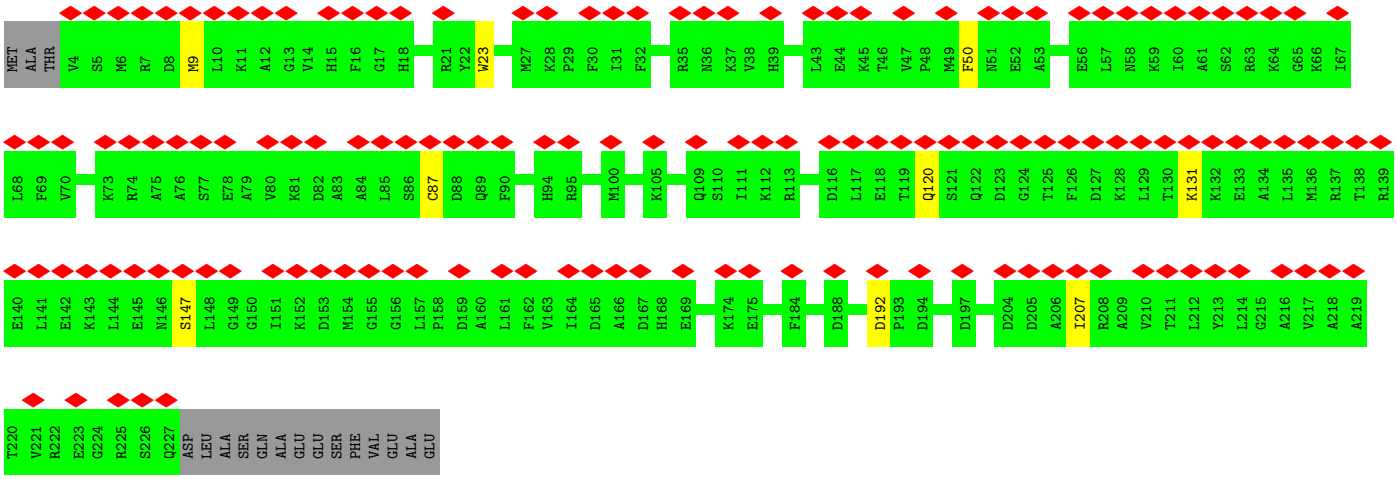
Chain 16:





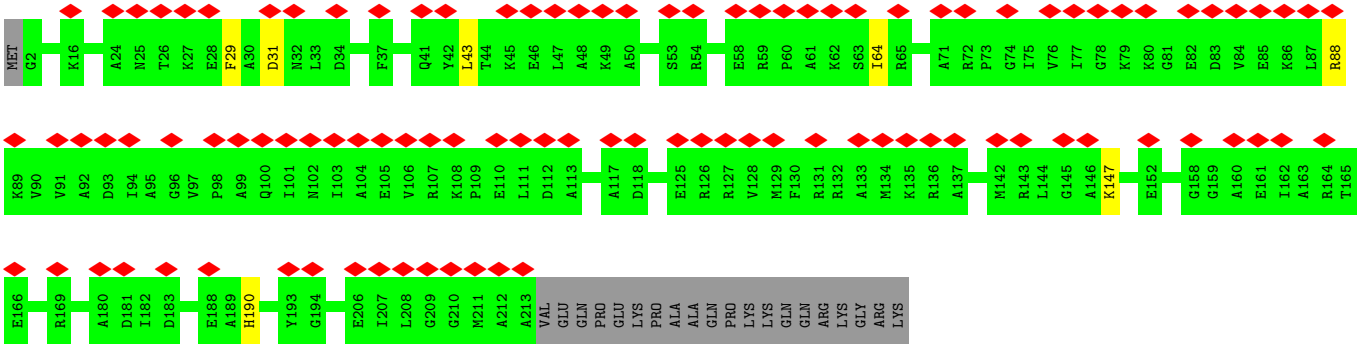
- Molecule 2: 30S ribosomal protein S2

Chain SB:



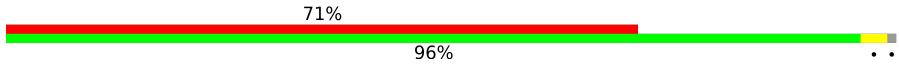
- Molecule 3: 30S ribosomal protein S3

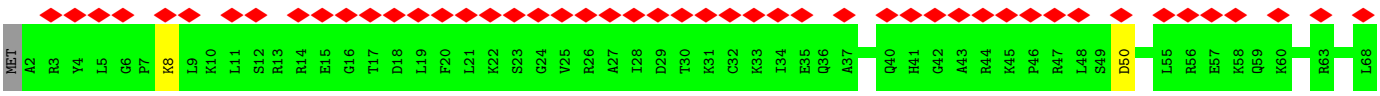
Chain SC:

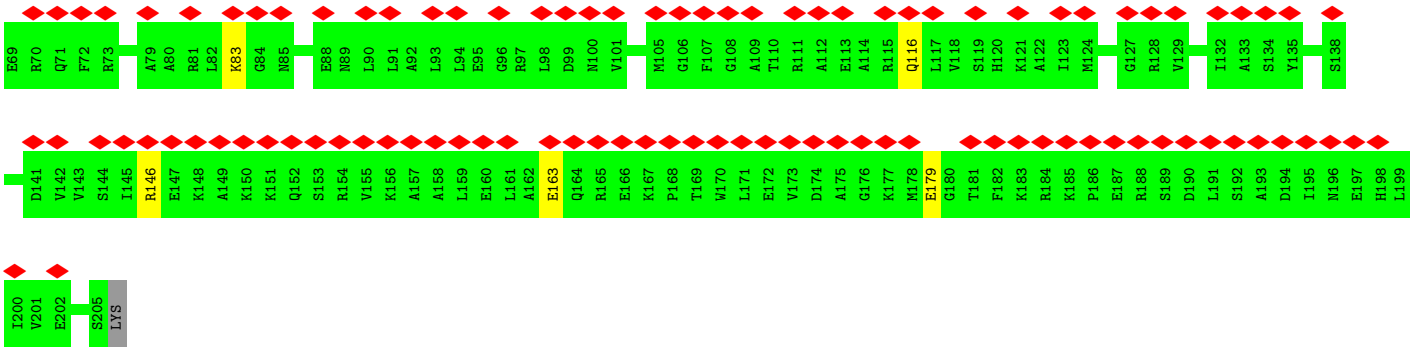


- Molecule 4: 30S ribosomal protein S4

Chain SD:

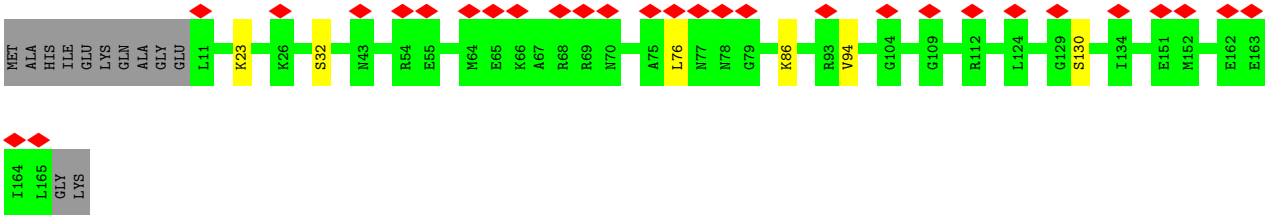






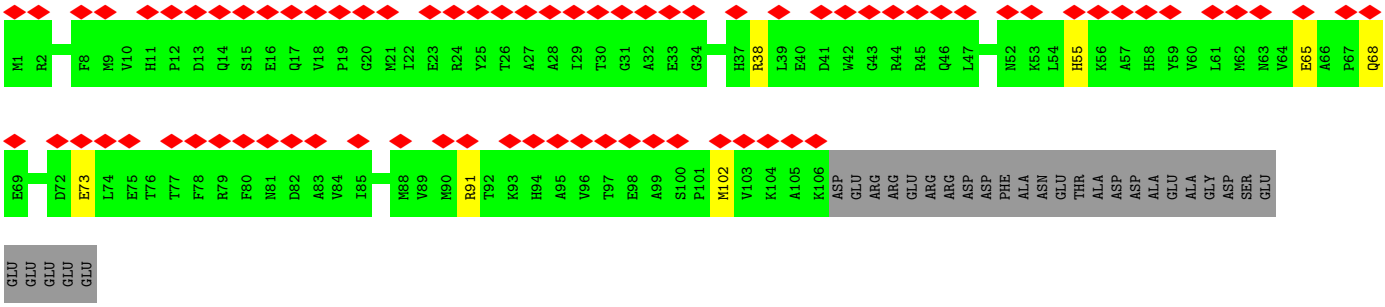
- Molecule 5: 30S ribosomal protein S5

Chain SE:



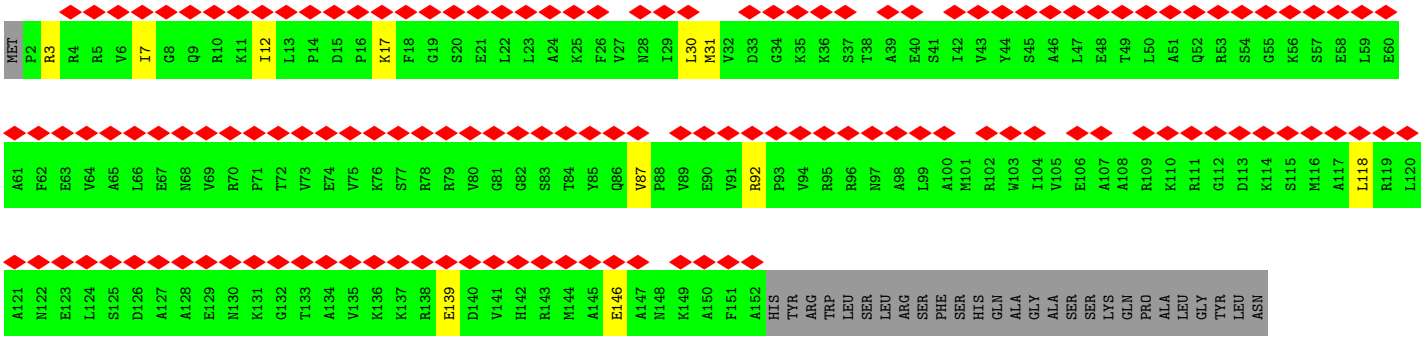
- Molecule 6: 30S ribosomal protein S6

Chain SF:



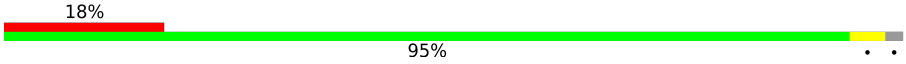
- Molecule 7: 30S ribosomal protein S7

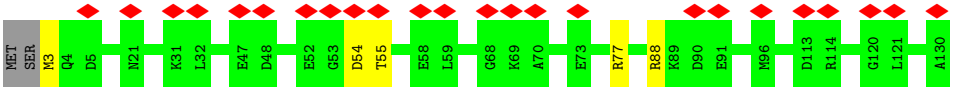
Chain SG:



- Molecule 8: 30S ribosomal protein S8

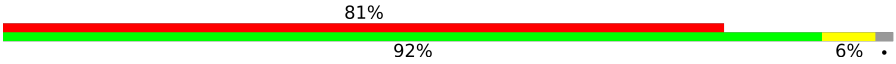
Chain SH:

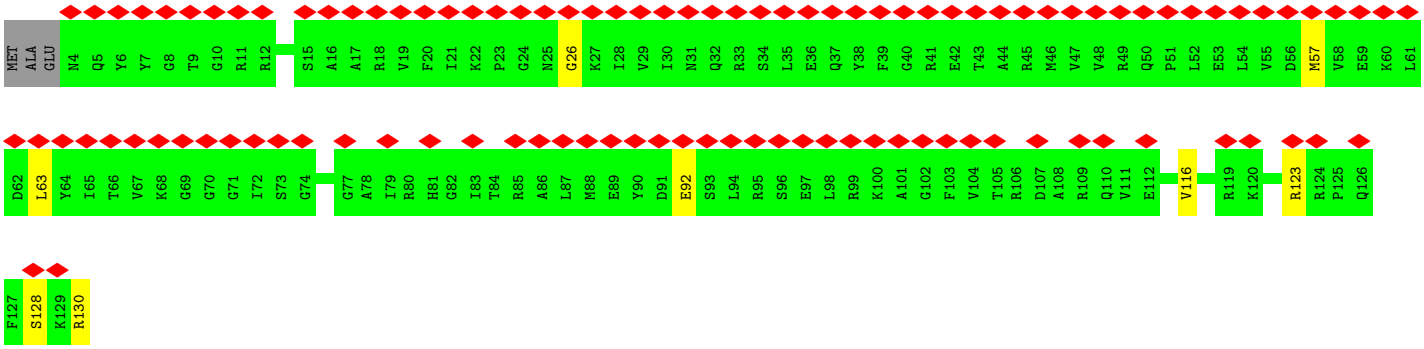




- Molecule 9: 30S ribosomal protein S9

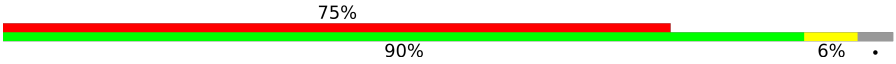
Chain SI:

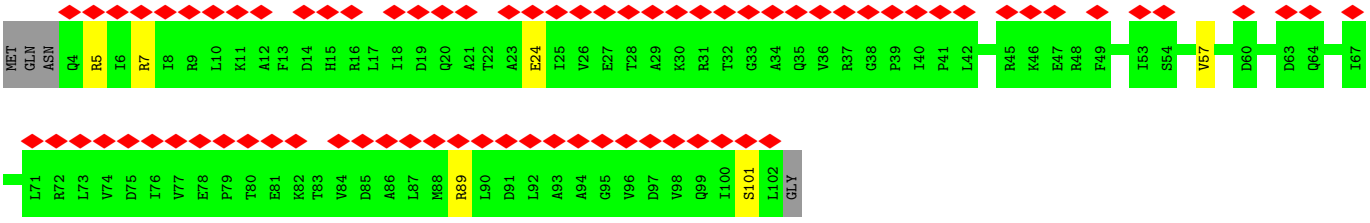




- Molecule 10: 30S ribosomal protein S10

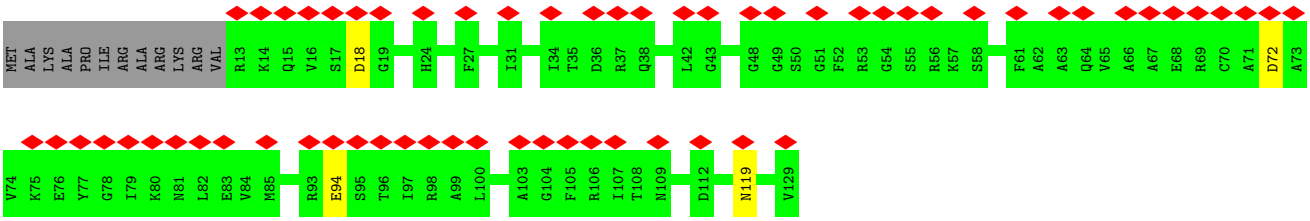
Chain SJ:





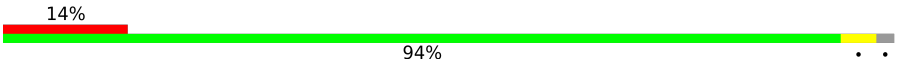
- Molecule 11: 30S ribosomal protein S11

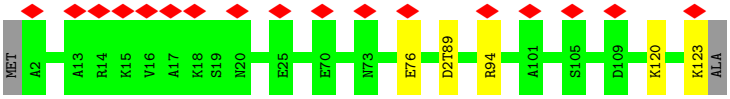
Chain SK:



- Molecule 12: 30S ribosomal protein S12

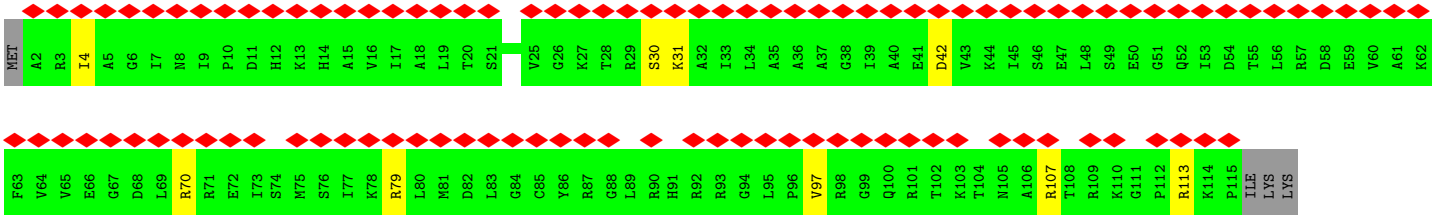
Chain SL:





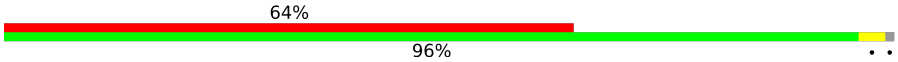
• Molecule 13: 30S ribosomal protein S13

Chain SM:



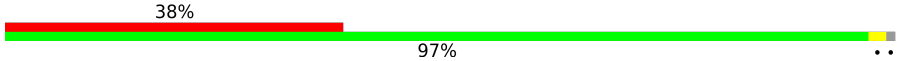
• Molecule 14: 30S ribosomal protein S14

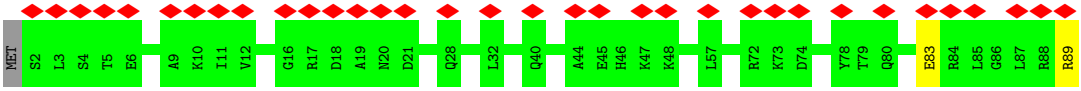
Chain SN:



• Molecule 15: 30S ribosomal protein S15

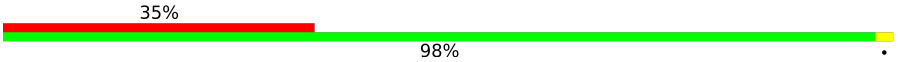
Chain SO:

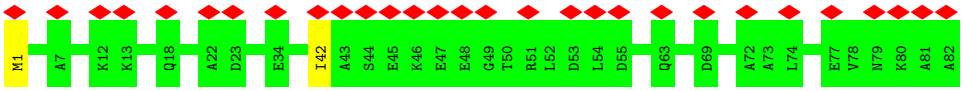




• Molecule 16: 30S ribosomal protein S16

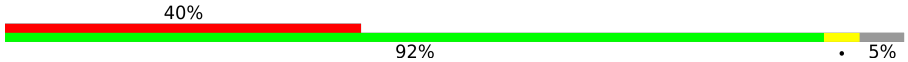
Chain SP:

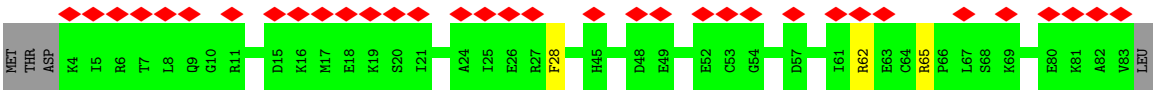




• Molecule 17: 30S ribosomal protein S17

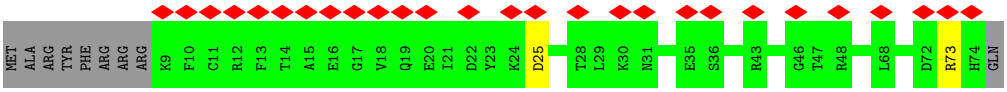
Chain SQ:





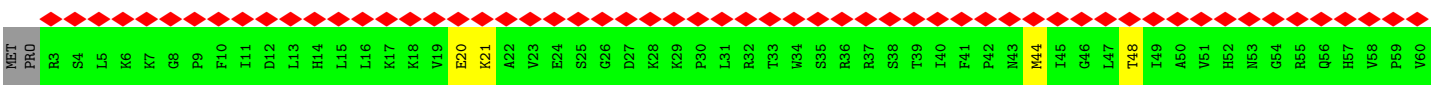
• Molecule 18: 30S ribosomal protein S18

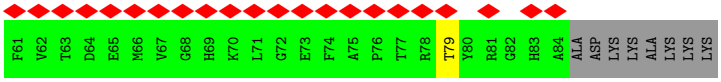
Chain SR:



- Molecule 19: 30S ribosomal protein S19

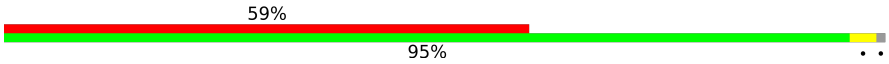
Chain SS:

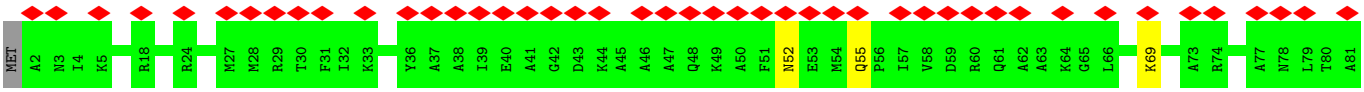


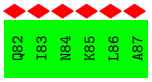


- Molecule 20: 30S ribosomal protein S20

Chain ST:

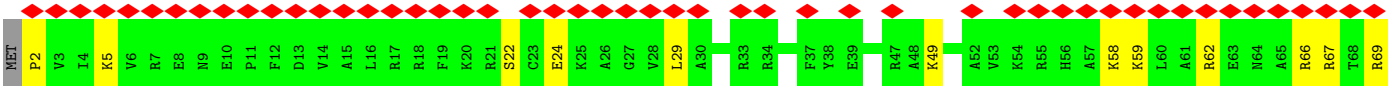






- Molecule 21: 30S ribosomal protein S21

Chain SU:

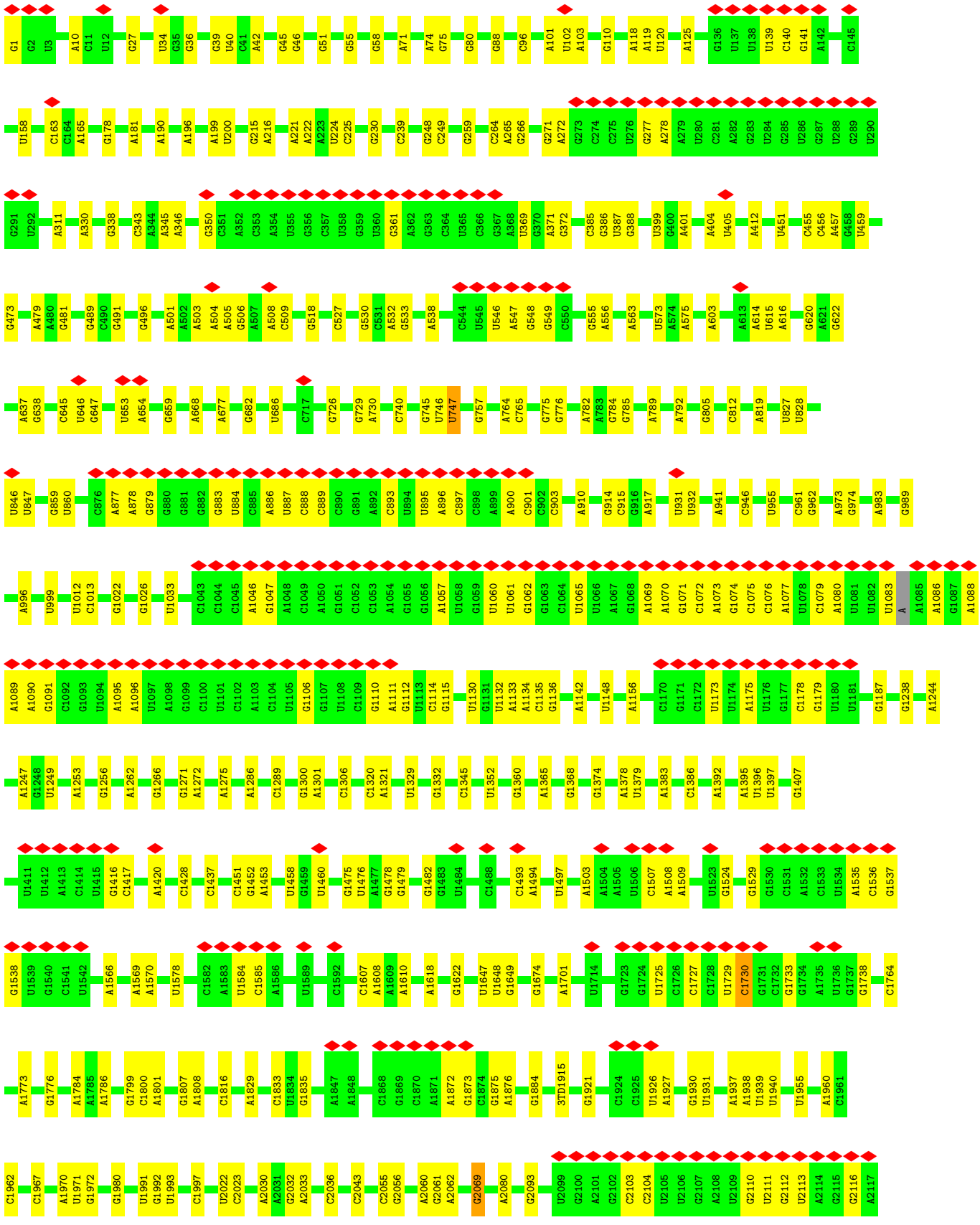


- Molecule 22: mRNA

Chain mR:

- Molecule 23: 23S rRNA

Chain 23: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U158 C163 C164 A165 G178 A181 A190 A196 A199 U200 G215 A216 A221 A222 A223 U224 C225 G230 C239 G248 C249 G259 C264 A265 C266 G271 A272 G273 C274 C275 U276 G277 A278 A279 U280 C281 A282 G283 U284 G285 U286 G287 U288 G289 U290
G291 U292 A311 A330 G338 C343 A344 A345 A346 G350 C351 A352 C353 A354 U355 C356 C357 U358 C359 U360 G361 A362 G363 C364 U365 C366 G367 A368 U369 G370 A371 G372 C385 G386 U387 G388 U399 G400 A401 A404 U405 A412 U451 C455 C456 A457 G458 U459
G473 A479 A480 G481 G489 C490 G491 G496 A501 A502 A503 A504 A505 G506 A507 A508 C509 G518 C527 G530 C531 A532 G533 A538 C544 U545 U546 A547 G548 G549 C550 G555 A556 A563 U573 A574 A575 A603 A613 A614 U615 A616 G620 A621 G622
A637 G638 C645 U646 G647 U653 A654 G659 A668 A677 G682 U686 C717 G726 G729 A730 C740 G745 U746 U747 G757 A764 C765 G775 G776 A782 A783 G784 G785 A789 A792 G805 C812 A819 U827 U828
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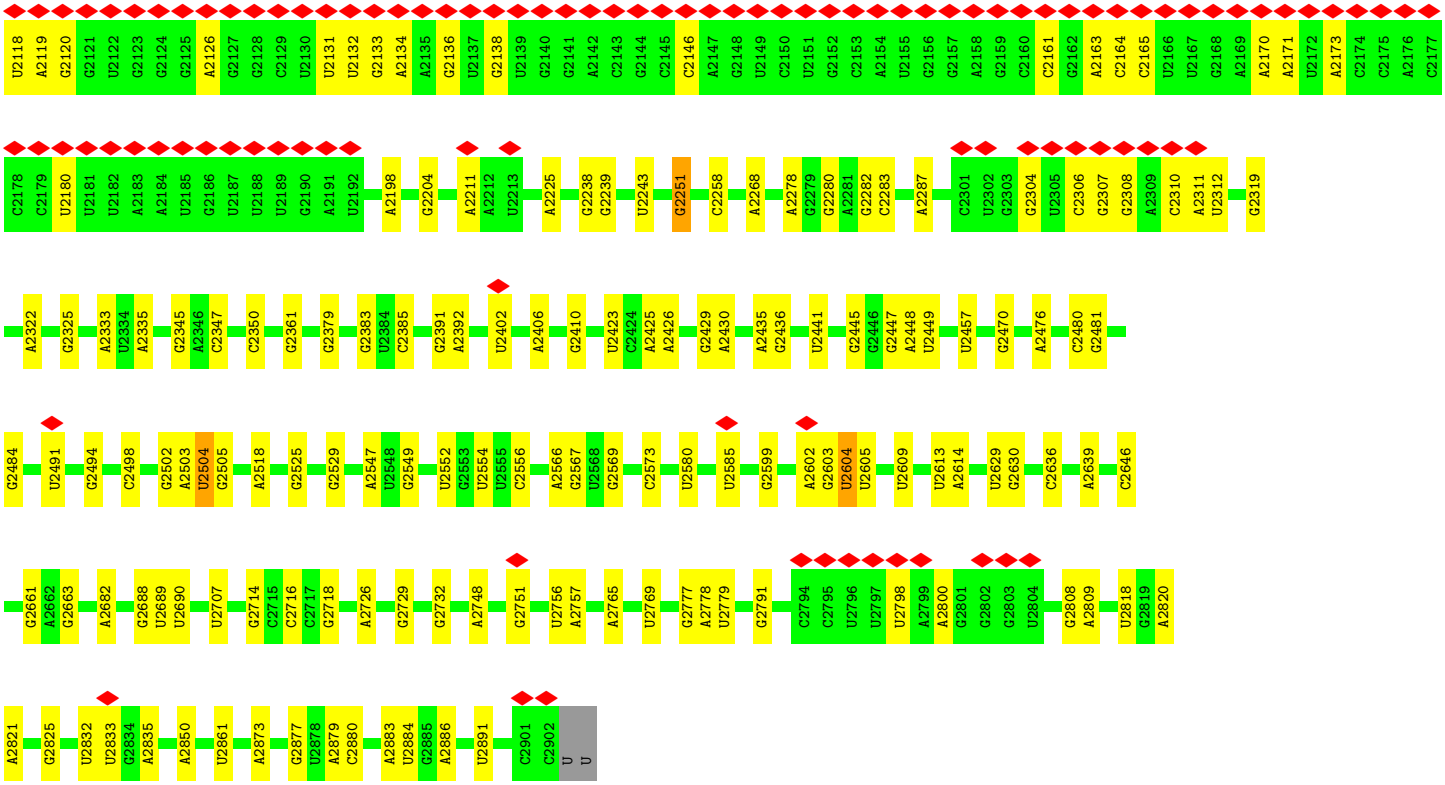
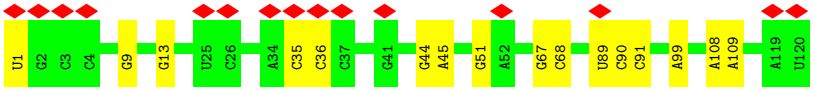
A996 U999 U1012 C1013 G1022 G1026 U1033 C1043 C1044 C1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A A1085 A1086 G1087 A1088
A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 U1130 G1131 U1132 A1133 A1134 C1135 G1136 A1142 U1148 A1156 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1187 G1238 A1244
A1247 G1248 U1249 A1253 G1256 A1262 G1266 G1271 A1272 A1275 A1286 C1289 G1300 A1301 C1306 C1320 A1321 U1329 G1332 C1345 U1352 G1360 A1365 G1368 G1374 A1378 U1379 A1383 C1386 A1392 A1395 U1396 U1397 G1407
U1411 U1412 A1413 C1414 U1415 G1416 C1417 A1420 C1428 C1437 C1451 G1452 A1453 U1458 G1459 U1460 G1475 U1476 A1477 G1478 G1479 G1482 G1483 U1484 C1488 C1493 A1494 U1497 A1503 A1504 A1505 U1506 C1507 A1508 A1509 U1523 G1524 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537
G1538 U1539 G1540 C1541 U1542 A1566 A1569 A1570 U1578 C1582 A1583 U1584 C1585 A1586 U1589 C1592 C1607 A1608 A1609 A1610 A1618 G1622 U1647 U1648 G1649 G1674 A1701 U1714 G1723 G1724 U1725 C1726 C1727 C1728 U1729 C1730 G1731 C1732 G1733 G1734 A1735 U1736 G1737 G1738 C1764
A1773 G1776 A1784 A1785 A1786 G1799 C1800 A1801 G1807 A1808 C1816 A1829 C1833 U1834 G1835 A1847 A1848 C1868 G1869 C1870 A1871 A1872 G1873 C1874 G1875 A1876 G1884 3TD1915 G1921 C1924 C1925 U1926 A1927 G1930 U1931 A1937 A1938 U1939 U1940 U1955 A1960 C1961
C1962 C1967 A1970 U1971 G1972 G1980 U1991 G1992 U1993 C1997 U2022 C2023 A2030 A2031 G2032 A2033 C2036 C2043 C2055 G2056 A2060 G2061 A2062 G2069 A2080 G2093 U2099 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117



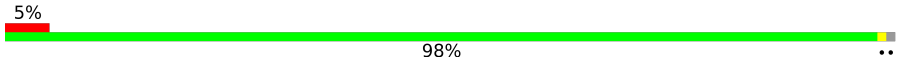
- Molecule 24: 5S rRNA

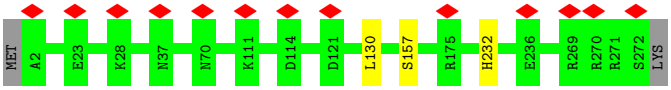
Chain 5:



- Molecule 25: 50S ribosomal protein L2

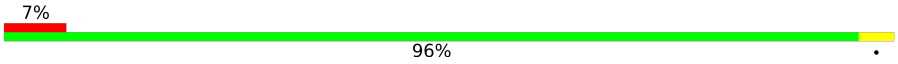
Chain LB:

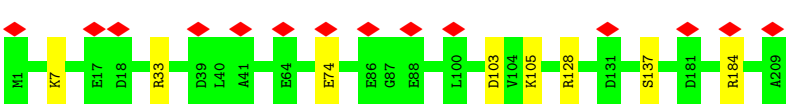




- Molecule 26: 50S ribosomal protein L3

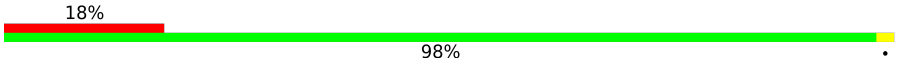
Chain LC:

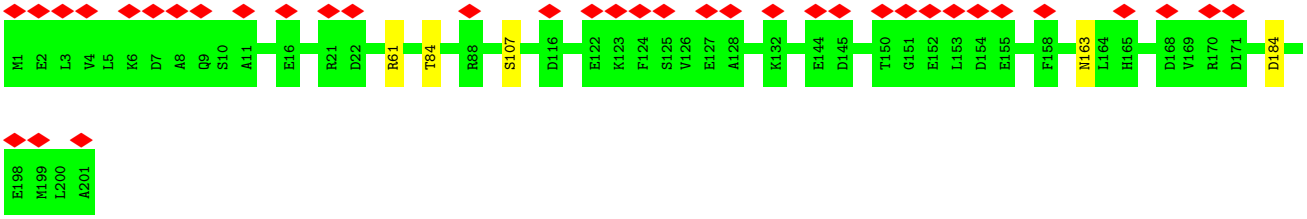




- Molecule 27: 50S ribosomal protein L4

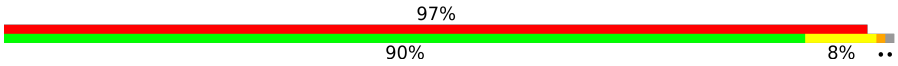
Chain LD:

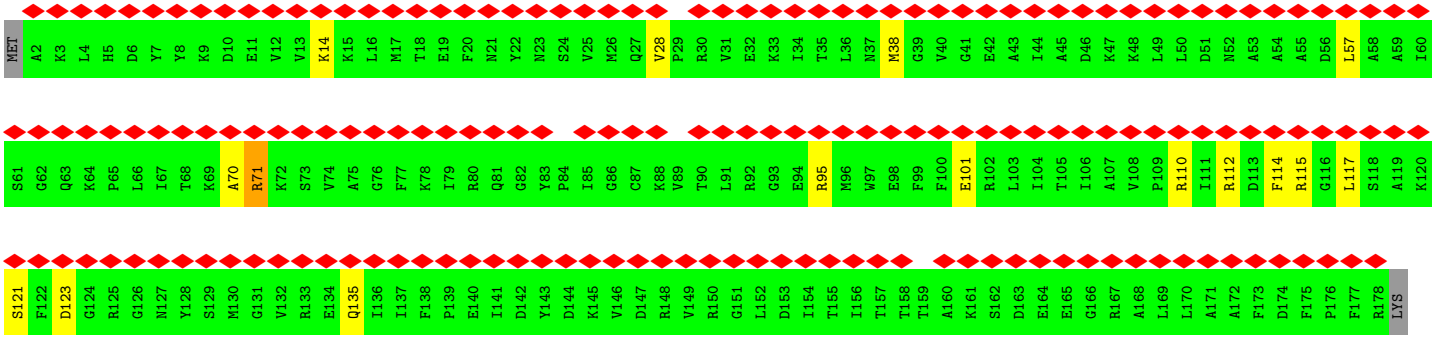




- Molecule 28: 50S ribosomal protein L5

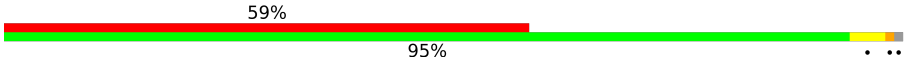
Chain LE:

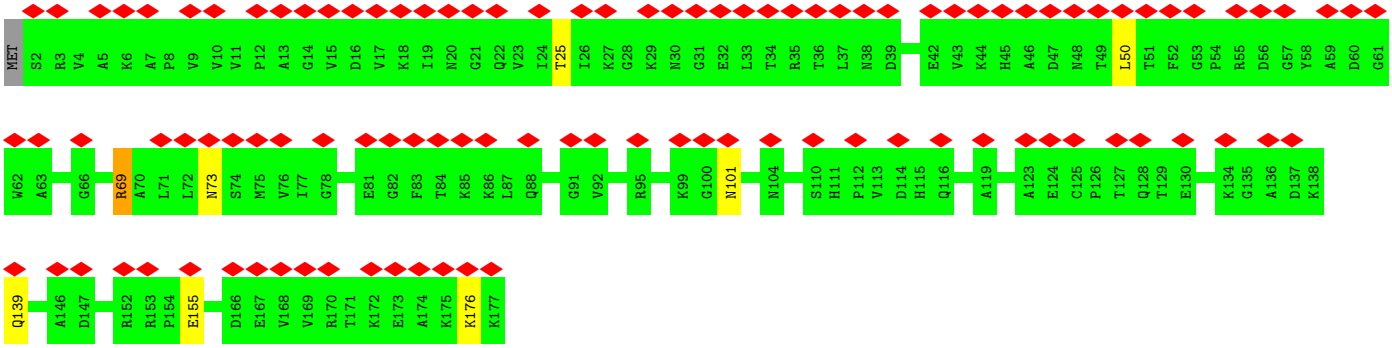




- Molecule 29: 50S ribosomal protein L6

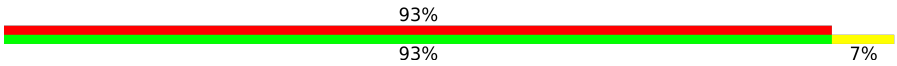
Chain LF:

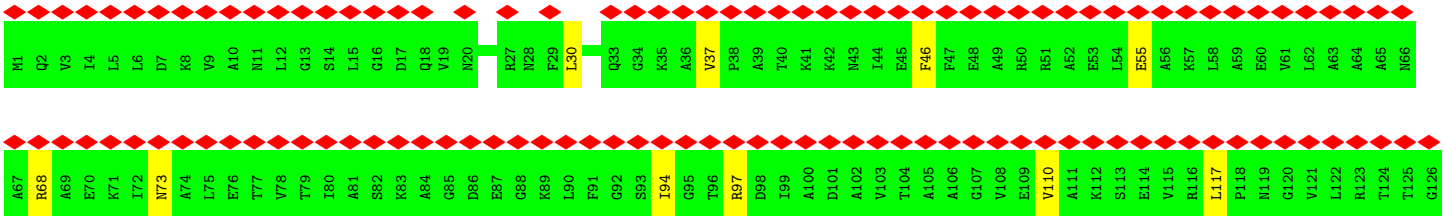


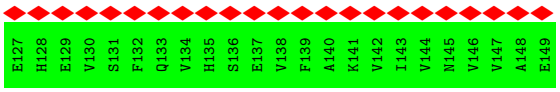


- Molecule 30: 50S ribosomal protein L9

Chain LI:

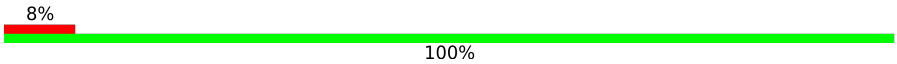


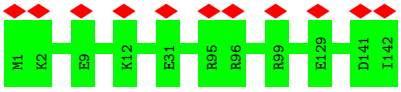




• Molecule 31: 50S ribosomal protein L13

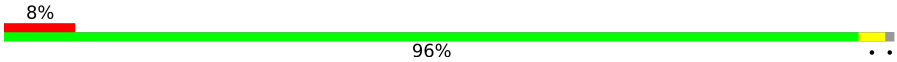
Chain LM:

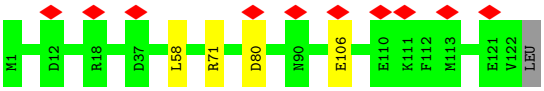




• Molecule 32: 50S ribosomal protein L14

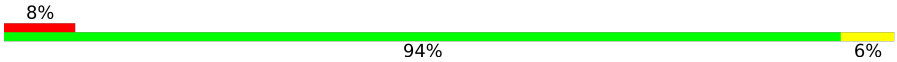
Chain LN:

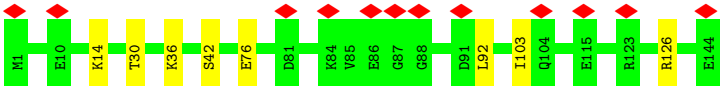




• Molecule 33: 50S ribosomal protein L15

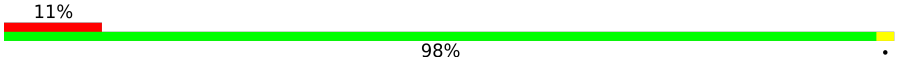
Chain LO:

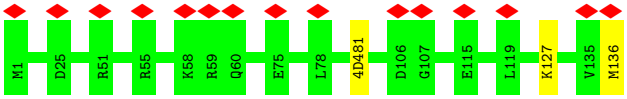




• Molecule 34: 50S ribosomal protein L16

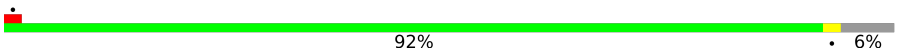
Chain LP:

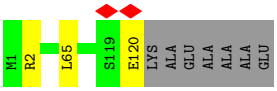




• Molecule 35: 50S ribosomal protein L17

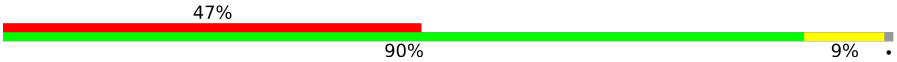
Chain LQ:

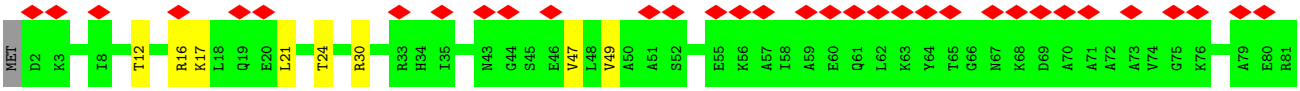


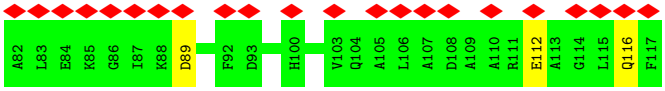


• Molecule 36: 50S ribosomal protein L18

Chain LR:

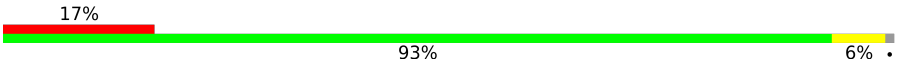


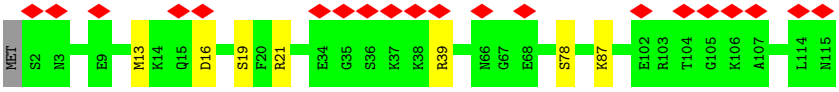




• Molecule 37: 50S ribosomal protein L19

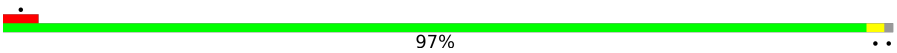
Chain LS:

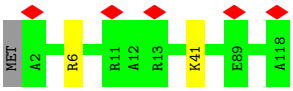




• Molecule 38: 50S ribosomal protein L20

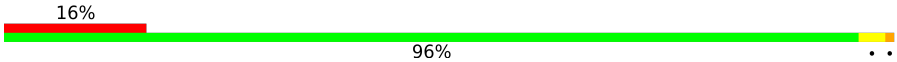
Chain LT:

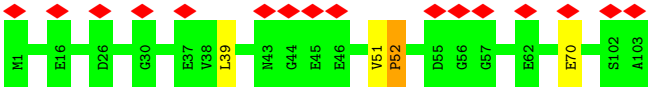




• Molecule 39: 50S ribosomal protein L21

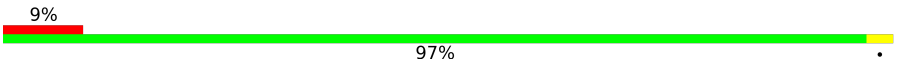
Chain LU:

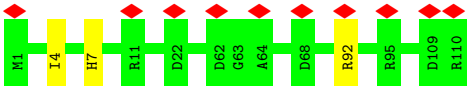




• Molecule 40: 50S ribosomal protein L22

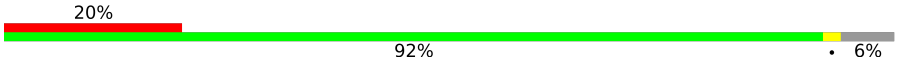
Chain LV:

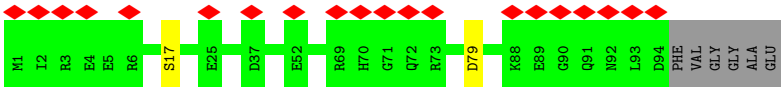




• Molecule 41: 50S ribosomal protein L23

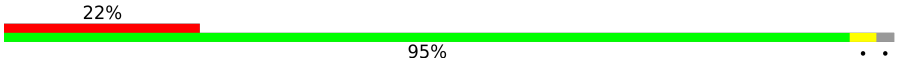
Chain LW:

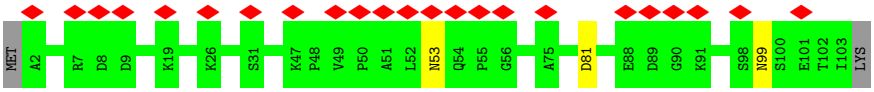




• Molecule 42: 50S ribosomal protein L24

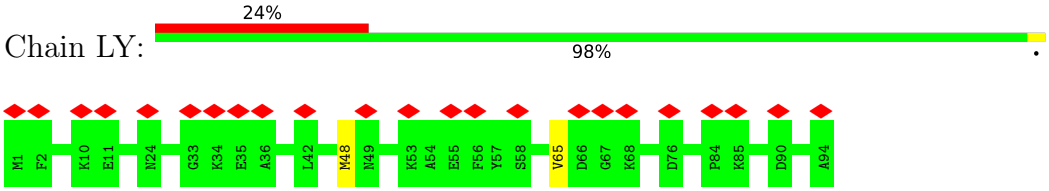
Chain LX:





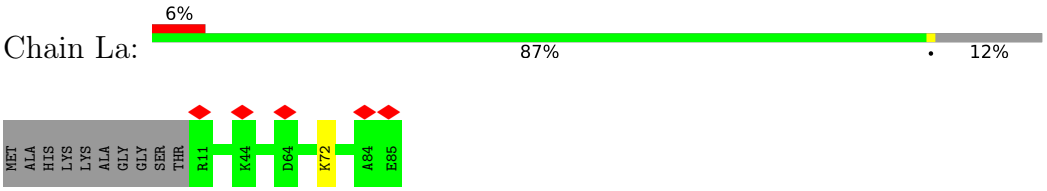
• Molecule 43: 50S ribosomal protein L25

Chain LY:



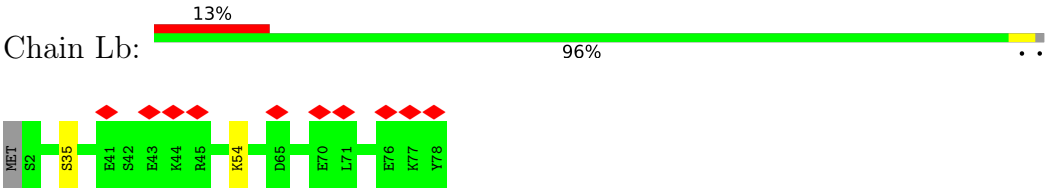
- Molecule 44: 50S ribosomal protein L27

Chain La:



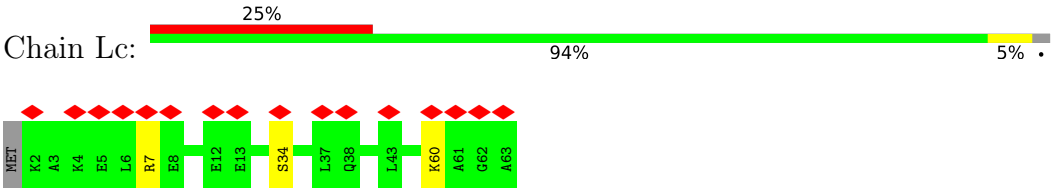
- Molecule 45: 50S ribosomal protein L28

Chain Lb:



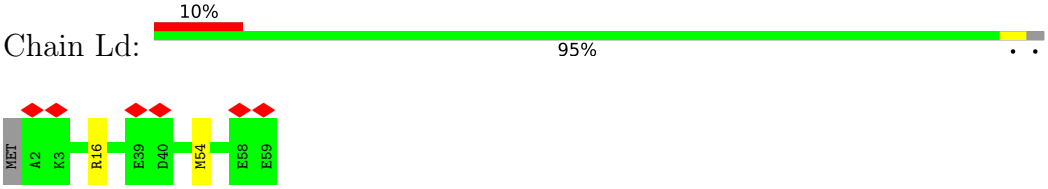
- Molecule 46: 50S ribosomal protein L29

Chain Lc:



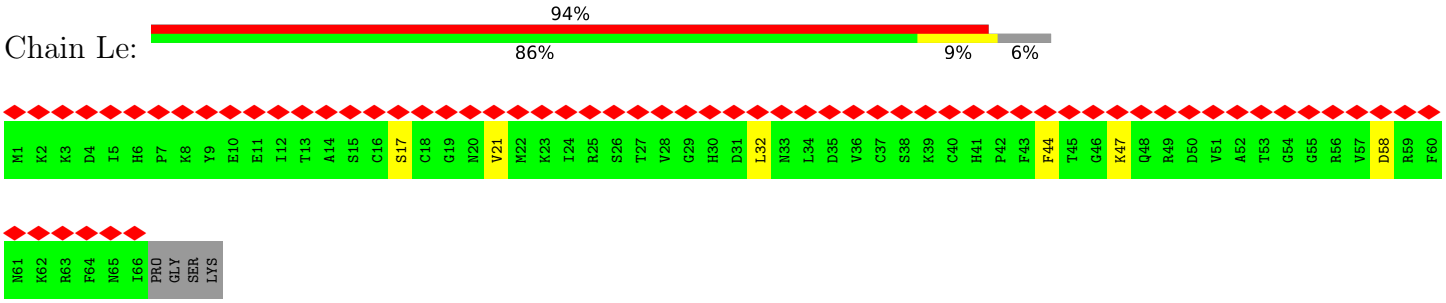
- Molecule 47: 50S ribosomal protein L30

Chain Ld:



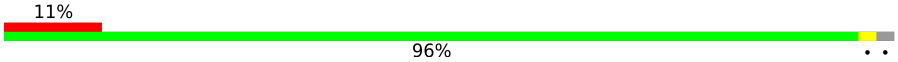
- Molecule 48: 50S ribosomal protein L31

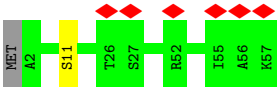
Chain Le:



- Molecule 49: 50S ribosomal protein L32

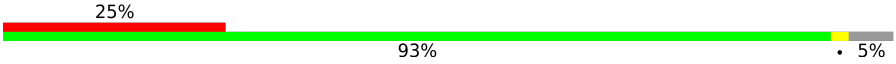
Chain Lf:

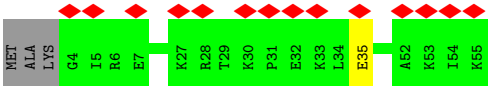




• Molecule 50: 50S ribosomal protein L33

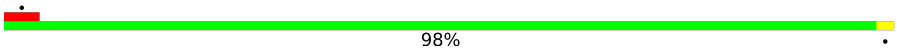
Chain Lg:

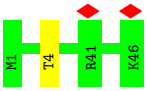




• Molecule 51: 50S ribosomal protein L34

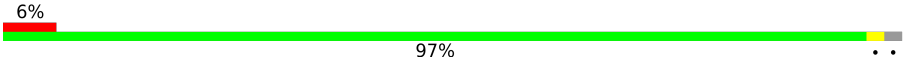
Chain Lh:

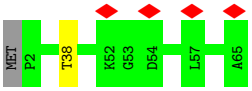




• Molecule 52: 50S ribosomal protein L35

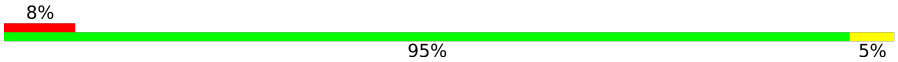
Chain Li:

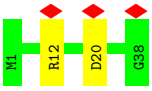




• Molecule 53: 50S ribosomal protein L36

Chain Lj:



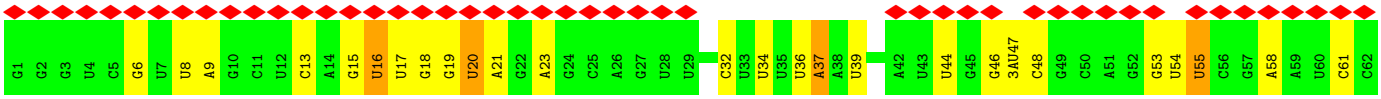


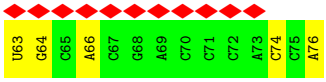
• Molecule 54: Nascent peptide

Chain Pp:

• Molecule 55: tRNA

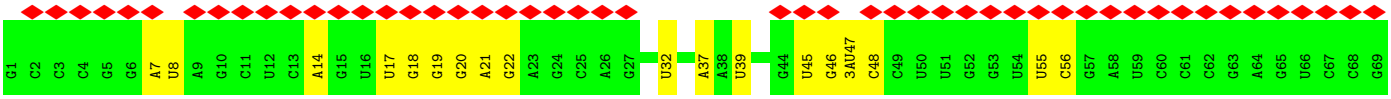
Chain Pt:





• Molecule 56: tRNA

Chain Dt:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	87	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0193	Depositor
Map size (Å)	610.55994, 610.55994, 610.55994	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: OMU, 5MU, 2MG, PUT, OMC, ZN, 5MC, PSU, 2MA, MA6, U8U, SPD, 4OC, UR3, 4D4, MG, 1MG, G7M, 3TD, 6MZ, H2U, T6A, MIA, D2T, ATP, OMG, 4SU, 3AU

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	16	0.52	0/36405	0.69	1/56786 (0.0%)
2	SB	0.43	0/1784	0.62	0/2403
3	SC	0.45	0/1685	0.62	0/2270
4	SD	0.45	0/1655	0.63	1/2216 (0.0%)
5	SE	0.48	0/1156	0.64	0/1556
6	SF	0.43	0/881	0.62	0/1189
7	SG	0.49	0/1195	0.64	0/1602
8	SH	0.45	0/983	0.63	0/1318
9	SI	0.42	0/1034	0.70	0/1375
10	SJ	0.48	0/805	0.70	0/1089
11	SK	0.47	0/893	0.65	0/1205
12	SL	0.44	0/954	0.67	0/1279
13	SM	0.48	0/892	0.71	0/1193
14	SN	0.43	0/817	0.58	0/1088
15	SO	0.45	0/721	0.61	0/964
16	SP	0.49	0/658	0.73	0/884
17	SQ	0.45	0/657	0.65	0/881
18	SR	0.45	0/553	0.63	1/742 (0.1%)
19	SS	0.45	0/672	0.65	0/904
20	ST	0.37	0/676	0.56	0/895
21	SU	0.46	0/598	0.68	0/792
22	mR	0.45	0/261	0.61	0/404
23	23	0.56	1/69236 (0.0%)	0.70	1/108005 (0.0%)
24	5	0.59	1/2873 (0.0%)	0.71	0/4478
25	LB	0.45	0/2121	0.69	1/2852 (0.0%)
26	LC	0.45	0/1586	0.65	0/2134
27	LD	0.40	0/1571	0.61	0/2113
28	LE	0.54	0/1434	0.69	0/1926
29	LF	0.45	0/1343	0.63	0/1816
30	LI	0.49	0/1122	0.63	0/1515
31	LM	0.44	0/1152	0.58	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LN	0.45	0/947	0.67	0/1268
33	LO	0.43	0/1062	0.70	1/1413 (0.1%)
34	LP	0.43	0/1081	0.64	0/1443
35	LQ	0.43	0/973	0.62	0/1301
36	LR	0.43	0/901	0.68	0/1209
37	LS	0.44	0/940	0.64	0/1256
38	LT	0.47	0/960	0.69	0/1278
39	LU	0.52	1/829 (0.1%)	0.98	3/1107 (0.3%)
40	LV	0.46	0/864	0.65	0/1156
41	LW	0.41	0/752	0.62	0/1005
42	LX	0.47	0/787	0.65	0/1051
43	LY	0.45	0/765	0.63	0/1025
44	La	0.39	0/582	0.63	0/769
45	Lb	0.49	0/634	0.73	0/848
46	Lc	0.39	0/502	0.59	0/667
47	Ld	0.41	0/453	0.61	0/605
48	Le	0.58	0/531	0.66	0/709
49	Lf	0.51	0/449	0.72	0/599
50	Lg	0.45	0/434	0.63	0/576
51	Lh	0.47	0/380	0.79	0/498
52	Li	0.44	0/513	0.66	0/676
53	Lj	0.43	0/303	0.65	0/397
54	Pp	0.56	0/28	1.13	0/34
55	Pt	0.34	0/1573	0.68	0/2445
56	Dt	0.40	0/1650	0.65	0/2568
All	All	0.52	3/157266 (0.0%)	0.69	9/235328 (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
8	SH	0	1
12	SL	0	1
13	SM	0	1
26	LC	0	1
28	LE	0	1
29	LF	0	1
46	Lc	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	1	U	OP3-P	-10.72	1.48	1.61
23	23	1	G	OP3-P	-10.30	1.48	1.61
39	LU	52	PRO	N-CD	-7.29	1.37	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	LU	51	VAL	C-N-CD	-23.12	69.73	120.60
23	23	1730	C	N1-C1'-C2'	6.15	122.00	114.00
33	LO	36	LYS	N-CA-C	5.80	126.66	111.00
39	LU	52	PRO	CA-N-CD	5.54	119.46	111.70
18	SR	25	ASP	CB-CG-OD1	5.24	123.02	118.30
1	16	1158	C	N1-C2-O2	5.08	121.95	118.90
25	LB	232	HIS	CB-CA-C	5.04	120.48	110.40
4	SD	50	ASP	CB-CG-OD1	5.04	122.83	118.30
39	LU	51	VAL	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	LC	128	ARG	Sidechain
28	LE	112	ARG	Sidechain
29	LF	69	ARG	Sidechain
46	Lc	7	ARG	Sidechain
8	SH	77	ARG	Sidechain
12	SL	94	ARG	Sidechain
13	SM	70	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SB	222/241 (92%)	208 (94%)	13 (6%)	1 (0%)	29	43
3	SC	210/233 (90%)	203 (97%)	7 (3%)	0	100	100
4	SD	202/206 (98%)	200 (99%)	2 (1%)	0	100	100
5	SE	153/167 (92%)	146 (95%)	7 (5%)	0	100	100
6	SF	104/135 (77%)	100 (96%)	4 (4%)	0	100	100
7	SG	149/179 (83%)	144 (97%)	5 (3%)	0	100	100
8	SH	126/130 (97%)	119 (94%)	7 (6%)	0	100	100
9	SI	125/130 (96%)	114 (91%)	10 (8%)	1 (1%)	19	29
10	SJ	97/103 (94%)	91 (94%)	5 (5%)	1 (1%)	15	23
11	SK	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	SL	119/124 (96%)	117 (98%)	2 (2%)	0	100	100
13	SM	112/118 (95%)	107 (96%)	4 (4%)	1 (1%)	17	26
14	SN	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	SO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	SP	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	SQ	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
18	SR	64/75 (85%)	64 (100%)	0	0	100	100
19	SS	80/92 (87%)	78 (98%)	2 (2%)	0	100	100
20	ST	84/87 (97%)	84 (100%)	0	0	100	100
21	SU	68/71 (96%)	68 (100%)	0	0	100	100
25	LB	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
26	LC	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
27	LD	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
28	LE	175/179 (98%)	167 (95%)	6 (3%)	2 (1%)	14	21
29	LF	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
30	LI	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
31	LM	140/142 (99%)	140 (100%)	0	0	100	100
32	LN	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
33	LO	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
34	LP	133/136 (98%)	131 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	LQ	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
36	LR	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
37	LS	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
38	LT	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
39	LU	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	15	23
40	LV	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	LW	92/100 (92%)	91 (99%)	1 (1%)	0	100	100
42	LX	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
43	LY	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
44	La	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
45	Lb	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
46	Lc	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
47	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	Le	64/70 (91%)	57 (89%)	6 (9%)	1 (2%)	9	14
49	Lf	54/57 (95%)	54 (100%)	0	0	100	100
50	Lg	50/55 (91%)	47 (94%)	3 (6%)	0	100	100
51	Lh	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	Li	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
53	Lj	36/38 (95%)	36 (100%)	0	0	100	100
54	Pp	1/3 (33%)	1 (100%)	0	0	100	100
All	All	5606/5916 (95%)	5404 (96%)	194 (4%)	8 (0%)	54	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	SB	131	LYS
10	SJ	57	VAL
39	LU	52	PRO
28	LE	70	ALA
48	Le	47	LYS
28	LE	71	ARG
9	SI	26	GLY
13	SM	4	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SB	186/199 (94%)	178 (96%)	8 (4%)	29	44
3	SC	172/190 (90%)	165 (96%)	7 (4%)	30	46
4	SD	171/173 (99%)	165 (96%)	6 (4%)	36	52
5	SE	118/126 (94%)	112 (95%)	6 (5%)	24	37
6	SF	92/116 (79%)	85 (92%)	7 (8%)	13	21
7	SG	124/147 (84%)	113 (91%)	11 (9%)	9	14
8	SH	103/105 (98%)	99 (96%)	4 (4%)	32	48
9	SI	105/107 (98%)	98 (93%)	7 (7%)	16	25
10	SJ	87/90 (97%)	82 (94%)	5 (6%)	20	31
11	SK	90/99 (91%)	86 (96%)	4 (4%)	28	43
12	SL	102/103 (99%)	99 (97%)	3 (3%)	42	60
13	SM	92/96 (96%)	85 (92%)	7 (8%)	13	21
14	SN	83/84 (99%)	80 (96%)	3 (4%)	35	51
15	SO	76/77 (99%)	74 (97%)	2 (3%)	46	64
16	SP	65/65 (100%)	63 (97%)	2 (3%)	40	57
17	SQ	74/78 (95%)	71 (96%)	3 (4%)	30	46
18	SR	57/65 (88%)	56 (98%)	1 (2%)	59	75
19	SS	71/79 (90%)	66 (93%)	5 (7%)	15	23
20	ST	65/66 (98%)	62 (95%)	3 (5%)	27	41
21	SU	60/61 (98%)	47 (78%)	13 (22%)	1	1
25	LB	216/218 (99%)	214 (99%)	2 (1%)	78	87
26	LC	164/164 (100%)	157 (96%)	7 (4%)	29	44
27	LD	165/165 (100%)	160 (97%)	5 (3%)	41	59
28	LE	148/150 (99%)	134 (90%)	14 (10%)	8	12
29	LF	137/138 (99%)	129 (94%)	8 (6%)	20	31
30	LI	114/114 (100%)	104 (91%)	10 (9%)	10	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	LM	116/116 (100%)	116 (100%)	0	100	100
32	LN	103/104 (99%)	99 (96%)	4 (4%)	32	48
33	LO	103/103 (100%)	96 (93%)	7 (7%)	16	24
34	LP	108/108 (100%)	106 (98%)	2 (2%)	57	74
35	LQ	100/103 (97%)	97 (97%)	3 (3%)	41	59
36	LR	86/87 (99%)	75 (87%)	11 (13%)	4	5
37	LS	100/100 (100%)	92 (92%)	8 (8%)	12	18
38	LT	89/90 (99%)	87 (98%)	2 (2%)	52	70
39	LU	84/84 (100%)	82 (98%)	2 (2%)	49	67
40	LV	93/93 (100%)	90 (97%)	3 (3%)	39	56
41	LW	81/84 (96%)	79 (98%)	2 (2%)	47	66
42	LX	83/85 (98%)	80 (96%)	3 (4%)	35	51
43	LY	78/78 (100%)	76 (97%)	2 (3%)	46	64
44	La	57/63 (90%)	56 (98%)	1 (2%)	59	75
45	Lb	67/68 (98%)	65 (97%)	2 (3%)	41	59
46	Lc	54/55 (98%)	52 (96%)	2 (4%)	34	50
47	Ld	48/49 (98%)	46 (96%)	2 (4%)	30	45
48	Le	59/62 (95%)	54 (92%)	5 (8%)	10	15
49	Lf	47/48 (98%)	46 (98%)	1 (2%)	53	72
50	Lg	47/49 (96%)	46 (98%)	1 (2%)	53	72
51	Lh	38/38 (100%)	37 (97%)	1 (3%)	46	64
52	Li	51/52 (98%)	50 (98%)	1 (2%)	55	73
53	Lj	34/34 (100%)	32 (94%)	2 (6%)	19	30
54	Pp	3/3 (100%)	3 (100%)	0	100	100
All	All	4666/4831 (97%)	4446 (95%)	220 (5%)	30	40

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	9	MET
2	SB	23	TRP
2	SB	50	PHE
2	SB	87	CYS
2	SB	120	GLN

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Mol	Chain	Res	Type
2	SB	147	SER
2	SB	192	ASP
2	SB	207	ILE
3	SC	29	PHE
3	SC	31	ASP
3	SC	43	LEU
3	SC	64	ILE
3	SC	88	ARG
3	SC	147	LYS
3	SC	190	HIS
4	SD	8	LYS
4	SD	83	LYS
4	SD	116	GLN
4	SD	146	ARG
4	SD	163	GLU
4	SD	179	GLU
5	SE	23	LYS
5	SE	32	SER
5	SE	76	LEU
5	SE	86	LYS
5	SE	94	VAL
5	SE	130	SER
6	SF	38	ARG
6	SF	55	HIS
6	SF	65	GLU
6	SF	68	GLN
6	SF	73	GLU
6	SF	91	ARG
6	SF	102	MET
7	SG	3	ARG
7	SG	7	ILE
7	SG	12	ILE
7	SG	17	LYS
7	SG	30	LEU
7	SG	31	MET
7	SG	87	VAL
7	SG	92	ARG
7	SG	118	LEU
7	SG	139	GLU
7	SG	146	GLU
8	SH	3	MET
8	SH	54	ASP

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Mol	Chain	Res	Type
8	SH	55	THR
8	SH	88	ARG
9	SI	57	MET
9	SI	63	LEU
9	SI	92	GLU
9	SI	116	VAL
9	SI	123	ARG
9	SI	128	SER
9	SI	130	ARG
10	SJ	5	ARG
10	SJ	7	ARG
10	SJ	24	GLU
10	SJ	89	ARG
10	SJ	101	SER
11	SK	18	ASP
11	SK	72	ASP
11	SK	94	GLU
11	SK	119	ASN
12	SL	76	GLU
12	SL	120	LYS
12	SL	123	LYS
13	SM	30	SER
13	SM	31	LYS
13	SM	42	ASP
13	SM	79	ARG
13	SM	97	VAL
13	SM	107	ARG
13	SM	113	ARG
14	SN	19	LYS
14	SN	47	LYS
14	SN	76	LYS
15	SO	83	GLU
15	SO	89	ARG
16	SP	1	MET
16	SP	42	ILE
17	SQ	28	PHE
17	SQ	62	ARG
17	SQ	65	ARG
18	SR	73	ARG
19	SS	20	GLU
19	SS	21	LYS
19	SS	44	MET

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Mol	Chain	Res	Type
19	SS	48	THR
19	SS	79	THR
20	ST	52	ASN
20	ST	55	GLN
20	ST	69	LYS
21	SU	2	PRO
21	SU	5	LYS
21	SU	22	SER
21	SU	24	GLU
21	SU	29	LEU
21	SU	49	LYS
21	SU	58	LYS
21	SU	59	LYS
21	SU	62	ARG
21	SU	66	ARG
21	SU	67	ARG
21	SU	69	ARG
21	SU	70	LEU
25	LB	130	LEU
25	LB	157	SER
26	LC	7	LYS
26	LC	33	ARG
26	LC	74	GLU
26	LC	103	ASP
26	LC	105	LYS
26	LC	137	SER
26	LC	184	ARG
27	LD	61	ARG
27	LD	84	THR
27	LD	107	SER
27	LD	163	ASN
27	LD	184	ASP
28	LE	14	LYS
28	LE	28	VAL
28	LE	38	MET
28	LE	57	LEU
28	LE	71	ARG
28	LE	95	ARG
28	LE	101	GLU
28	LE	110	ARG
28	LE	114	PHE
28	LE	115	ARG

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Mol	Chain	Res	Type
28	LE	117	LEU
28	LE	121	SER
28	LE	123	ASP
28	LE	135	GLN
29	LF	25	THR
29	LF	50	LEU
29	LF	69	ARG
29	LF	73	ASN
29	LF	101	ASN
29	LF	139	GLN
29	LF	155	GLU
29	LF	176	LYS
30	LI	30	LEU
30	LI	37	VAL
30	LI	46	PHE
30	LI	55	GLU
30	LI	68	ARG
30	LI	73	ASN
30	LI	94	ILE
30	LI	97	ARG
30	LI	110	VAL
30	LI	117	LEU
32	LN	58	LEU
32	LN	71	ARG
32	LN	80	ASP
32	LN	106	GLU
33	LO	14	LYS
33	LO	30	THR
33	LO	42	SER
33	LO	76	GLU
33	LO	92	LEU
33	LO	103	ILE
33	LO	126	ARG
34	LP	127	LYS
34	LP	136	MET
35	LQ	2	ARG
35	LQ	65	LEU
35	LQ	120	GLU
36	LR	12	THR
36	LR	16	ARG
36	LR	17	LYS
36	LR	21	LEU

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Mol	Chain	Res	Type
36	LR	24	THR
36	LR	30	ARG
36	LR	47	VAL
36	LR	49	VAL
36	LR	89	ASP
36	LR	112	GLU
36	LR	116	GLN
37	LS	13	MET
37	LS	16	ASP
37	LS	19	SER
37	LS	21	ARG
37	LS	39[A]	ARG
37	LS	39[B]	ARG
37	LS	78	SER
37	LS	87	LYS
38	LT	6	ARG
38	LT	41	LYS
39	LU	39	LEU
39	LU	70	GLU
40	LV	4	ILE
40	LV	7	HIS
40	LV	92	ARG
41	LW	17	SER
41	LW	79	ASP
42	LX	53	ASN
42	LX	81	ASP
42	LX	99	ASN
43	LY	48	MET
43	LY	65	VAL
44	La	72	LYS
45	Lb	35	SER
45	Lb	54	LYS
46	Lc	34	SER
46	Lc	60	LYS
47	Ld	16	ARG
47	Ld	54	MET
48	Le	17	SER
48	Le	21	VAL
48	Le	32	LEU
48	Le	44	PHE
48	Le	58	ASP
49	Lf	11	SER

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Mol	Chain	Res	Type
50	Lg	35	GLU
51	Lh	4	THR
52	Li	38	THR
53	Lj	12	ARG
53	Lj	20	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	177	ASN
3	SC	176	HIS
5	SE	78	ASN
5	SE	82	GLN
6	SF	14	GLN
6	SF	46	GLN
6	SF	68	GLN
10	SJ	58	ASN
11	SK	119	ASN
14	SN	66	GLN
16	SP	63	GLN
16	SP	79	ASN
19	SS	57	HIS
20	ST	55	GLN
26	LC	49	GLN
26	LC	150	GLN
27	LD	163	ASN
28	LE	37	ASN
29	LF	30	ASN
29	LF	101	ASN
29	LF	116	GLN
30	LI	11	ASN
30	LI	66	ASN
30	LI	133	GLN
36	LR	38	GLN
36	LR	116	GLN
38	LT	52	GLN
39	LU	86	GLN
41	LW	91	GLN
43	LY	24	ASN
48	Le	33	ASN
50	Lg	45	GLN
52	Li	31	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1521/1534 (99%)	252 (16%)	20 (1%)
22	mR	10/60 (16%)	0	0
23	23	2895/2904 (99%)	511 (17%)	41 (1%)
24	5	119/120 (99%)	15 (12%)	1 (0%)
55	Pt	73/76 (96%)	25 (34%)	0
56	Dt	73/76 (96%)	12 (16%)	0
All	All	4691/4770 (98%)	815 (17%)	62 (1%)

All (815) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	5	U
1	16	6	G
1	16	7	A
1	16	9	G
1	16	15	G
1	16	17	U
1	16	22	G
1	16	32	A
1	16	39	G
1	16	44	A
1	16	48	C
1	16	50	A
1	16	51	A
1	16	52	C
1	16	58	C
1	16	69	G
1	16	71	A
1	16	72	A
1	16	78	A
1	16	79	G
1	16	80	A
1	16	90	C
1	16	91	U
1	16	92	U
1	16	95	C
1	16	97	G
1	16	108	G
1	16	116	A
1	16	120	A
1	16	130	A

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Mol	Chain	Res	Type
1	16	131	A
1	16	138	G
1	16	141	G
1	16	143	A
1	16	144	G
1	16	149	A
1	16	163	C
1	16	164	G
1	16	167	A
1	16	173	U
1	16	182	A
1	16	183	C
1	16	191	G
1	16	197	A
1	16	204	G
1	16	205	A
1	16	210	C
1	16	212	G
1	16	226	G
1	16	240	G
1	16	245	U
1	16	247	G
1	16	250	A
1	16	251	G
1	16	266	G
1	16	267	C
1	16	280	C
1	16	281	G
1	16	289	G
1	16	316	C
1	16	321	A
1	16	328	C
1	16	329	A
1	16	332	G
1	16	345	C
1	16	348	G
1	16	352	C
1	16	354	G
1	16	365	U
1	16	367	U
1	16	372	C
1	16	382	A

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Mol	Chain	Res	Type
1	16	384	G
1	16	392	C
1	16	406	G
1	16	412	A
1	16	413	G
1	16	421	U
1	16	423	G
1	16	429	U
1	16	435	A
1	16	439	U
1	16	457	G
1	16	463	U
1	16	467	U
1	16	468	A
1	16	479	U
1	16	481	G
1	16	482	A
1	16	483	C
1	16	486	U
1	16	495	A
1	16	496	A
1	16	509	A
1	16	511	C
1	16	516	PSU
1	16	518	C
1	16	521	G
1	16	527	G7M
1	16	531	U
1	16	533	A
1	16	547	A
1	16	559	A
1	16	562	U
1	16	572	A
1	16	573	A
1	16	576	C
1	16	579	A
1	16	596	A
1	16	633	G
1	16	653	U
1	16	665	A
1	16	687	A
1	16	703	G

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Mol	Chain	Res	Type
1	16	721	G
1	16	723	U
1	16	724	G
1	16	734	G
1	16	748	G
1	16	753	A
1	16	755	G
1	16	777	A
1	16	790	A
1	16	792	A
1	16	793	U
1	16	794	A
1	16	810	C
1	16	814	A
1	16	815	A
1	16	817	C
1	16	821	G
1	16	828	U
1	16	832	G
1	16	836	G
1	16	841	C
1	16	842	U
1	16	843	U
1	16	845	A
1	16	846	G
1	16	870	U
1	16	876	C
1	16	902	G
1	16	914	A
1	16	919	A
1	16	927	G
1	16	934	C
1	16	935	A
1	16	958	A
1	16	960	U
1	16	969	A
1	16	975	A
1	16	976	G
1	16	977	A
1	16	992	U
1	16	993	G
1	16	999	C

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Mol	Chain	Res	Type
1	16	1000	A
1	16	1003	G
1	16	1004	A
1	16	1005	A
1	16	1017	U
1	16	1018	G
1	16	1019	A
1	16	1020	G
1	16	1021	A
1	16	1025	U
1	16	1026	G
1	16	1028	C
1	16	1030	U
1	16	1031	C
1	16	1033	G
1	16	1036	A
1	16	1043	G
1	16	1045	C
1	16	1065	U
1	16	1085	U
1	16	1086	U
1	16	1094	G
1	16	1095	U
1	16	1101	A
1	16	1123	U
1	16	1124	G
1	16	1125	U
1	16	1129	C
1	16	1130	A
1	16	1133	G
1	16	1136	C
1	16	1137	C
1	16	1139	G
1	16	1140	C
1	16	1141	C
1	16	1142	G
1	16	1145	A
1	16	1158	C
1	16	1159	U
1	16	1167	A
1	16	1168	U
1	16	1184	G

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Mol	Chain	Res	Type
1	16	1196	A
1	16	1197	A
1	16	1199	U
1	16	1212	U
1	16	1227	A
1	16	1228	C
1	16	1238	A
1	16	1239	A
1	16	1240	U
1	16	1256	A
1	16	1257	A
1	16	1260	G
1	16	1279	G
1	16	1280	A
1	16	1286	U
1	16	1287	A
1	16	1289	A
1	16	1300	G
1	16	1302	C
1	16	1312	G
1	16	1320	C
1	16	1338	G
1	16	1340	A
1	16	1346	A
1	16	1353	G
1	16	1357	A
1	16	1363	A
1	16	1370	G
1	16	1379	G
1	16	1380	U
1	16	1395	C
1	16	1396	A
1	16	1397	C
1	16	1398	A
1	16	1399	C
1	16	1429	A
1	16	1432	G
1	16	1433	A
1	16	1441	A
1	16	1442	G
1	16	1446	A
1	16	1452	C

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Mol	Chain	Res	Type
1	16	1453	G
1	16	1492	A
1	16	1493	A
1	16	1497	G
1	16	1499	A
1	16	1503	A
1	16	1505	G
1	16	1506	U
1	16	1517	G
1	16	1529	G
1	16	1530	G
1	16	1534	A
23	23	10	A
23	23	27	G
23	23	34	U
23	23	36	G
23	23	39	G
23	23	40	U
23	23	42	A
23	23	45	G
23	23	46	G
23	23	51	G
23	23	55	G
23	23	58	G
23	23	71	A
23	23	74	A
23	23	75	G
23	23	80	G
23	23	88	G
23	23	96	C
23	23	101	A
23	23	102	U
23	23	103	A
23	23	110	G
23	23	118	A
23	23	119	A
23	23	120	U
23	23	125	A
23	23	139	U
23	23	140	C
23	23	141	G
23	23	158	U

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Mol	Chain	Res	Type
23	23	163	C
23	23	165	A
23	23	178	G
23	23	181	A
23	23	190	A
23	23	196	A
23	23	199	A
23	23	200	U
23	23	215	G
23	23	216	A
23	23	221	A
23	23	222	A
23	23	224	U
23	23	225	C
23	23	230	G
23	23	239	C
23	23	248	G
23	23	259	G
23	23	264	C
23	23	265	A
23	23	266	G
23	23	271	G
23	23	272	A
23	23	278	A
23	23	311	A
23	23	330	A
23	23	338	G
23	23	343	C
23	23	345	A
23	23	346	A
23	23	350	G
23	23	361	G
23	23	371	A
23	23	372	G
23	23	385	C
23	23	386	G
23	23	387	U
23	23	388	G
23	23	399	U
23	23	401	A
23	23	405	U
23	23	412	A

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Mol	Chain	Res	Type
23	23	451	U
23	23	455	C
23	23	456	C
23	23	457	A
23	23	459	U
23	23	473	G
23	23	481	G
23	23	489	G
23	23	491	G
23	23	496	G
23	23	501	A
23	23	503	A
23	23	504	A
23	23	505	A
23	23	506	G
23	23	508	A
23	23	509	C
23	23	518	G
23	23	527	C
23	23	530	G
23	23	532	A
23	23	533	G
23	23	538	A
23	23	546	U
23	23	547	A
23	23	548	G
23	23	549	G
23	23	556	A
23	23	563	A
23	23	573	U
23	23	575	A
23	23	603	A
23	23	614	A
23	23	615	U
23	23	616	A
23	23	622	G
23	23	637	A
23	23	638	G
23	23	645	C
23	23	646	U
23	23	647	G
23	23	653	U

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Mol	Chain	Res	Type
23	23	654	A
23	23	659	G
23	23	668	A
23	23	677	A
23	23	682	G
23	23	686	U
23	23	726	G
23	23	729	G
23	23	730	A
23	23	740	C
23	23	747	5MU
23	23	757	G
23	23	764	A
23	23	765	C
23	23	775	G
23	23	776	G
23	23	782	A
23	23	784	G
23	23	785	G
23	23	789	A
23	23	792	A
23	23	805	G
23	23	812	C
23	23	819	A
23	23	827	U
23	23	828	U
23	23	846	U
23	23	847	U
23	23	859	G
23	23	860	U
23	23	877	A
23	23	878	A
23	23	879	G
23	23	883	G
23	23	884	U
23	23	886	A
23	23	887	U
23	23	888	C
23	23	889	C
23	23	893	C
23	23	895	U
23	23	896	A

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Mol	Chain	Res	Type
23	23	897	C
23	23	900	A
23	23	901	C
23	23	903	C
23	23	910	A
23	23	914	G
23	23	915	C
23	23	917	A
23	23	931	U
23	23	932	U
23	23	941	A
23	23	946	C
23	23	961	C
23	23	962	G
23	23	973	A
23	23	974	G
23	23	983	A
23	23	989	G
23	23	996	A
23	23	999	U
23	23	1012	U
23	23	1013	C
23	23	1022	G
23	23	1026	G
23	23	1033	U
23	23	1046	A
23	23	1047	G
23	23	1057	A
23	23	1060	U
23	23	1061	U
23	23	1062	G
23	23	1065	U
23	23	1069	A
23	23	1070	A
23	23	1071	G
23	23	1072	C
23	23	1073	A
23	23	1074	G
23	23	1075	C
23	23	1076	C
23	23	1077	A
23	23	1079	C

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Mol	Chain	Res	Type
23	23	1080	A
23	23	1083	U
23	23	1086	A
23	23	1088	A
23	23	1089	A
23	23	1090	A
23	23	1091	G
23	23	1095	A
23	23	1096	A
23	23	1106	G
23	23	1110	G
23	23	1111	A
23	23	1112	G
23	23	1114	C
23	23	1115	G
23	23	1130	U
23	23	1132	U
23	23	1133	A
23	23	1134	A
23	23	1135	C
23	23	1136	G
23	23	1142	A
23	23	1148	U
23	23	1156	A
23	23	1173	U
23	23	1175	A
23	23	1178	C
23	23	1179	G
23	23	1187	G
23	23	1238	G
23	23	1244	A
23	23	1247	A
23	23	1249	U
23	23	1253	A
23	23	1256	G
23	23	1262	A
23	23	1266	G
23	23	1271	G
23	23	1272	A
23	23	1275	A
23	23	1289	C
23	23	1300	G

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Mol	Chain	Res	Type
23	23	1301	A
23	23	1306	C
23	23	1320	C
23	23	1321	A
23	23	1329	U
23	23	1332	G
23	23	1345	C
23	23	1352	U
23	23	1360	G
23	23	1365	A
23	23	1368	G
23	23	1374	G
23	23	1378	A
23	23	1379	U
23	23	1383	A
23	23	1386	C
23	23	1392	A
23	23	1395	A
23	23	1396	U
23	23	1397	U
23	23	1407	G
23	23	1416	G
23	23	1417	C
23	23	1420	A
23	23	1428	C
23	23	1437	C
23	23	1451	C
23	23	1452	G
23	23	1453	A
23	23	1458	U
23	23	1460	U
23	23	1475	G
23	23	1476	U
23	23	1478	G
23	23	1479	G
23	23	1482	G
23	23	1493	C
23	23	1494	A
23	23	1497	U
23	23	1503	A
23	23	1507	C
23	23	1508	A

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Mol	Chain	Res	Type
23	23	1509	A
23	23	1524	G
23	23	1529	G
23	23	1535	A
23	23	1536	C
23	23	1537	G
23	23	1538	G
23	23	1566	A
23	23	1569	A
23	23	1570	A
23	23	1578	U
23	23	1584	U
23	23	1585	C
23	23	1607	C
23	23	1608	A
23	23	1610	A
23	23	1622	G
23	23	1647	U
23	23	1648	U
23	23	1649	G
23	23	1674	G
23	23	1701	A
23	23	1725	U
23	23	1727	C
23	23	1729	U
23	23	1730	C
23	23	1733	G
23	23	1738	G
23	23	1764	C
23	23	1773	A
23	23	1776	G
23	23	1784	A
23	23	1786	A
23	23	1799	G
23	23	1800	C
23	23	1801	A
23	23	1807	G
23	23	1808	A
23	23	1816	C
23	23	1829	A
23	23	1833	C
23	23	1872	A

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Mol	Chain	Res	Type
23	23	1873	G
23	23	1875	G
23	23	1876	A
23	23	1884	G
23	23	1921	G
23	23	1926	U
23	23	1927	A
23	23	1930	G
23	23	1931	U
23	23	1937	A
23	23	1938	A
23	23	1940	U
23	23	1955	U
23	23	1960	A
23	23	1967	C
23	23	1970	A
23	23	1971	U
23	23	1972	G
23	23	1980	G
23	23	1991	U
23	23	1992	G
23	23	1993	U
23	23	1997	C
23	23	2022	U
23	23	2023	C
23	23	2032	G
23	23	2033	A
23	23	2036	C
23	23	2043	C
23	23	2055	C
23	23	2056	G
23	23	2060	A
23	23	2061	G
23	23	2062	A
23	23	2069	G7M
23	23	2080	A
23	23	2093	G
23	23	2103	C
23	23	2104	C
23	23	2110	G
23	23	2111	U
23	23	2112	G

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Mol	Chain	Res	Type
23	23	2113	U
23	23	2116	G
23	23	2118	U
23	23	2119	A
23	23	2120	G
23	23	2126	A
23	23	2131	U
23	23	2132	U
23	23	2133	G
23	23	2134	A
23	23	2136	G
23	23	2138	G
23	23	2146	C
23	23	2161	C
23	23	2163	A
23	23	2164	C
23	23	2165	C
23	23	2170	A
23	23	2171	A
23	23	2173	A
23	23	2180	U
23	23	2198	A
23	23	2204	G
23	23	2211	A
23	23	2225	A
23	23	2238	G
23	23	2239	G
23	23	2243	U
23	23	2251	OMG
23	23	2258	C
23	23	2268	A
23	23	2278	A
23	23	2280	G
23	23	2283	C
23	23	2287	A
23	23	2304	G
23	23	2306	C
23	23	2307	G
23	23	2308	G
23	23	2310	C
23	23	2311	A
23	23	2312	U

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Mol	Chain	Res	Type
23	23	2319	G
23	23	2322	A
23	23	2325	G
23	23	2333	A
23	23	2335	A
23	23	2345	G
23	23	2347	C
23	23	2350	C
23	23	2361	G
23	23	2379	G
23	23	2383	G
23	23	2385	C
23	23	2391	G
23	23	2392	A
23	23	2402	U
23	23	2406	A
23	23	2410	G
23	23	2423	U
23	23	2425	A
23	23	2426	A
23	23	2429	G
23	23	2430	A
23	23	2435	A
23	23	2436	G
23	23	2441	U
23	23	2448	A
23	23	2470	G
23	23	2476	A
23	23	2480	C
23	23	2481	G
23	23	2484	G
23	23	2491	U
23	23	2494	G
23	23	2502	G
23	23	2504	PSU
23	23	2505	G
23	23	2518	A
23	23	2525	G
23	23	2529	G
23	23	2547	A
23	23	2549	G
23	23	2554	U

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Mol	Chain	Res	Type
23	23	2556	C
23	23	2566	A
23	23	2567	G
23	23	2569	G
23	23	2573	C
23	23	2585	U
23	23	2599	G
23	23	2602	A
23	23	2603	G
23	23	2604	PSU
23	23	2609	U
23	23	2613	U
23	23	2614	A
23	23	2629	U
23	23	2630	G
23	23	2636	C
23	23	2639	A
23	23	2646	C
23	23	2661	G
23	23	2663	G
23	23	2682	A
23	23	2688	G
23	23	2689	U
23	23	2690	U
23	23	2707	U
23	23	2714	G
23	23	2716	C
23	23	2718	G
23	23	2726	A
23	23	2729	G
23	23	2732	G
23	23	2748	A
23	23	2751	G
23	23	2757	A
23	23	2765	A
23	23	2769	U
23	23	2777	G
23	23	2778	A
23	23	2779	U
23	23	2791	G
23	23	2798	U
23	23	2800	A

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Mol	Chain	Res	Type
23	23	2808	G
23	23	2809	A
23	23	2818	U
23	23	2820	A
23	23	2821	A
23	23	2825	G
23	23	2832	U
23	23	2833	U
23	23	2835	A
23	23	2850	A
23	23	2861	U
23	23	2873	A
23	23	2877	G
23	23	2879	A
23	23	2880	C
23	23	2883	A
23	23	2884	U
23	23	2886	A
23	23	2891	U
24	5	9	G
24	5	13	G
24	5	35	C
24	5	36	C
24	5	44	G
24	5	45	A
24	5	51	G
24	5	67	G
24	5	68	C
24	5	89	U
24	5	90	C
24	5	91	C
24	5	99	A
24	5	108	A
24	5	109	A
55	Pt	6	G
55	Pt	8	U
55	Pt	9	A
55	Pt	13	C
55	Pt	15	G
55	Pt	16	H2U
55	Pt	18	G
55	Pt	19	G

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Mol	Chain	Res	Type
55	Pt	20	H2U
55	Pt	21	A
55	Pt	23	A
55	Pt	32	C
55	Pt	36	U
55	Pt	37	T6A
55	Pt	44	U
55	Pt	48	C
55	Pt	53	G
55	Pt	55	PSU
55	Pt	58	A
55	Pt	61	C
55	Pt	63	U
55	Pt	64	G
55	Pt	66	A
55	Pt	74	C
55	Pt	76	A
56	Dt	7	A
56	Dt	14	A
56	Dt	17	U
56	Dt	18	G
56	Dt	19	G
56	Dt	20	G
56	Dt	21	A
56	Dt	22	G
56	Dt	45	U
56	Dt	48	C
56	Dt	56	C
56	Dt	76	A

All (62) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16	181	A
1	16	251	G
1	16	329	A
1	16	413	G
1	16	428	G
1	16	438	U
1	16	530	G
1	16	1024	G
1	16	1124	G

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Mol	Chain	Res	Type
1	16	1129	C
1	16	1137	C
1	16	1145	A
1	16	1183	U
1	16	1225	A
1	16	1239	A
1	16	1346	A
1	16	1432	G
1	16	1452	C
1	16	1492	A
1	16	1505	G
23	23	140	C
23	23	196	A
23	23	199	A
23	23	221	A
23	23	249	C
23	23	277	G
23	23	278	A
23	23	345	A
23	23	369	U
23	23	387	U
23	23	404	A
23	23	479	A
23	23	503	A
23	23	504	A
23	23	555	G
23	23	620	G
23	23	784	G
23	23	895	U
23	23	1060	U
23	23	1069	A
23	23	1070	A
23	23	1079	C
23	23	1110	G
23	23	1178	C
23	23	1286	A
23	23	1416	G
23	23	1451	C
23	23	1535	A
23	23	1584	U
23	23	1647	U
23	23	2111	U

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Mol	Chain	Res	Type
23	23	2119	A
23	23	2282	G
23	23	2308	G
23	23	2311	A
23	23	2430	A
23	23	2447	G
23	23	2481	G
23	23	2756	U
23	23	2779	U
23	23	2820	A
24	5	108	A

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

52 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
34	4D4	LP	81	34	9,11,12	2.05	2 (22%)	8,13,15	2.14	4 (50%)
55	PSU	Pt	39	55	18,21,22	1.52	4 (22%)	22,30,33	1.88	3 (13%)
23	5MU	23	1939	23,58	19,22,23	1.48	4 (21%)	28,32,35	2.30	6 (21%)
23	PSU	23	2605	23	18,21,22	1.60	5 (27%)	22,30,33	1.93	4 (18%)
55	H2U	Pt	17	55	18,21,22	1.07	2 (11%)	21,30,33	1.90	2 (9%)
1	5MC	16	967	1	18,22,23	0.96	2 (11%)	26,32,35	1.15	2 (7%)
1	5MC	16	1407	1	18,22,23	0.96	2 (11%)	26,32,35	1.32	3 (11%)
56	MIA	Dt	37	56	24,31,32	2.35	3 (12%)	26,44,47	2.58	10 (38%)
23	PSU	23	2580	23	18,21,22	1.72	6 (33%)	22,30,33	2.13	6 (27%)
55	H2U	Pt	20	55	18,21,22	1.11	2 (11%)	21,30,33	2.77	2 (9%)
1	4OC	16	1402	1	20,23,24	0.81	0	26,32,35	1.15	2 (7%)
23	PSU	23	2457	23	18,21,22	1.63	4 (22%)	22,30,33	2.14	5 (22%)
23	3TD	23	1915	23	18,22,23	1.28	2 (11%)	22,32,35	1.94	3 (13%)
23	G7M	23	2069	23	20,26,27	2.47	5 (25%)	17,39,42	1.15	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
55	5MU	Pt	54	55	19,22,23	1.43	5 (26%)	28,32,35	1.96	5 (17%)
23	1MG	23	745	23	18,26,27	0.79	0	19,39,42	1.49	3 (15%)
55	U8U	Pt	34	55,22	19,24,25	1.80	3 (15%)	23,34,37	1.34	4 (17%)
55	G7M	Pt	46	55	20,26,27	2.62	4 (20%)	17,39,42	1.05	1 (5%)
23	H2U	23	2449	23	18,21,22	1.27	3 (16%)	21,30,33	1.55	3 (14%)
23	OMC	23	2498	23,58	19,22,23	0.90	0	26,31,34	0.96	1 (3%)
1	PSU	16	516	58,1	18,21,22	1.54	5 (27%)	22,30,33	2.11	4 (18%)
1	MA6	16	1518	1	19,26,27	1.11	2 (10%)	18,38,41	1.43	2 (11%)
23	PSU	23	955	23	18,21,22	1.54	5 (27%)	22,30,33	2.08	5 (22%)
12	D2T	SL	89	12	7,9,10	1.36	1 (14%)	6,11,13	1.62	3 (50%)
56	4SU	Dt	8	56	18,21,22	1.84	5 (27%)	26,30,33	2.14	5 (19%)
56	3AU	Dt	47	56	24,28,29	1.06	1 (4%)	33,40,43	1.48	5 (15%)
55	T6A	Pt	37	55	27,34,35	1.09	1 (3%)	29,49,52	2.15	6 (20%)
56	G7M	Dt	46	56	20,26,27	2.65	4 (20%)	17,39,42	1.13	1 (5%)
23	6MZ	23	2030	23	18,25,26	0.97	1 (5%)	16,36,39	2.59	5 (31%)
23	5MU	23	747	23	19,22,23	1.54	6 (31%)	28,32,35	2.19	8 (28%)
23	PSU	23	2604	23	18,21,22	1.66	5 (27%)	22,30,33	2.16	5 (22%)
23	6MZ	23	1618	23	18,25,26	0.97	0	16,36,39	2.35	5 (31%)
23	OMU	23	2552	23	19,22,23	1.41	3 (15%)	26,31,34	2.05	7 (26%)
56	PSU	Dt	32	56	18,21,22	1.47	4 (22%)	22,30,33	2.02	3 (13%)
1	2MG	16	966	1	18,26,27	1.20	1 (5%)	16,38,41	1.30	3 (18%)
1	2MG	16	1516	1	18,26,27	1.12	1 (5%)	16,38,41	1.28	2 (12%)
55	3AU	Pt	47	55	24,28,29	1.02	0	33,40,43	1.37	3 (9%)
1	MA6	16	1519	1	19,26,27	0.94	1 (5%)	18,38,41	1.49	4 (22%)
56	PSU	Dt	39	56	18,21,22	1.55	5 (27%)	22,30,33	1.84	3 (13%)
1	2MG	16	1207	1	18,26,27	1.20	2 (11%)	16,38,41	1.38	3 (18%)
23	OMG	23	2251	55,23	18,26,27	1.10	1 (5%)	19,38,41	1.39	2 (10%)
56	PSU	Dt	55	56	18,21,22	1.40	3 (16%)	22,30,33	1.96	4 (18%)
55	H2U	Pt	16	55	18,21,22	0.99	2 (11%)	21,30,33	1.38	4 (19%)
23	2MG	23	2445	23	18,26,27	1.18	2 (11%)	16,38,41	1.27	2 (12%)
23	PSU	23	2504	23,58	18,21,22	1.49	3 (16%)	22,30,33	2.09	6 (27%)
23	2MA	23	2503	23,58	17,25,26	1.13	1 (5%)	17,37,40	1.30	4 (23%)
23	PSU	23	746	23,58	18,21,22	1.44	3 (16%)	22,30,33	2.02	4 (18%)
1	UR3	16	1498	1	19,22,23	0.94	0	26,32,35	1.64	2 (7%)
1	G7M	16	527	1	20,26,27	2.59	4 (20%)	17,39,42	1.48	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	PSU	Pt	55	55	18,21,22	1.38	3 (16%)	22,30,33	1.91	4 (18%)
23	5MC	23	1962	23	18,22,23	0.98	2 (11%)	26,32,35	1.21	2 (7%)
23	2MG	23	1835	23	18,26,27	1.08	1 (5%)	16,38,41	1.35	4 (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
34	4D4	LP	81	34	-	3/11/12/14	-
55	PSU	Pt	39	55	-	0/7/25/26	0/2/2/2
23	5MU	23	1939	23,58	-	0/7/25/26	0/2/2/2
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
55	H2U	Pt	17	55	-	5/7/38/39	0/2/2/2
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
56	MIA	Dt	37	56	-	3/11/33/34	0/3/3/3
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
55	H2U	Pt	20	55	-	5/7/38/39	0/2/2/2
1	4OC	16	1402	1	-	1/9/29/30	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
23	3TD	23	1915	23	-	0/7/25/26	0/2/2/2
23	G7M	23	2069	23	-	2/3/25/26	0/3/3/3
55	5MU	Pt	54	55	-	0/7/25/26	0/2/2/2
23	1MG	23	745	23	-	0/3/25/26	0/3/3/3
55	U8U	Pt	34	55,22	-	0/9/28/29	0/2/2/2
55	G7M	Pt	46	55	-	0/3/25/26	0/3/3/3
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
23	OMC	23	2498	23,58	-	0/9/27/28	0/2/2/2
1	PSU	16	516	58,1	-	2/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	0/7/29/30	0/3/3/3
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	1/7/12/14	-
56	4SU	Dt	8	56	-	0/7/25/26	0/2/2/2
56	3AU	Dt	47	56	-	6/16/34/35	0/2/2/2
55	T6A	Pt	37	55	-	4/19/41/42	0/3/3/3
56	G7M	Dt	46	56	-	0/3/25/26	0/3/3/3
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
23	6MZ	23	1618	23	-	0/5/27/28	0/3/3/3
23	OMU	23	2552	23	-	0/9/27/28	0/2/2/2
56	PSU	Dt	32	56	-	0/7/25/26	0/2/2/2
1	2MG	16	966	1	-	0/5/27/28	0/3/3/3
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3
55	3AU	Pt	47	55	-	9/16/34/35	0/2/2/2
1	MA6	16	1519	1	-	0/7/29/30	0/3/3/3
56	PSU	Dt	39	56	-	0/7/25/26	0/2/2/2
1	2MG	16	1207	1	-	0/5/27/28	0/3/3/3
23	OMG	23	2251	55,23	-	3/5/27/28	0/3/3/3
56	PSU	Dt	55	56	-	0/7/25/26	0/2/2/2
55	H2U	Pt	16	55	-	4/7/38/39	0/2/2/2
23	2MG	23	2445	23	-	1/5/27/28	0/3/3/3
23	PSU	23	2504	23,58	-	0/7/25/26	0/2/2/2
23	2MA	23	2503	23,58	-	0/3/25/26	0/3/3/3
23	PSU	23	746	23,58	-	1/7/25/26	0/2/2/2
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
1	G7M	16	527	1	-	2/3/25/26	0/3/3/3
55	PSU	Pt	55	55	-	1/7/25/26	0/2/2/2
23	5MC	23	1962	23	-	0/7/25/26	0/2/2/2
23	2MG	23	1835	23	-	0/5/27/28	0/3/3/3

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Dt	37	MIA	C2-S10	-7.94	1.69	1.75
56	Dt	46	G7M	C8-N9	7.45	1.46	1.33
1	16	527	G7M	C8-N9	7.33	1.46	1.33
55	Pt	46	G7M	C8-N9	7.21	1.46	1.33
55	Pt	46	G7M	C8-N7	7.11	1.46	1.33
56	Dt	46	G7M	C8-N7	7.09	1.46	1.33
56	Dt	37	MIA	C13-C14	6.99	1.52	1.32
23	23	2069	G7M	C8-N9	6.82	1.45	1.33
1	16	527	G7M	C8-N7	6.63	1.45	1.33
23	23	2069	G7M	C8-N7	6.54	1.45	1.33
55	Pt	34	U8U	C2-S2	-5.53	1.59	1.67
34	LP	81	4D4	CZ-NE	4.88	1.42	1.33
56	Dt	8	4SU	C4-S4	-4.62	1.59	1.68
56	Dt	46	G7M	C5-C4	4.33	1.47	1.39
55	Pt	46	G7M	C5-C4	4.18	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	527	G7M	C5-C4	4.04	1.47	1.39
23	23	2580	PSU	C4-N3	-3.87	1.31	1.38
23	23	2457	PSU	C4-N3	-3.64	1.32	1.38
23	23	2552	OMU	C4-N3	-3.55	1.32	1.38
23	23	2604	PSU	C4-N3	-3.53	1.32	1.38
23	23	2605	PSU	C4-N3	-3.52	1.32	1.38
56	Dt	8	4SU	C4-N3	-3.47	1.33	1.37
23	23	2069	G7M	C5-C4	3.46	1.46	1.39
55	Pt	34	U8U	C6-N1	-3.34	1.32	1.38
23	23	2504	PSU	C4-N3	-3.33	1.32	1.38
23	23	955	PSU	C4-N3	-3.30	1.32	1.38
23	23	747	5MU	C4-N3	-3.27	1.32	1.38
23	23	1939	5MU	C4-N3	-3.25	1.32	1.38
1	16	516	PSU	C4-N3	-3.21	1.32	1.38
23	23	1915	3TD	C6-C5	3.19	1.39	1.35
55	Pt	39	PSU	C4-N3	-3.17	1.32	1.38
56	Dt	55	PSU	C6-C5	3.17	1.39	1.35
23	23	2504	PSU	C6-C5	3.14	1.39	1.35
1	16	966	2MG	C6-N1	-3.09	1.33	1.37
34	LP	81	4D4	CZ-NH2	3.06	1.44	1.32
56	Dt	39	PSU	C4-N3	-3.06	1.33	1.38
1	16	1516	2MG	C6-N1	-3.03	1.33	1.37
55	Pt	39	PSU	C6-C5	3.01	1.38	1.35
23	23	2457	PSU	C6-C5	3.00	1.38	1.35
23	23	746	PSU	C4-N3	-3.00	1.33	1.38
55	Pt	20	H2U	C2-N3	-2.99	1.32	1.38
23	23	2604	PSU	C2-N3	-2.99	1.32	1.37
55	Pt	55	PSU	C6-C5	2.99	1.38	1.35
56	Dt	39	PSU	C6-C5	2.97	1.38	1.35
23	23	2251	OMG	C6-N1	-2.97	1.33	1.37
56	Dt	32	PSU	C4-N3	-2.95	1.33	1.38
23	23	955	PSU	C2-N3	-2.93	1.32	1.37
23	23	2605	PSU	C2-N3	-2.93	1.32	1.37
23	23	2445	2MG	C6-N1	-2.92	1.33	1.37
23	23	2552	OMU	C2-N3	-2.92	1.32	1.38
23	23	2449	H2U	C2-N3	-2.91	1.32	1.38
55	Pt	54	5MU	C4-N3	-2.90	1.33	1.38
55	Pt	34	U8U	C4-N3	-2.89	1.33	1.38
1	16	1207	2MG	C6-N1	-2.89	1.33	1.37
56	Dt	32	PSU	C6-C5	2.85	1.38	1.35
1	16	527	G7M	C6-N1	-2.85	1.33	1.37
55	Pt	55	PSU	C4-N3	-2.84	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Dt	55	PSU	C4-N3	-2.83	1.33	1.38
56	Dt	8	4SU	C5-C4	-2.78	1.39	1.42
23	23	1835	2MG	C6-N1	-2.77	1.33	1.37
23	23	2580	PSU	C2-N3	-2.76	1.32	1.37
23	23	2449	H2U	C4-N3	-2.75	1.32	1.37
55	Pt	20	H2U	C4-N3	-2.73	1.32	1.37
55	Pt	17	H2U	C2-N3	-2.73	1.33	1.38
23	23	2604	PSU	C6-C5	2.72	1.38	1.35
23	23	1939	5MU	C2-N3	-2.71	1.33	1.38
23	23	2605	PSU	C6-C5	2.68	1.38	1.35
1	16	1518	MA6	C2'-C1'	-2.68	1.49	1.53
23	23	2580	PSU	C6-C5	2.65	1.38	1.35
23	23	1962	5MC	C6-N1	-2.64	1.33	1.38
1	16	516	PSU	C6-C5	2.64	1.38	1.35
23	23	747	5MU	C6-N1	-2.62	1.33	1.38
23	23	1939	5MU	C6-C5	2.62	1.38	1.34
23	23	747	5MU	C2-N3	-2.61	1.33	1.38
23	23	1915	3TD	C2-N1	-2.59	1.33	1.37
23	23	2457	PSU	C2-N3	-2.58	1.33	1.37
1	16	967	5MC	C6-N1	-2.56	1.33	1.38
55	Pt	16	H2U	C2-N3	-2.53	1.33	1.38
23	23	2503	2MA	C6-N1	-2.51	1.32	1.38
23	23	2552	OMU	C5-C4	-2.51	1.38	1.43
55	Pt	46	G7M	C6-N1	-2.51	1.34	1.37
55	Pt	17	H2U	C4-N3	-2.47	1.33	1.37
55	Pt	54	5MU	C6-C5	2.46	1.38	1.34
23	23	2069	G7M	C6-N1	-2.42	1.34	1.37
1	16	516	PSU	C2-N1	-2.41	1.33	1.36
23	23	2604	PSU	C2-N1	-2.41	1.33	1.36
23	23	1939	5MU	C6-N1	-2.39	1.34	1.38
56	Dt	8	4SU	C2-N1	2.37	1.42	1.38
1	16	1407	5MC	C6-C5	2.37	1.38	1.34
55	Pt	39	PSU	C2-N3	-2.37	1.33	1.37
23	23	747	5MU	C4-C5	2.37	1.48	1.44
23	23	1962	5MC	C6-C5	2.36	1.38	1.34
1	16	516	PSU	C2-N3	-2.35	1.33	1.37
23	23	2504	PSU	C2-N3	-2.35	1.33	1.37
56	Dt	39	PSU	C2-N1	-2.35	1.33	1.36
23	23	2580	PSU	C2'-C1'	-2.33	1.50	1.53
23	23	746	PSU	C6-C5	2.32	1.38	1.35
23	23	2605	PSU	C2-N1	-2.31	1.33	1.36
56	Dt	39	PSU	C2-N3	-2.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	955	PSU	C6-C5	2.29	1.38	1.35
55	Pt	54	5MU	C6-N1	-2.28	1.34	1.38
1	16	1407	5MC	C6-N1	-2.28	1.34	1.38
23	23	746	PSU	C2-N3	-2.28	1.33	1.37
56	Dt	47	3AU	C2-N1	2.27	1.41	1.38
55	Pt	39	PSU	C2-N1	-2.25	1.33	1.36
23	23	955	PSU	C2'-C1'	-2.24	1.50	1.53
55	Pt	54	5MU	C2-N3	-2.24	1.34	1.38
23	23	2449	H2U	C2-N1	-2.23	1.32	1.35
23	23	2445	2MG	C2-N1	-2.23	1.33	1.36
55	Pt	37	T6A	C2'-C1'	-2.22	1.50	1.53
56	Dt	8	4SU	C2-N3	-2.21	1.34	1.38
55	Pt	16	H2U	C4-N3	-2.21	1.33	1.37
1	16	1518	MA6	C5-C4	2.21	1.46	1.40
56	Dt	32	PSU	C2-N3	-2.20	1.33	1.37
23	23	747	5MU	C6-C5	2.19	1.38	1.34
23	23	955	PSU	C2-N1	-2.16	1.33	1.36
23	23	2457	PSU	C2-N1	-2.16	1.33	1.36
56	Dt	46	G7M	C6-N1	-2.15	1.34	1.37
12	SL	89	D2T	CB1-SB	-2.14	1.75	1.79
56	Dt	32	PSU	C2-N1	-2.13	1.33	1.36
1	16	967	5MC	C6-C5	2.12	1.38	1.34
23	23	2604	PSU	C2'-C1'	-2.12	1.51	1.53
23	23	2605	PSU	C2'-C1'	-2.11	1.51	1.53
55	Pt	54	5MU	C2-N1	2.11	1.41	1.38
23	23	747	5MU	C2-N1	2.10	1.41	1.38
56	Dt	39	PSU	C2'-C1'	-2.09	1.51	1.53
1	16	1207	2MG	C2'-C1'	-2.07	1.50	1.53
55	Pt	55	PSU	C2-N3	-2.06	1.34	1.37
23	23	2580	PSU	C2-N1	-2.04	1.34	1.36
56	Dt	37	MIA	C5-C4	2.04	1.46	1.40
23	23	2580	PSU	C6-N1	-2.03	1.32	1.36
23	23	2069	G7M	C2'-C1'	-2.02	1.50	1.53
1	16	516	PSU	C2'-C1'	-2.02	1.51	1.53
56	Dt	55	PSU	C2-N3	-2.02	1.34	1.37
23	23	2030	6MZ	C2'-C1'	-2.01	1.50	1.53
1	16	1519	MA6	C5-C4	2.00	1.46	1.40

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	Pt	20	H2U	C4-N3-C2	-12.10	115.75	125.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Dt	37	MIA	C12-C13-C14	-8.44	110.72	127.14
55	Pt	17	H2U	C4-N3-C2	-7.54	119.54	125.79
55	Pt	37	T6A	C2-N1-C6	6.97	122.57	116.59
23	23	2457	PSU	N1-C2-N3	6.77	122.80	115.13
23	23	955	PSU	N1-C2-N3	6.72	122.75	115.13
23	23	2580	PSU	N1-C2-N3	6.65	122.66	115.13
1	16	516	PSU	N1-C2-N3	6.63	122.64	115.13
23	23	2504	PSU	N1-C2-N3	6.56	122.56	115.13
23	23	1618	6MZ	C2-N1-C6	6.50	122.16	116.59
1	16	1498	UR3	C4-N3-C2	-6.50	118.45	124.56
23	23	2604	PSU	N1-C2-N3	6.40	122.38	115.13
56	Dt	32	PSU	N1-C2-N3	6.34	122.31	115.13
23	23	1915	3TD	N1-C2-N3	6.29	121.10	116.14
55	Pt	39	PSU	N1-C2-N3	6.22	122.17	115.13
23	23	2030	6MZ	C2-N1-C6	6.18	121.89	116.59
23	23	2605	PSU	N1-C2-N3	6.17	122.12	115.13
23	23	746	PSU	N1-C2-N3	6.07	122.00	115.13
56	Dt	39	PSU	N1-C2-N3	5.95	121.88	115.13
55	Pt	55	PSU	N1-C2-N3	5.95	121.87	115.13
56	Dt	8	4SU	C4-N3-C2	-5.86	121.65	127.34
56	Dt	55	PSU	N1-C2-N3	5.85	121.76	115.13
23	23	1939	5MU	C4-N3-C2	-5.75	119.91	127.35
56	Dt	8	4SU	C5-C4-N3	5.71	119.99	114.69
23	23	1939	5MU	N3-C2-N1	5.51	122.21	114.89
23	23	747	5MU	N3-C2-N1	5.27	121.89	114.89
23	23	747	5MU	C4-N3-C2	-5.18	120.65	127.35
23	23	1939	5MU	C5-C4-N3	5.17	119.73	115.31
55	Pt	37	T6A	N6-C10-N11	5.16	120.96	113.76
23	23	1915	3TD	C4-N3-C2	-5.06	119.12	124.61
23	23	2552	OMU	C2'-C1'-N1	-4.89	104.73	114.22
23	23	2030	6MZ	C9-N6-C6	-4.89	118.66	122.87
23	23	746	PSU	C4-N3-C2	-4.69	119.58	126.34
55	Pt	54	5MU	N3-C2-N1	4.61	121.01	114.89
55	Pt	54	5MU	C4-N3-C2	-4.60	121.40	127.35
55	Pt	47	3AU	C4-N3-C2	-4.59	118.87	124.63
23	23	2552	OMU	N3-C2-N1	4.58	120.97	114.89
23	23	955	PSU	C4-N3-C2	-4.58	119.74	126.34
56	Dt	47	3AU	C4-N3-C2	-4.57	118.90	124.63
23	23	2552	OMU	C4-N3-C2	-4.53	120.61	126.58
23	23	2449	H2U	C4-N3-C2	-4.52	122.04	125.79
23	23	1939	5MU	C5-C6-N1	-4.49	118.72	123.34
23	23	2504	PSU	C4-N3-C2	-4.48	119.88	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Dt	37	MIA	C2-N3-C4	4.29	121.24	115.32
23	23	747	5MU	C5-C4-N3	4.25	118.94	115.31
55	Pt	54	5MU	C5-C4-N3	4.14	118.84	115.31
56	Dt	37	MIA	C15-C14-C13	-4.09	110.83	122.65
23	23	1939	5MU	O4-C4-C5	-4.07	120.19	124.90
56	Dt	37	MIA	C16-C14-C13	-4.07	110.89	122.65
56	Dt	32	PSU	C4-N3-C2	-4.05	120.51	126.34
1	16	516	PSU	C4-N3-C2	-4.01	120.56	126.34
55	Pt	54	5MU	O4-C4-C5	-4.00	120.27	124.90
23	23	2457	PSU	C4-N3-C2	-4.00	120.58	126.34
23	23	2604	PSU	C3'-C2'-C1'	3.94	106.22	101.64
23	23	1618	6MZ	N3-C2-N1	-3.92	122.55	128.68
56	Dt	55	PSU	C4-N3-C2	-3.91	120.70	126.34
1	16	516	PSU	O2-C2-N1	-3.90	118.49	122.79
23	23	2604	PSU	C4-N3-C2	-3.90	120.73	126.34
23	23	1962	5MC	C5-C6-N1	-3.88	119.35	123.34
23	23	2580	PSU	C4-N3-C2	-3.83	120.82	126.34
23	23	2605	PSU	C4-N3-C2	-3.78	120.89	126.34
56	Dt	8	4SU	N3-C2-N1	3.78	119.90	114.89
55	Pt	55	PSU	C4-N3-C2	-3.77	120.91	126.34
56	Dt	32	PSU	O2-C2-N1	-3.77	118.64	122.79
55	Pt	37	T6A	N6-C6-N1	3.76	123.76	118.72
23	23	2552	OMU	C5-C4-N3	3.75	120.45	114.84
23	23	1618	6MZ	C9-N6-C6	-3.74	119.65	122.87
55	Pt	39	PSU	C4-N3-C2	-3.73	120.97	126.34
55	Pt	37	T6A	N3-C2-N1	-3.72	122.86	128.68
23	23	747	5MU	C5-C6-N1	-3.67	119.56	123.34
23	23	2030	6MZ	C4-C5-N7	-3.61	105.63	109.40
1	16	1518	MA6	N3-C2-N1	-3.59	123.06	128.68
56	Dt	8	4SU	C5-C4-S4	-3.55	119.90	124.47
23	23	2580	PSU	C3'-C2'-C1'	3.54	105.75	101.64
23	23	746	PSU	O2-C2-N1	-3.53	118.90	122.79
34	LP	81	4D4	NE-CZ-NH2	-3.50	114.54	120.70
55	Pt	16	H2U	C4-N3-C2	-3.50	122.89	125.79
56	Dt	39	PSU	C4-N3-C2	-3.46	121.35	126.34
55	Pt	55	PSU	O2-C2-N1	-3.44	119.00	122.79
23	23	2030	6MZ	O4'-C1'-C2'	-3.40	101.95	106.93
23	23	2030	6MZ	N3-C2-N1	-3.34	123.45	128.68
1	16	1519	MA6	C4-C5-N7	-3.33	105.93	109.40
23	23	2251	OMG	O6-C6-C5	-3.27	117.99	124.37
56	Dt	47	3AU	C5-C4-N3	3.26	119.80	115.50
34	LP	81	4D4	NH1-CZ-NE	3.26	126.72	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Dt	37	MIA	C5-C6-N1	-3.24	118.12	120.81
56	Dt	55	PSU	O2-C2-N1	-3.20	119.27	122.79
55	Pt	54	5MU	C5-C6-N1	-3.18	120.06	123.34
55	Pt	39	PSU	O2-C2-N1	-3.18	119.29	122.79
1	16	1519	MA6	N3-C2-N1	-3.17	123.72	128.68
55	Pt	47	3AU	C5-C4-N3	3.12	119.62	115.50
23	23	2251	OMG	C5-C6-N1	3.12	119.47	113.95
23	23	2457	PSU	O2-C2-N1	-3.08	119.40	122.79
55	Pt	34	U8U	C1'-N1-C6	-3.07	116.02	121.12
56	Dt	39	PSU	O2-C2-N1	-3.07	119.41	122.79
1	16	967	5MC	C5-C6-N1	-3.05	120.20	123.34
23	23	745	1MG	C5-C6-N1	3.00	118.41	113.90
23	23	747	5MU	O4-C4-C5	-2.99	121.44	124.90
56	Dt	8	4SU	C1'-N1-C2	2.99	122.98	117.57
1	16	1518	MA6	C4-C5-N7	-2.98	106.30	109.40
1	16	527	G7M	CN7-N7-C8	-2.92	111.36	125.43
23	23	2504	PSU	O2-C2-N1	-2.92	119.58	122.79
23	23	2580	PSU	O2-C2-N1	-2.88	119.62	122.79
23	23	745	1MG	CM1-N1-C6	2.88	121.49	117.55
55	Pt	34	U8U	O4-C4-C5	-2.85	120.72	124.96
23	23	2457	PSU	C3'-C2'-C1'	2.85	104.95	101.64
34	LP	81	4D4	CB-CA-C	-2.81	107.29	111.77
1	16	1407	5MC	C5-C6-N1	-2.79	120.46	123.34
56	Dt	46	G7M	CN7-N7-C8	-2.78	112.03	125.43
23	23	2069	G7M	CN7-N7-C8	-2.78	112.03	125.43
55	Pt	46	G7M	CN7-N7-C8	-2.76	112.13	125.43
23	23	746	PSU	C5-C6-N1	-2.75	117.99	122.11
55	Pt	55	PSU	C3'-C2'-C1'	2.74	104.83	101.64
23	23	1835	2MG	C5-C6-N1	2.74	118.79	113.95
1	16	1516	2MG	C5-C6-N1	2.72	118.75	113.95
23	23	2604	PSU	O2-C2-N1	-2.68	119.84	122.79
1	16	1402	4OC	O2-C2-N3	-2.68	117.98	122.33
56	Dt	37	MIA	C4-C5-N7	-2.67	106.61	109.40
55	Pt	16	H2U	O4'-C1'-N1	2.63	112.88	109.30
1	16	1407	5MC	O2-C2-N3	-2.61	118.08	122.33
23	23	747	5MU	C3'-C2'-C1'	2.60	106.36	101.43
1	16	1402	4OC	C6-C5-C4	2.59	120.13	116.96
23	23	2503	2MA	C5-C6-N1	2.58	118.47	114.02
23	23	1835	2MG	O6-C6-C5	-2.56	119.36	124.37
56	Dt	37	MIA	C2-N1-C6	2.56	121.77	117.19
23	23	2605	PSU	O2-C2-N3	-2.55	117.00	121.82
56	Dt	47	3AU	C10-N3-C2	2.55	121.48	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	955	PSU	O2-C2-N1	-2.54	120.00	122.79
23	23	2449	H2U	O4'-C1'-N1	2.54	112.75	109.30
23	23	2449	H2U	C5-C4-N3	2.53	119.49	116.65
1	16	1207	2MG	C5-C6-N1	2.52	118.41	113.95
23	23	2503	2MA	C8-N7-C5	2.52	107.78	102.99
23	23	2445	2MG	C8-N7-C5	2.50	107.75	102.99
1	16	1207	2MG	C8-N7-C5	2.49	107.74	102.99
23	23	1939	5MU	O2-C2-N1	-2.49	119.47	122.79
1	16	966	2MG	C5-C6-N1	2.48	118.34	113.95
23	23	2445	2MG	C5-C6-N1	2.48	118.33	113.95
1	16	967	5MC	C5-C4-N3	-2.48	119.00	121.67
56	Dt	37	MIA	C11-S10-C2	-2.45	100.44	102.27
23	23	1835	2MG	CM2-N2-C2	-2.43	118.50	123.86
56	Dt	47	3AU	C3'-C2'-C1'	2.42	106.03	101.43
23	23	955	PSU	O2-C2-N3	-2.42	117.25	121.82
1	16	527	G7M	O4'-C1'-C2'	-2.41	103.40	106.93
23	23	745	1MG	C8-N7-C5	2.41	107.57	102.99
23	23	747	5MU	C5M-C5-C4	2.40	121.41	118.77
23	23	1915	3TD	C3'-C2'-C1'	2.39	104.42	101.64
56	Dt	55	PSU	C6-C5-C4	-2.37	116.54	118.20
55	Pt	34	U8U	C5-C4-N3	2.36	118.29	114.97
1	16	1207	2MG	CM2-N2-C2	-2.35	118.67	123.86
1	16	1407	5MC	C5-C4-N3	-2.35	119.14	121.67
55	Pt	37	T6A	O10-C10-N6	-2.34	119.66	123.62
55	Pt	47	3AU	C10-N3-C2	2.32	121.15	117.67
56	Dt	47	3AU	C1'-N1-C2	2.31	120.88	116.99
1	16	1519	MA6	C1'-N9-C4	-2.30	122.61	126.64
55	Pt	16	H2U	C5-C6-N1	-2.29	104.06	111.61
1	16	966	2MG	C3'-C2'-C1'	2.29	104.43	100.98
56	Dt	37	MIA	N3-C2-N1	-2.28	122.79	126.98
55	Pt	37	T6A	C4-C5-N7	-2.28	107.03	109.40
55	Pt	16	H2U	C5-C4-N3	2.27	119.20	116.65
23	23	2552	OMU	O4-C4-C5	-2.25	121.20	125.16
23	23	747	5MU	C5M-C5-C6	-2.25	119.85	122.85
23	23	1962	5MC	C5-C4-N3	-2.24	119.25	121.67
23	23	1618	6MZ	C4-C5-N7	-2.22	107.08	109.40
1	16	516	PSU	C3'-C2'-C1'	2.21	104.21	101.64
1	16	1516	2MG	C8-N7-C5	2.21	107.19	102.99
23	23	2552	OMU	O4'-C1'-N1	2.20	113.39	108.36
23	23	2498	OMC	O2-C2-N3	-2.18	118.78	122.33
23	23	2580	PSU	C5-C6-N1	-2.18	118.84	122.11
1	16	1498	UR3	C3U-N3-C4	2.18	121.00	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2580	PSU	O2-C2-N3	-2.17	117.72	121.82
23	23	2504	PSU	C5-C6-N1	-2.17	118.85	122.11
56	Dt	37	MIA	C12-N6-C6	-2.17	119.33	122.55
1	16	966	2MG	C8-N7-C5	2.17	107.11	102.99
23	23	955	PSU	C5-C6-N1	-2.16	118.86	122.11
12	SL	89	D2T	OD2-CG-CB	2.16	117.83	113.15
1	16	1519	MA6	C3'-C2'-C1'	2.16	104.23	100.98
23	23	2604	PSU	O2-C2-N3	-2.14	117.77	121.82
23	23	2504	PSU	C3'-C2'-C1'	2.13	104.12	101.64
23	23	2457	PSU	O2-C2-N3	-2.13	117.80	121.82
23	23	2605	PSU	C5-C6-N1	-2.13	118.92	122.11
55	Pt	17	H2U	C3'-C2'-C1'	2.12	105.46	101.43
23	23	2504	PSU	O2-C2-N3	-2.12	117.83	121.82
55	Pt	34	U8U	C-C5-C6	-2.09	118.07	121.21
34	LP	81	4D4	O-C-CA	-2.07	119.34	124.78
23	23	1618	6MZ	O3'-C3'-C2'	-2.06	105.15	111.82
23	23	2503	2MA	O4'-C1'-C2'	-2.05	103.92	106.93
23	23	2503	2MA	C3'-C2'-C1'	2.05	104.07	100.98
55	Pt	20	H2U	C3'-C2'-C1'	2.03	105.29	101.43
1	16	527	G7M	C2'-C3'-C4'	-2.02	98.71	102.64
23	23	1835	2MG	C8-N7-C5	2.02	106.84	102.99
12	SL	89	D2T	CB-CA-N	2.02	113.41	109.10
12	SL	89	D2T	O-C-CA	-2.01	119.52	124.78
23	23	2552	OMU	O2-C2-N1	-2.01	120.12	122.79

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	516	PSU	O4'-C4'-C5'-O5'
1	16	527	G7M	O4'-C4'-C5'-O5'
1	16	527	G7M	C3'-C4'-C5'-O5'
23	23	2251	OMG	O4'-C4'-C5'-O5'
23	23	2251	OMG	C3'-C4'-C5'-O5'
23	23	2251	OMG	C1'-C2'-O2'-CM2
55	Pt	16	H2U	O4'-C4'-C5'-O5'
55	Pt	16	H2U	C3'-C4'-C5'-O5'
55	Pt	16	H2U	O4'-C1'-N1-C2
55	Pt	16	H2U	O4'-C1'-N1-C6
55	Pt	37	T6A	O4'-C4'-C5'-O5'
55	Pt	37	T6A	C3'-C4'-C5'-O5'
55	Pt	47	3AU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
55	Pt	47	3AU	C2'-C1'-N1-C6
55	Pt	55	PSU	C4'-C5'-O5'-P
56	Dt	37	MIA	O4'-C4'-C5'-O5'
56	Dt	37	MIA	C3'-C4'-C5'-O5'
56	Dt	37	MIA	C12-C13-C14-C16
56	Dt	47	3AU	C2'-C1'-N1-C2
56	Dt	47	3AU	C2'-C1'-N1-C6
56	Dt	47	3AU	C10-C11-C12-N40
23	23	2030	6MZ	O4'-C4'-C5'-O5'
23	23	2030	6MZ	C3'-C4'-C5'-O5'
55	Pt	47	3AU	C11-C12-C13-O31
1	16	516	PSU	C3'-C4'-C5'-O5'
55	Pt	47	3AU	C11-C12-C13-O30
55	Pt	47	3AU	N40-C12-C13-O31
55	Pt	17	H2U	C2'-C1'-N1-C6
55	Pt	20	H2U	C2'-C1'-N1-C6
34	LP	81	4D4	OB-CB-CG-CD
56	Dt	47	3AU	O4'-C1'-N1-C6
55	Pt	47	3AU	N40-C12-C13-O30
55	Pt	20	H2U	C2'-C1'-N1-C2
55	Pt	37	T6A	N11-C12-C13-ODB
56	Dt	47	3AU	O4'-C1'-N1-C2
55	Pt	17	H2U	C2'-C1'-N1-C2
55	Pt	20	H2U	O4'-C1'-N1-C6
55	Pt	47	3AU	C10-C11-C12-C13
56	Dt	47	3AU	C4'-C5'-O5'-P
55	Pt	47	3AU	O4'-C1'-N1-C6
55	Pt	20	H2U	O4'-C1'-N1-C2
23	23	2069	G7M	C4'-C5'-O5'-P
55	Pt	17	H2U	C4'-C5'-O5'-P
1	16	1402	4OC	O4'-C4'-C5'-O5'
23	23	2445	2MG	C3'-C4'-C5'-O5'
55	Pt	47	3AU	O4'-C1'-N1-C2
55	Pt	37	T6A	N11-C12-C13-ODA
55	Pt	17	H2U	O4'-C1'-N1-C2
55	Pt	20	H2U	C4'-C5'-O5'-P
34	LP	81	4D4	CA-CB-CG-CD
12	SL	89	D2T	CG-CB-SB-CB1
23	23	746	PSU	O4'-C1'-C5-C6
55	Pt	17	H2U	O4'-C1'-N1-C6
23	23	2069	G7M	O4'-C4'-C5'-O5'
34	LP	81	4D4	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 314 ligands modelled in this entry, 297 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
57	PUT	16	1601	-	5,5,5	0.15	0	4,4,4	0.23	0
61	SPD	23	3014	-	9,9,9	0.16	0	8,8,8	0.33	0
57	PUT	23	3006	-	5,5,5	0.13	0	4,4,4	0.20	0
57	PUT	23	3012	-	5,5,5	0.14	0	4,4,4	0.18	0
61	SPD	23	3016	-	9,9,9	0.32	0	8,8,8	0.90	0
57	PUT	23	3007	-	5,5,5	0.15	0	4,4,4	0.20	0
57	PUT	23	3003	-	5,5,5	0.15	0	4,4,4	0.17	0
57	PUT	23	3010	-	5,5,5	0.15	0	4,4,4	0.21	0
60	ATP	23	3002	-	26,33,33	0.68	0	31,52,52	0.85	1 (3%)
57	PUT	23	3004	-	5,5,5	0.14	0	4,4,4	0.21	0
61	SPD	23	3013	-	9,9,9	0.16	0	8,8,8	0.29	0
57	PUT	23	3011	-	5,5,5	0.15	0	4,4,4	0.20	0
57	PUT	23	3009	-	5,5,5	0.14	0	4,4,4	0.15	0
60	ATP	23	3001	-	26,33,33	0.67	0	31,52,52	0.81	1 (3%)
57	PUT	23	3005	-	5,5,5	0.14	0	4,4,4	0.22	0
61	SPD	23	3015	-	9,9,9	0.13	0	8,8,8	0.24	0
57	PUT	23	3008	-	5,5,5	0.14	0	4,4,4	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PUT	16	1601	-	-	0/3/3/3	-
61	SPD	23	3014	-	-	2/7/7/7	-
57	PUT	23	3006	-	-	2/3/3/3	-
57	PUT	23	3012	-	-	1/3/3/3	-
61	SPD	23	3016	-	-	1/7/7/7	-
57	PUT	23	3007	-	-	0/3/3/3	-
57	PUT	23	3003	-	-	0/3/3/3	-
57	PUT	23	3010	-	-	0/3/3/3	-
60	ATP	23	3002	-	-	5/18/38/38	0/3/3/3
57	PUT	23	3004	-	-	0/3/3/3	-
61	SPD	23	3013	-	-	3/7/7/7	-
57	PUT	23	3011	-	-	2/3/3/3	-
57	PUT	23	3009	-	-	1/3/3/3	-
60	ATP	23	3001	-	-	6/18/38/38	0/3/3/3
57	PUT	23	3005	-	-	0/3/3/3	-
61	SPD	23	3015	-	-	4/7/7/7	-
57	PUT	23	3008	-	-	0/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	23	3002	ATP	C5-C6-N6	2.44	124.06	120.35
60	23	3001	ATP	C5-C6-N6	2.32	123.88	120.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	23	3001	ATP	C5'-O5'-PA-O2A
60	23	3002	ATP	PB-O3B-PG-O2G
61	23	3013	SPD	N6-C7-C8-C9
57	23	3012	PUT	C2-C3-C4-N2
61	23	3014	SPD	C3-C4-C5-N6
61	23	3015	SPD	C2-C3-C4-C5
61	23	3015	SPD	N6-C7-C8-C9
60	23	3001	ATP	C4'-C5'-O5'-PA
60	23	3001	ATP	C5'-O5'-PA-O3A
61	23	3015	SPD	C7-C8-C9-N10
60	23	3002	ATP	PG-O3B-PB-O1B

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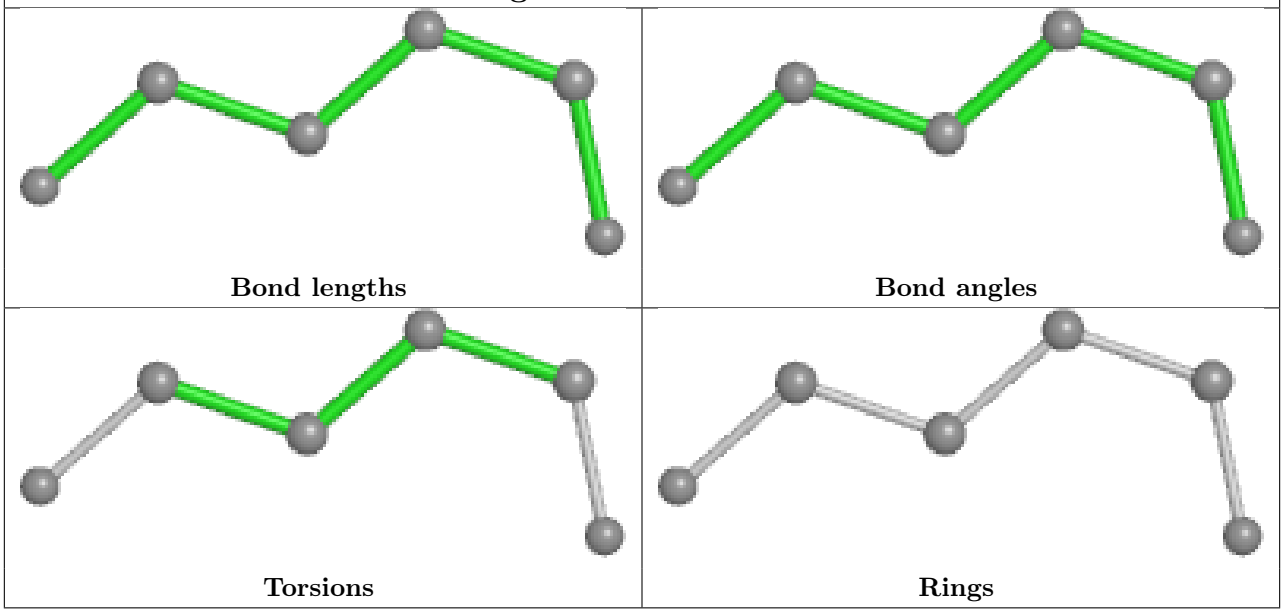
Mol	Chain	Res	Type	Atoms
60	23	3001	ATP	C5'-O5'-PA-O1A
57	23	3011	PUT	C2-C3-C4-N2
60	23	3001	ATP	O4'-C4'-C5'-O5'
60	23	3001	ATP	C3'-C4'-C5'-O5'
61	23	3014	SPD	C8-C7-N6-C5
57	23	3006	PUT	N1-C1-C2-C3
60	23	3002	ATP	PB-O3A-PA-O2A
61	23	3013	SPD	C8-C7-N6-C5
61	23	3013	SPD	C2-C3-C4-C5
61	23	3016	SPD	C7-C8-C9-N10
61	23	3015	SPD	C4-C5-N6-C7
57	23	3009	PUT	N1-C1-C2-C3
60	23	3002	ATP	PB-O3B-PG-O1G
57	23	3006	PUT	C2-C3-C4-N2
57	23	3011	PUT	N1-C1-C2-C3
60	23	3002	ATP	PG-O3B-PB-O2B

There are no ring outliers.

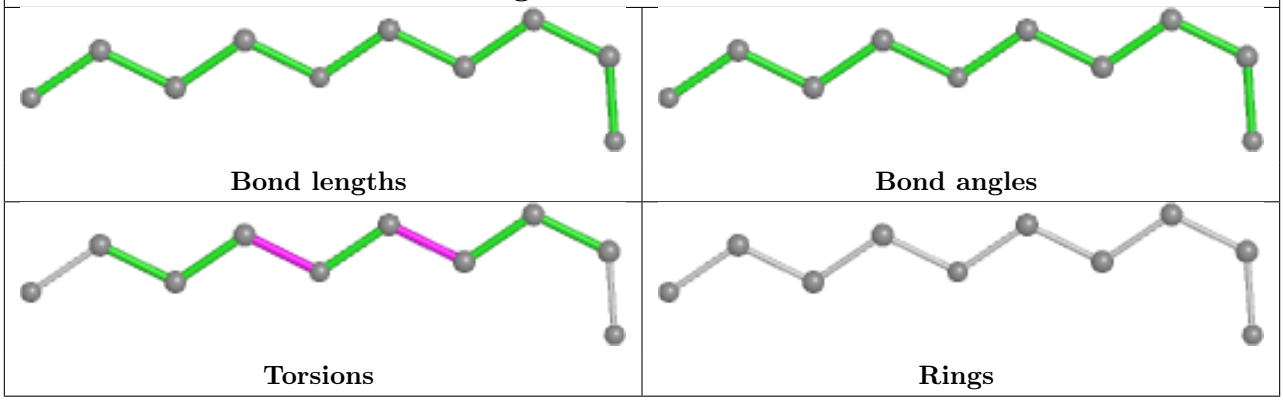
No monomer is involved in short contacts.

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.

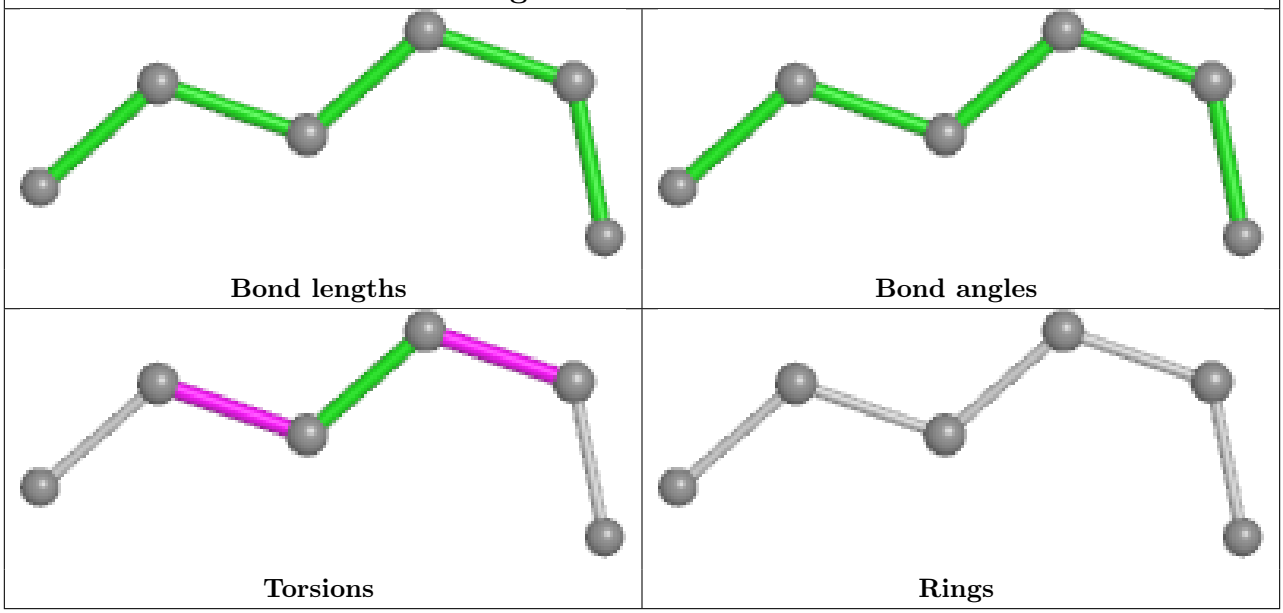
Ligand PUT 16 1601



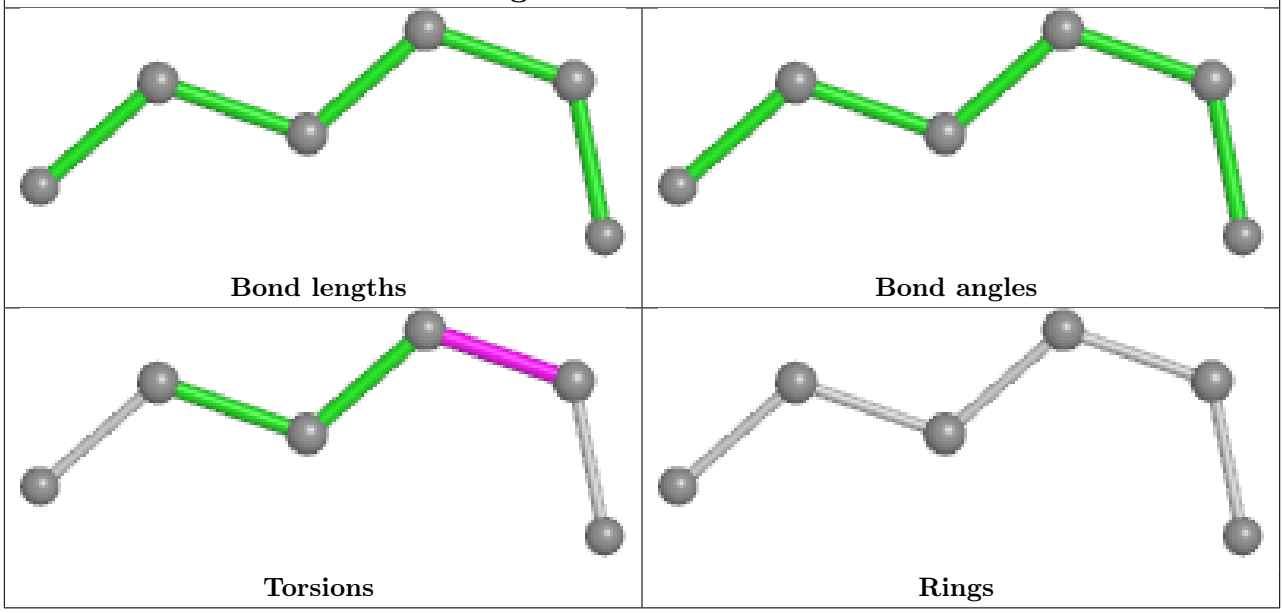
Ligand SPD 23 3014



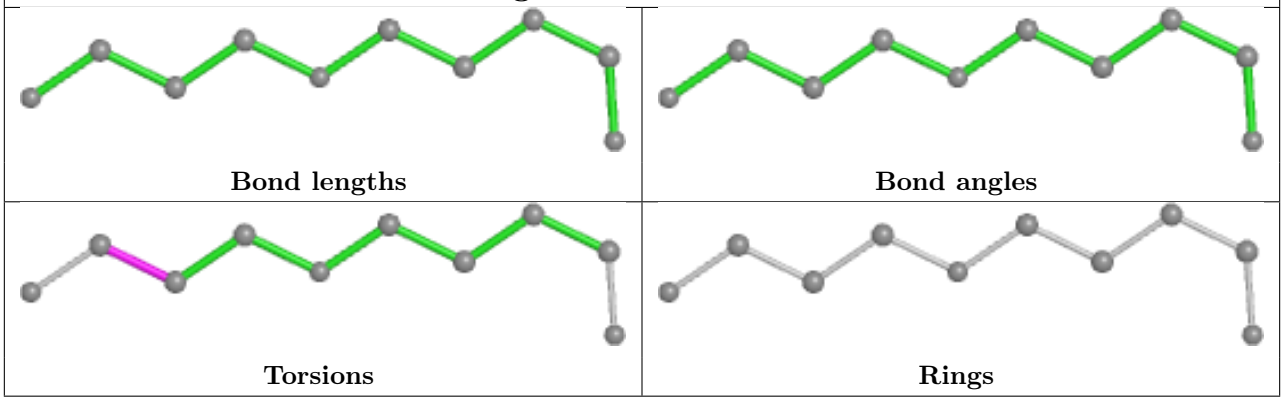
Ligand PUT 23 3006



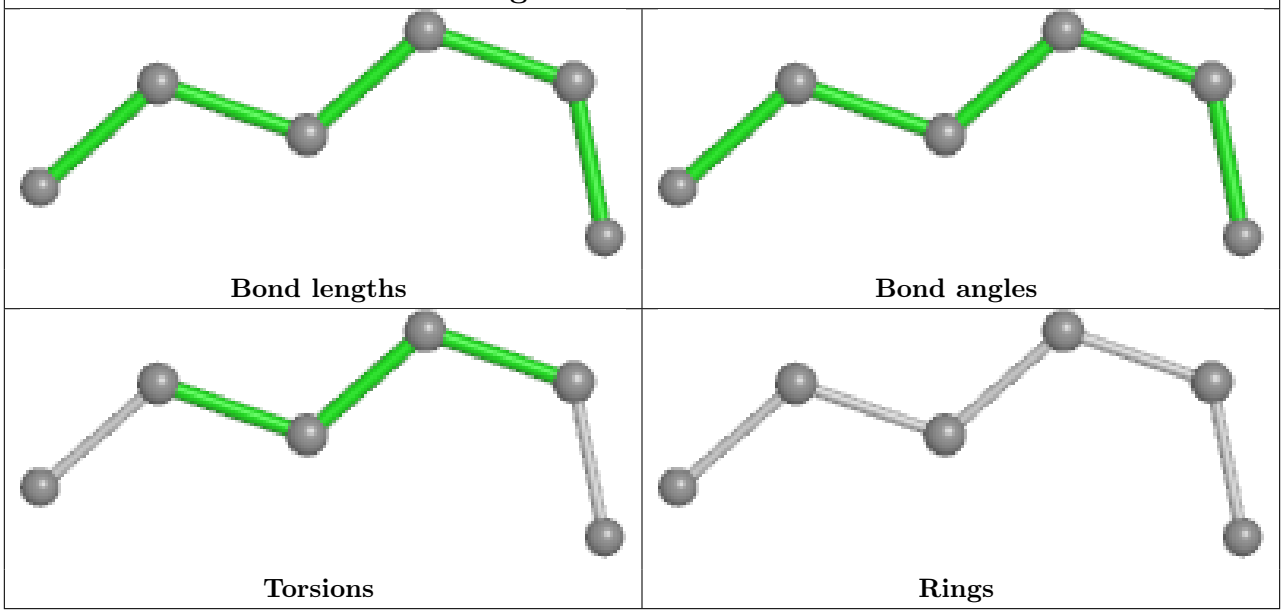
Ligand PUT 23 3012



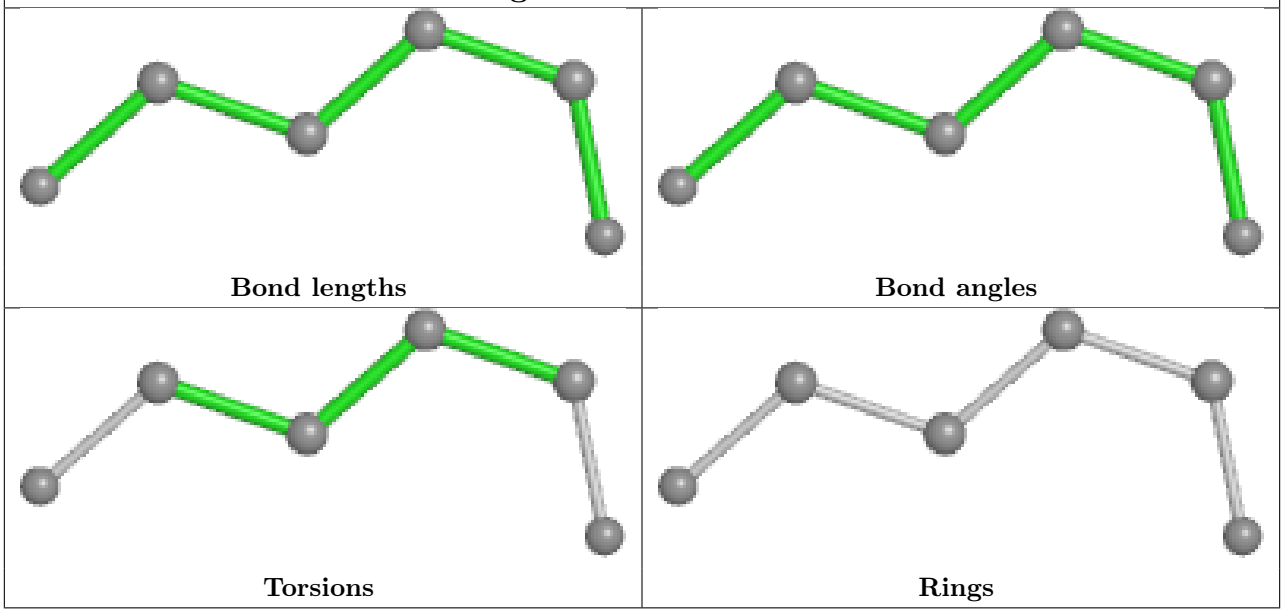
Ligand SPD 23 3016



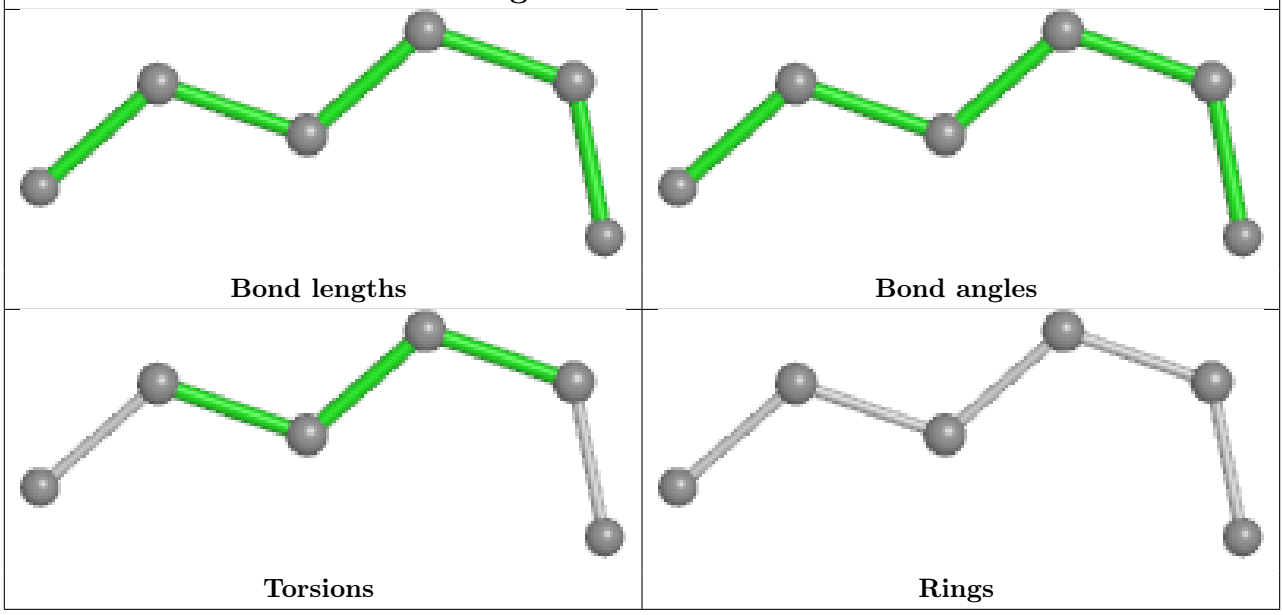
Ligand PUT 23 3007



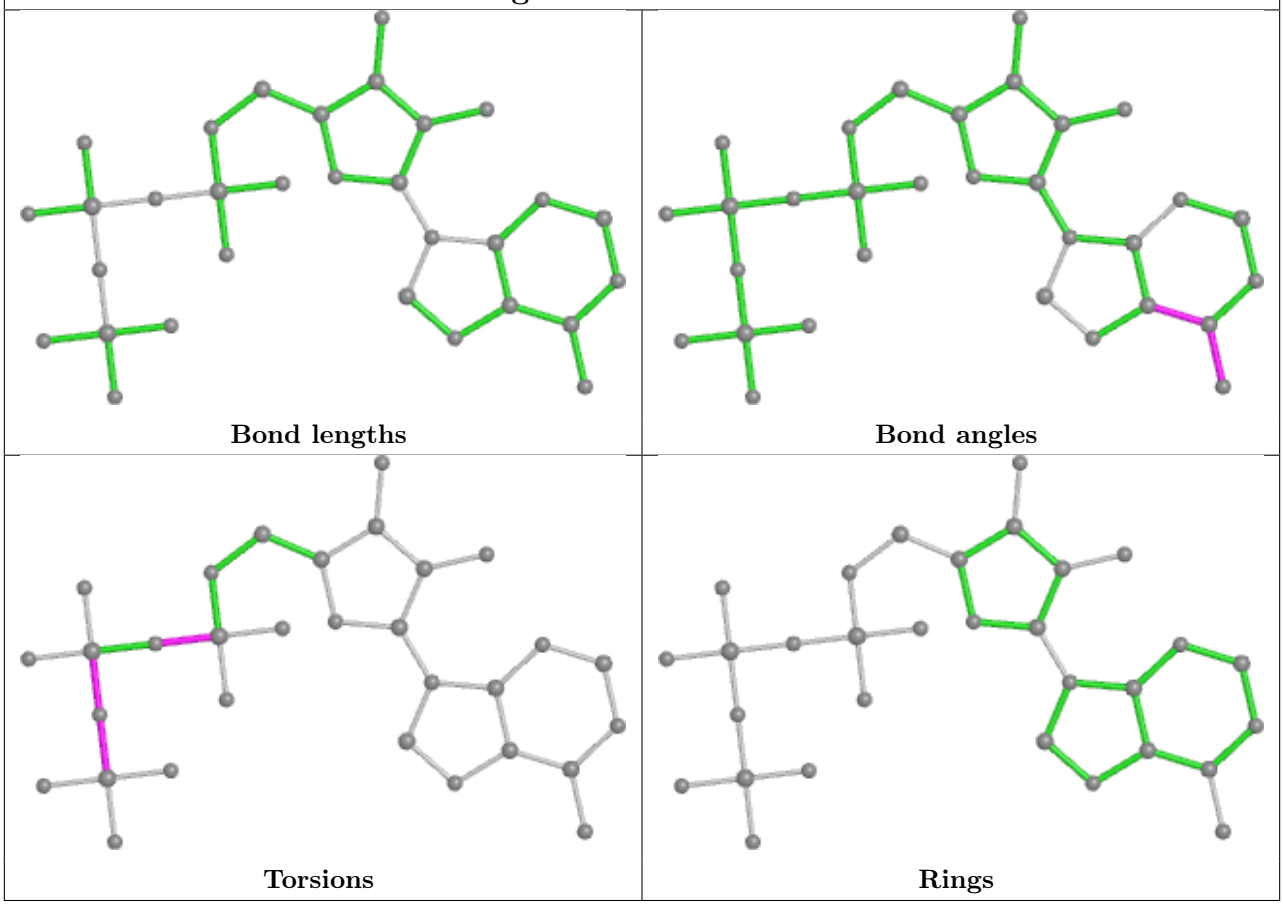
Ligand PUT 23 3003



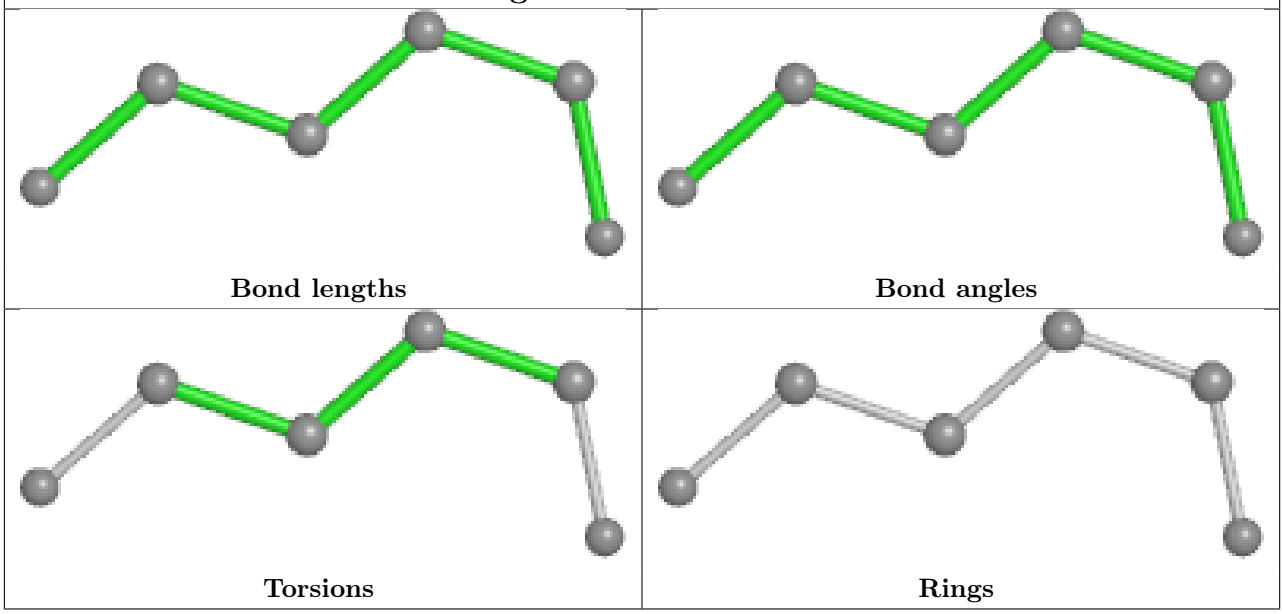
Ligand PUT 23 3010



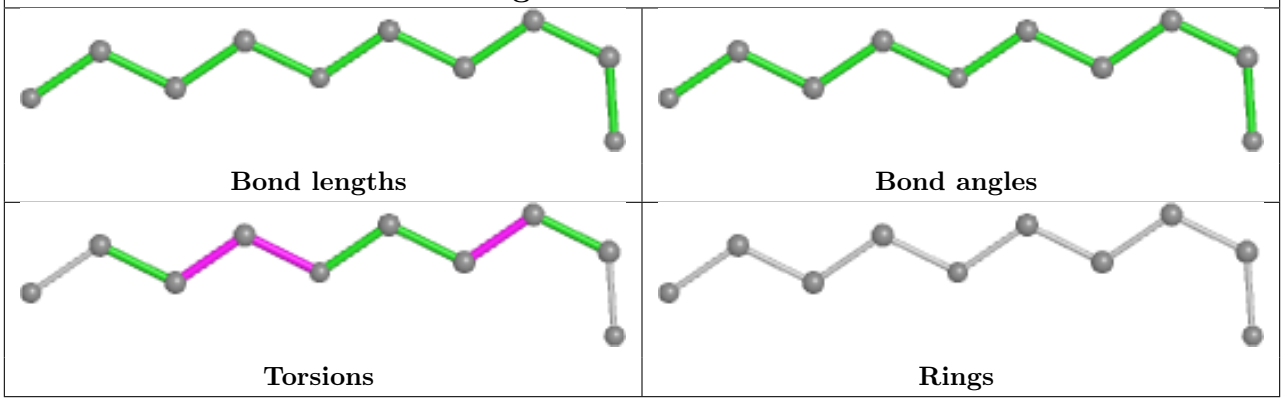
Ligand ATP 23 3002



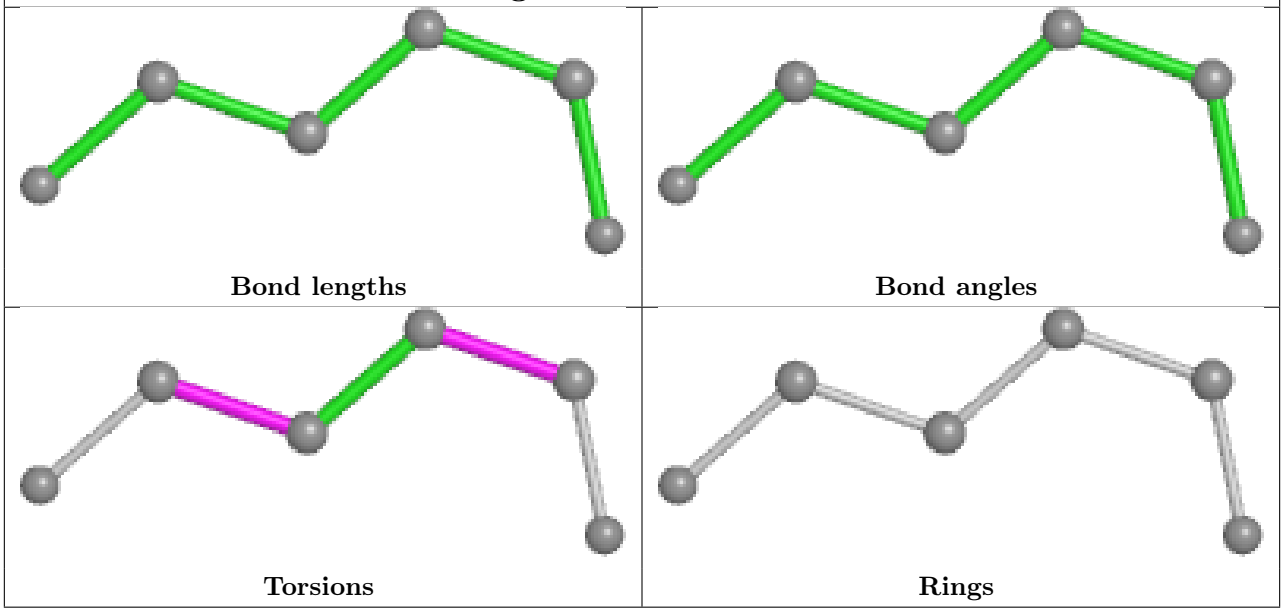
Ligand PUT 23 3004



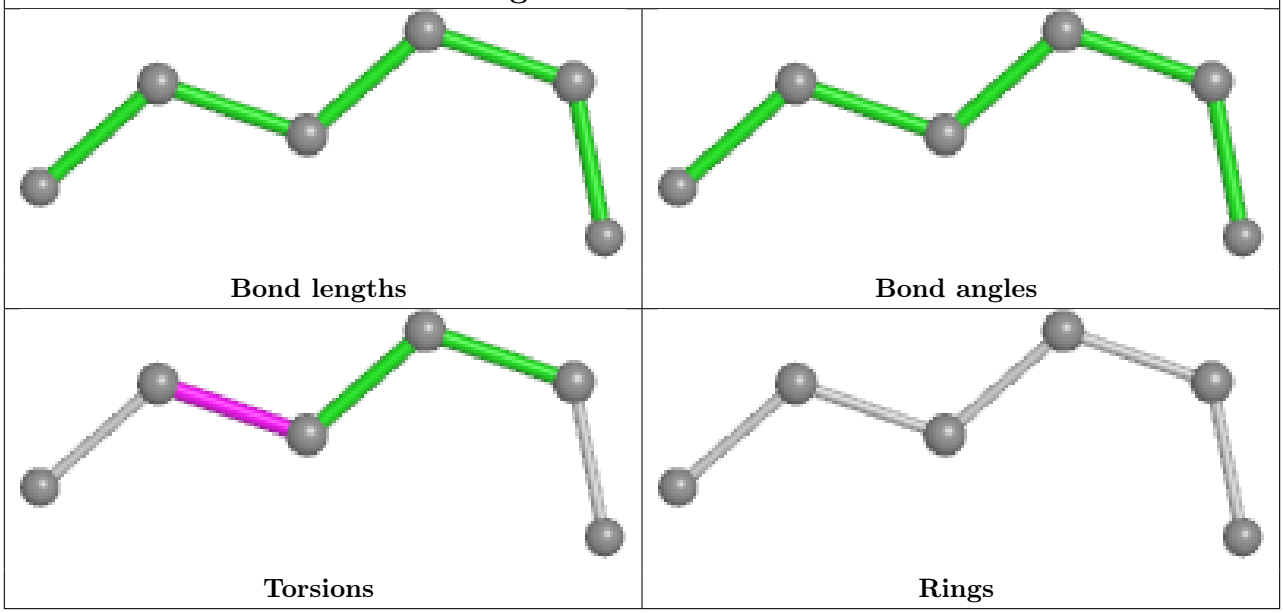
Ligand SPD 23 3013



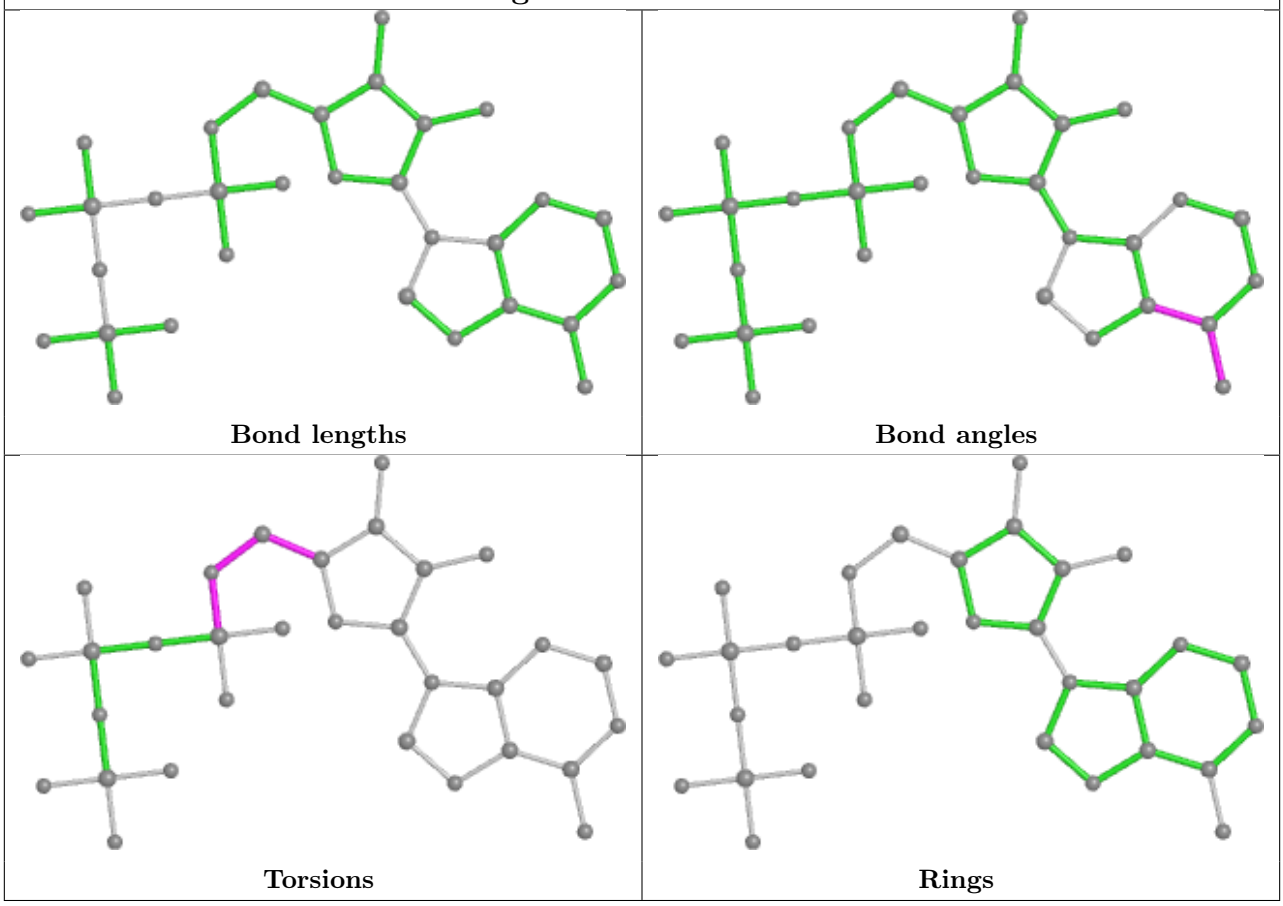
Ligand PUT 23 3011



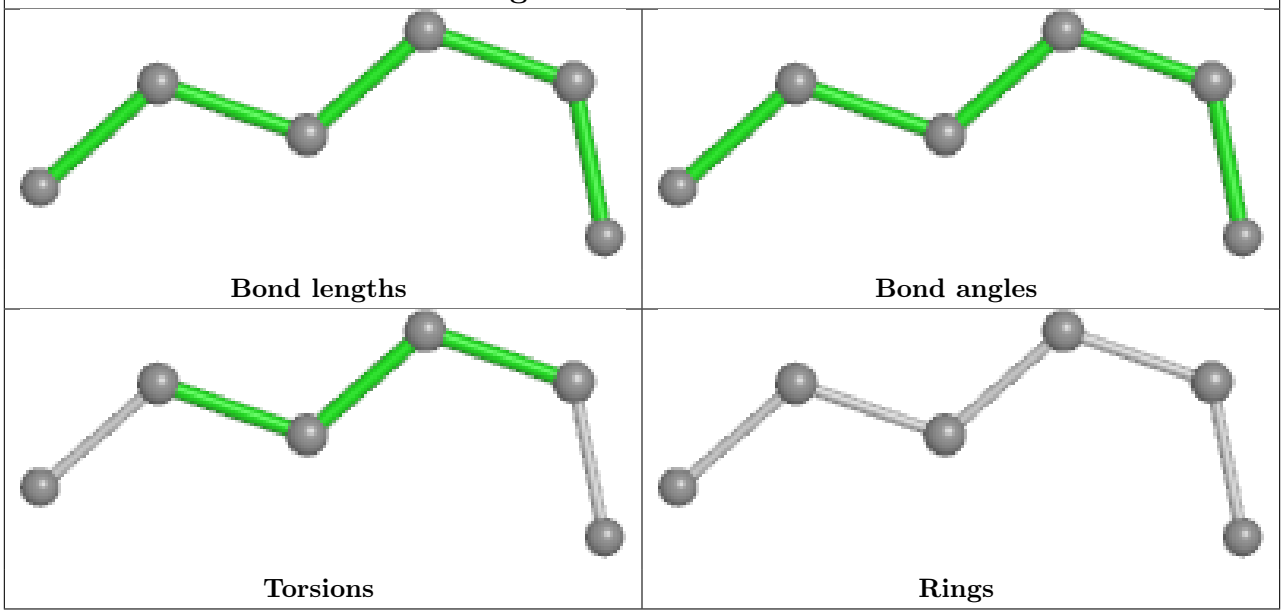
Ligand PUT 23 3009

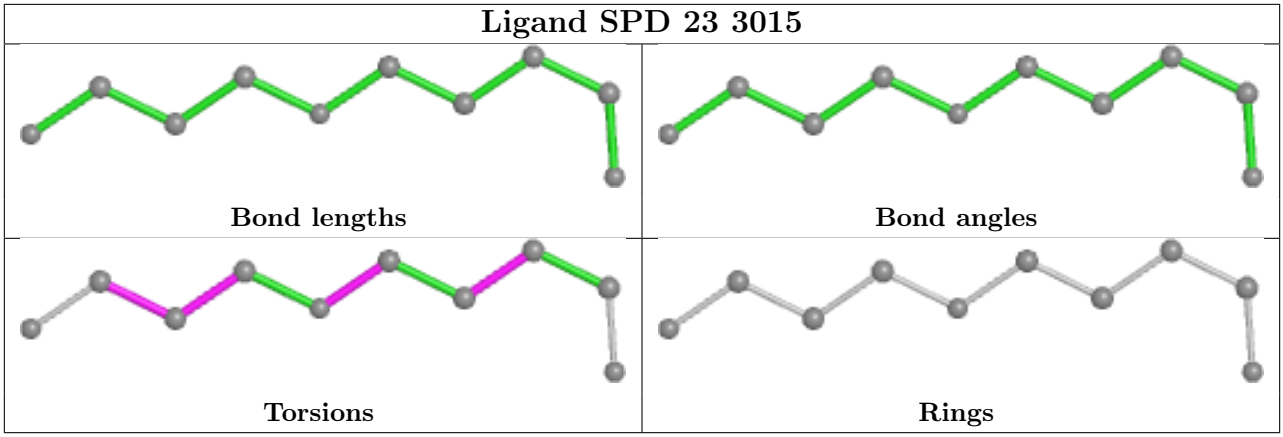


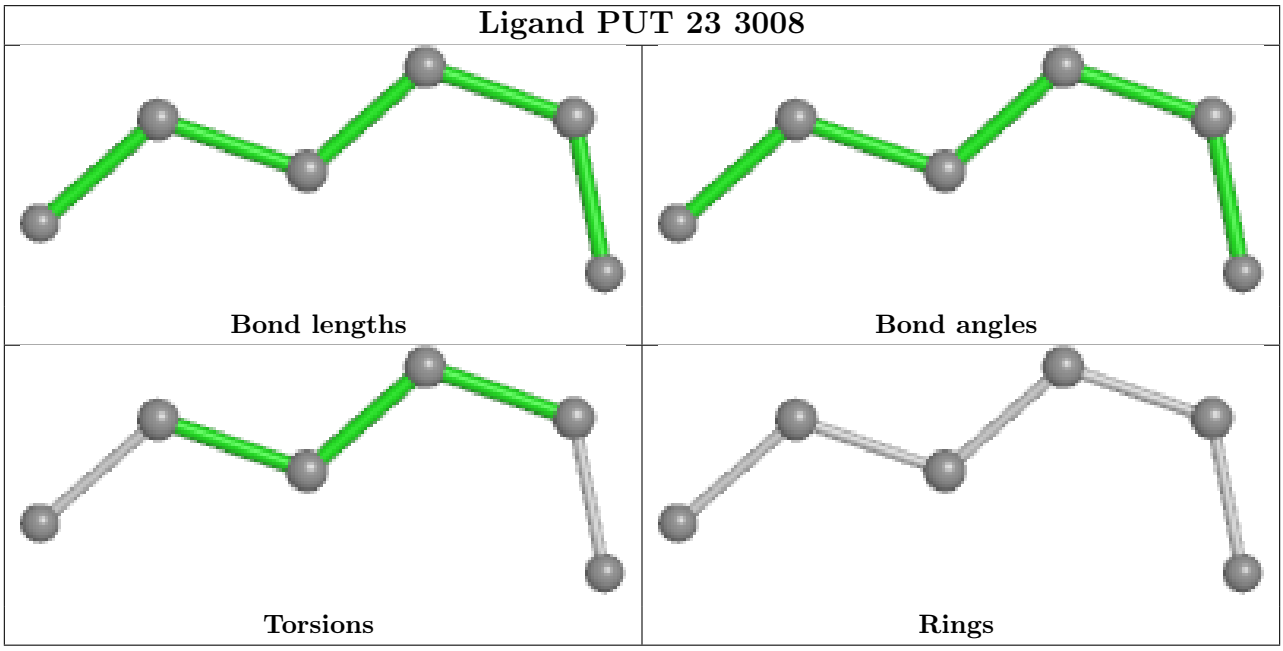
Ligand ATP 23 3001



Ligand PUT 23 3005







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

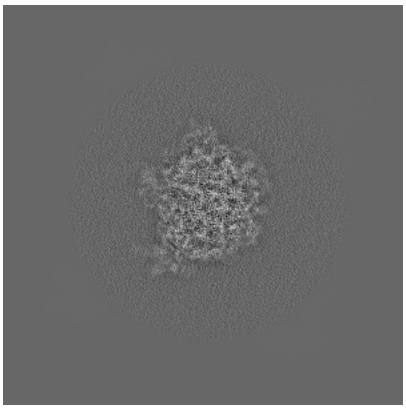
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24135. These allow visual inspection of the internal detail of the map and identification of artifacts.

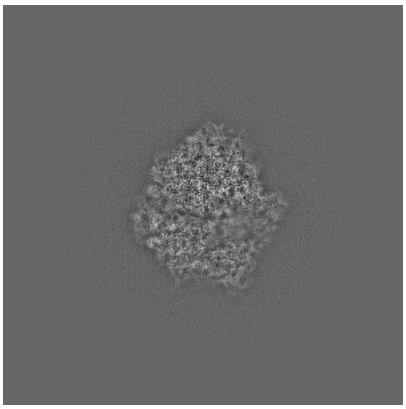
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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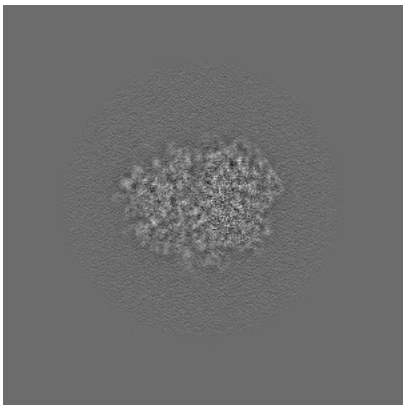
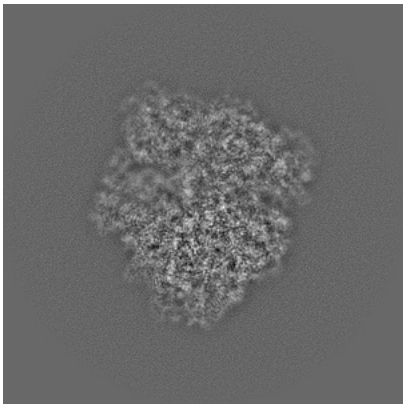
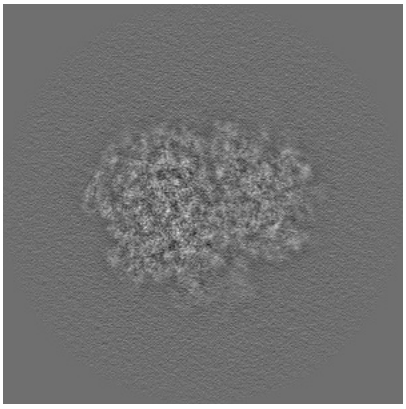


Z

6.1.2 Raw map



X



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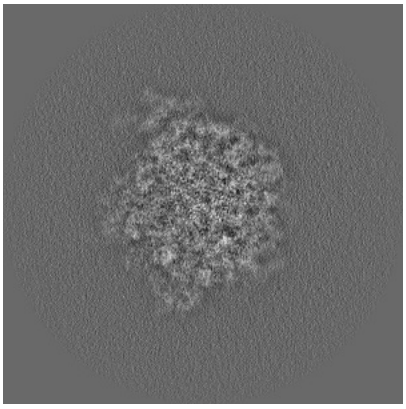
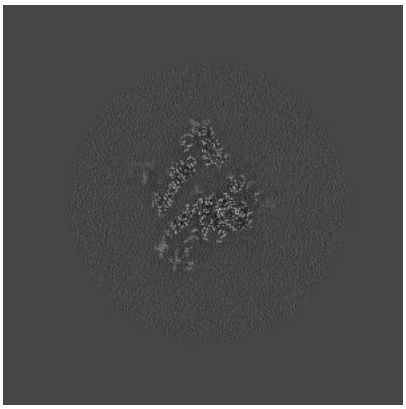


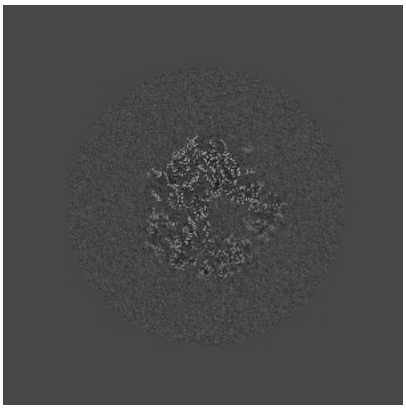
Z

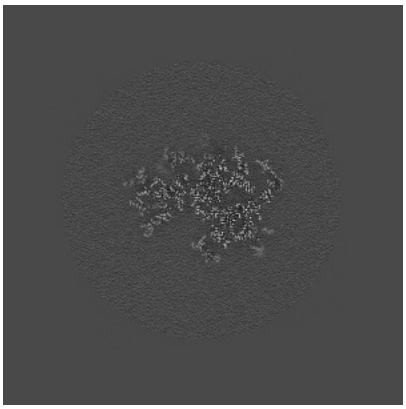
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

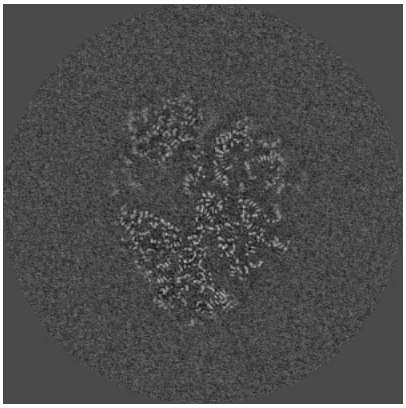
6.2.1 Primary map

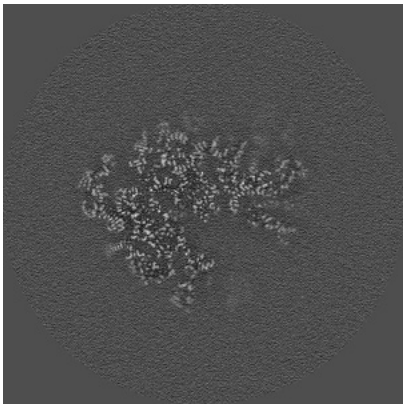

X Index: 288

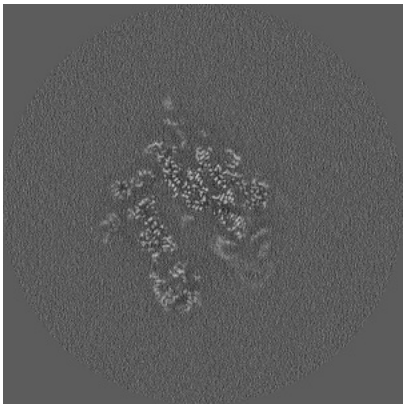

Y Index: 288


Z Index: 288

6.2.2 Raw map


X Index: 256

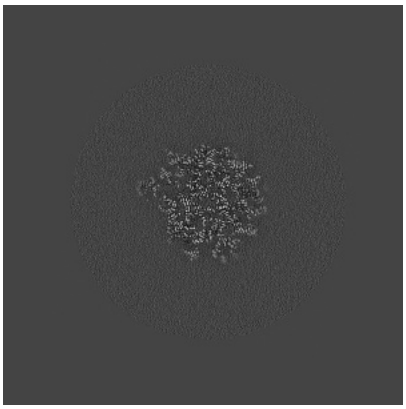

Y Index: 256

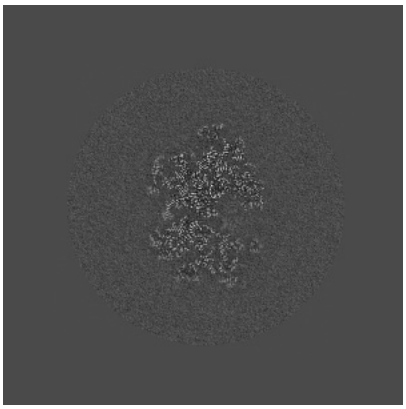

Z Index: 256

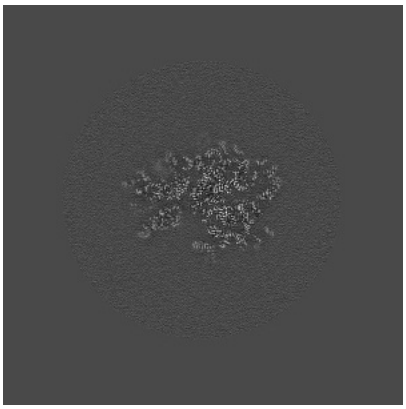
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

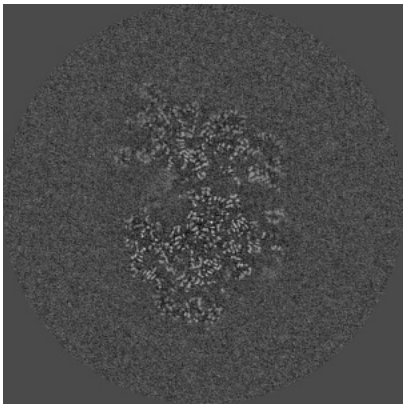
6.3.1 Primary map

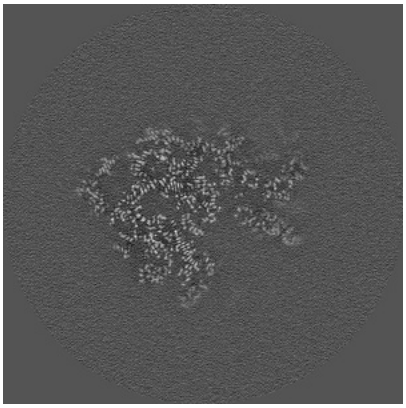

X Index: 315

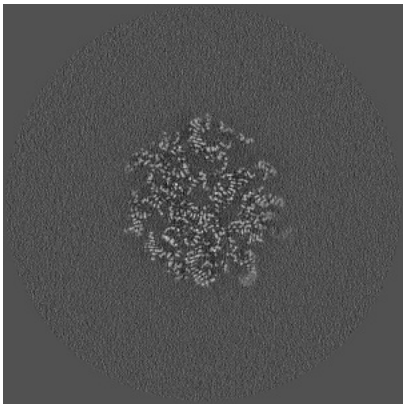

Y Index: 313


Z Index: 283

6.3.2 Raw map


X Index: 270

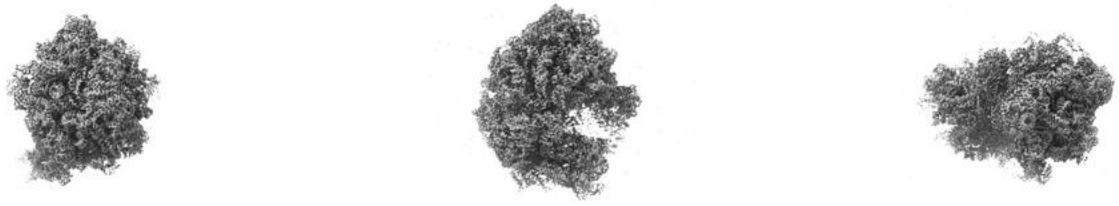

Y Index: 264


Z Index: 210

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0193. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

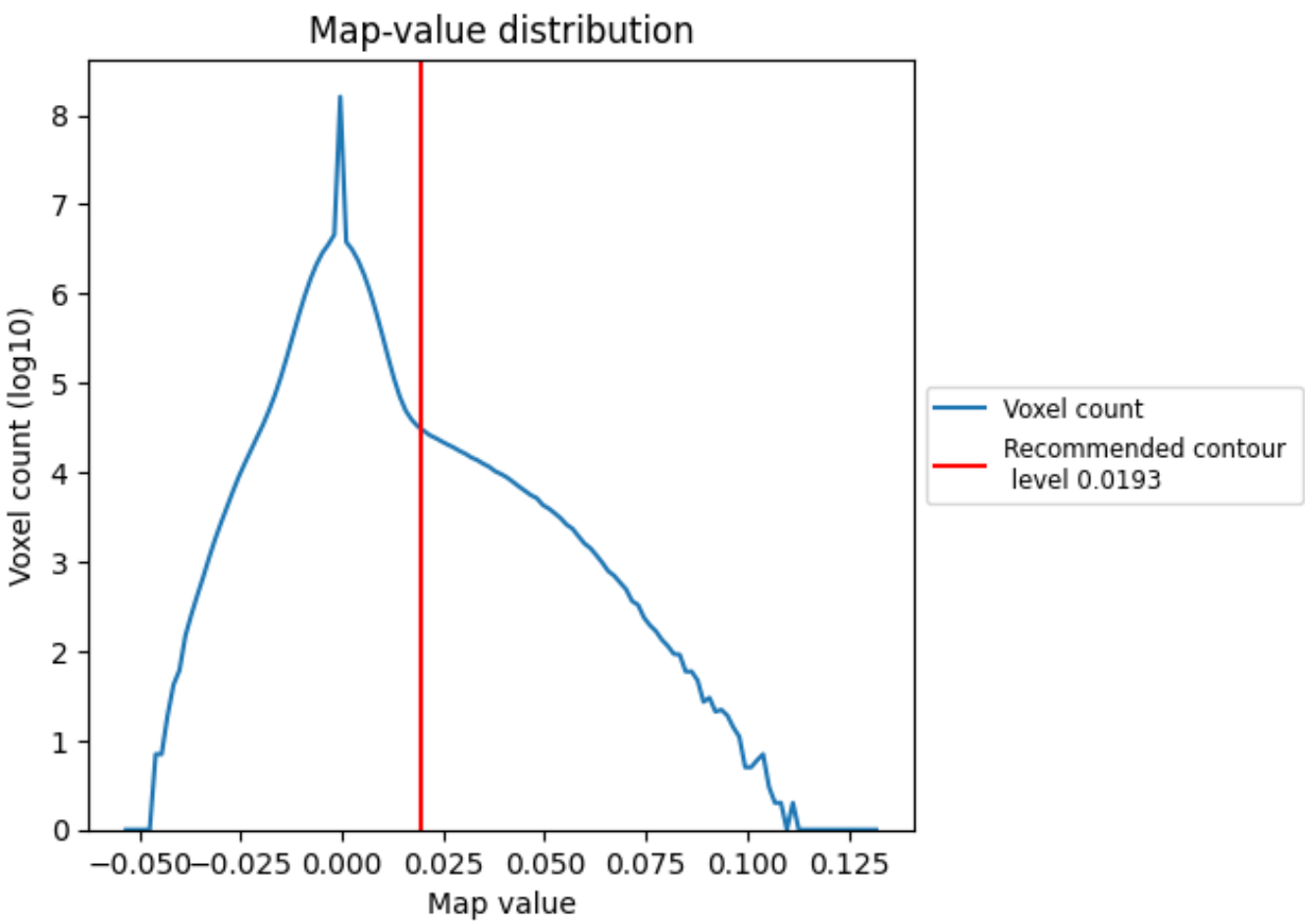
6.5 Mask visualisation (i)

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

7 Map analysis (i)

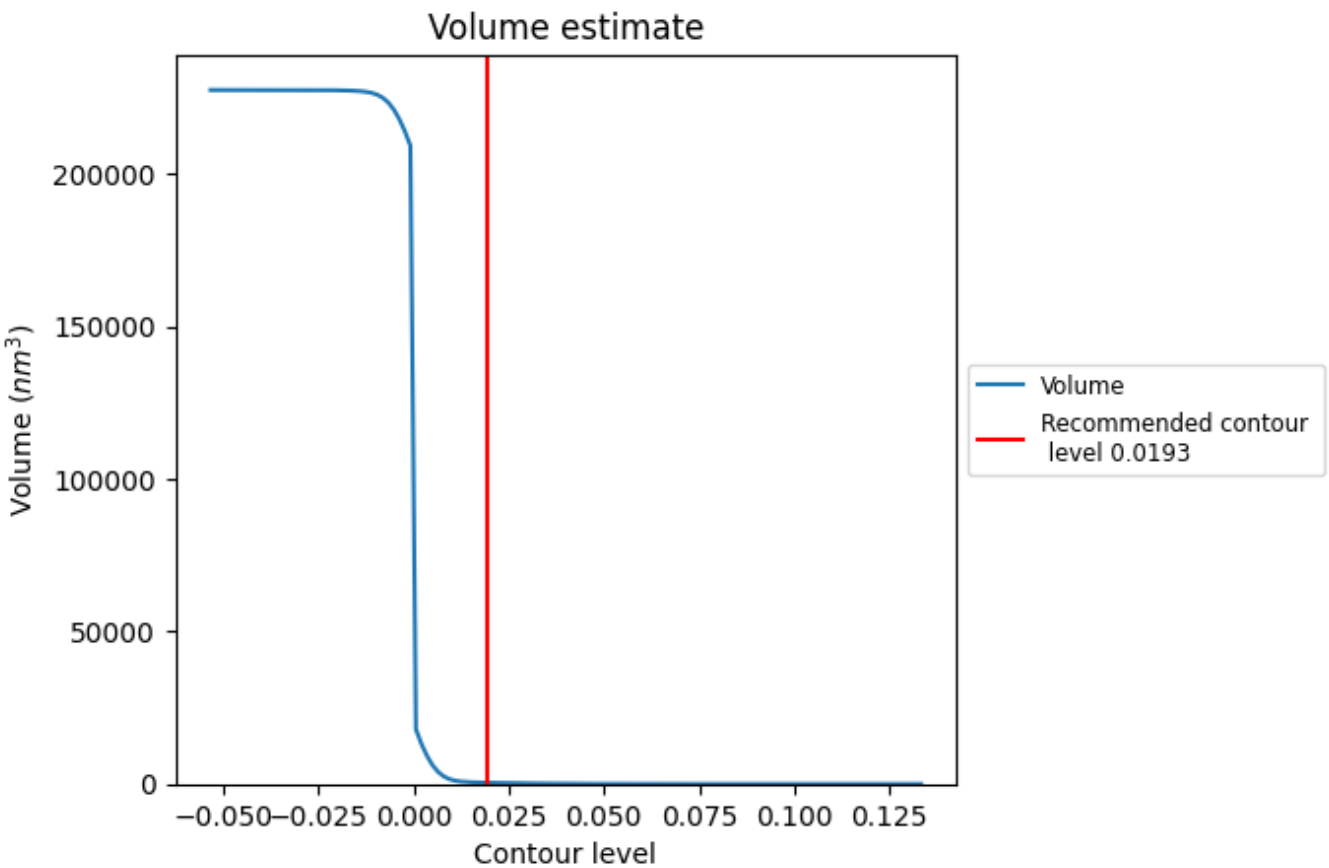
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

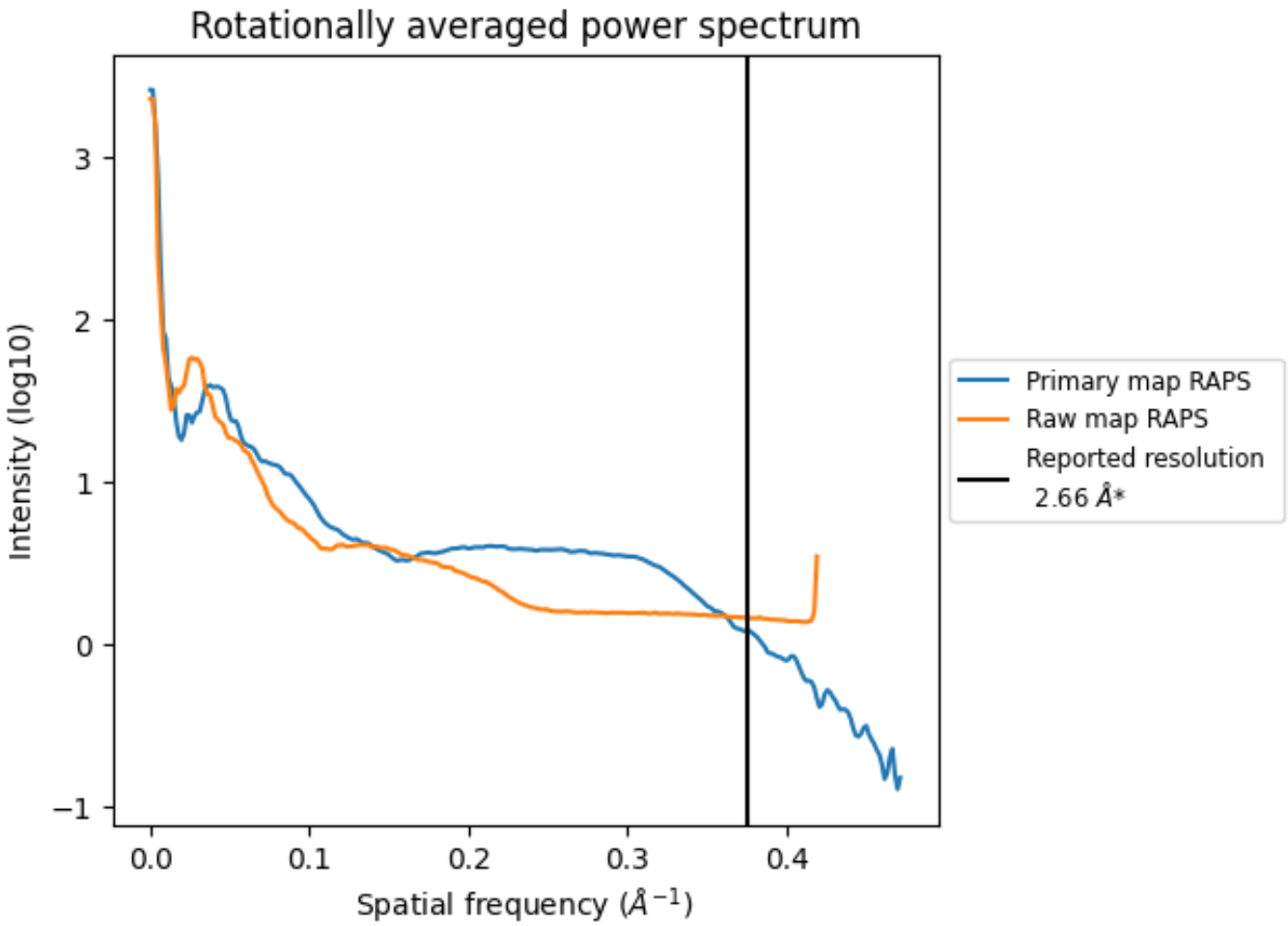
7.2 Volume estimate (i)



The volume at the recommended contour level is 403 nm^3; this corresponds to an approximate mass of 364 kDa.

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

7.3 Rotationally averaged power spectrum (i)

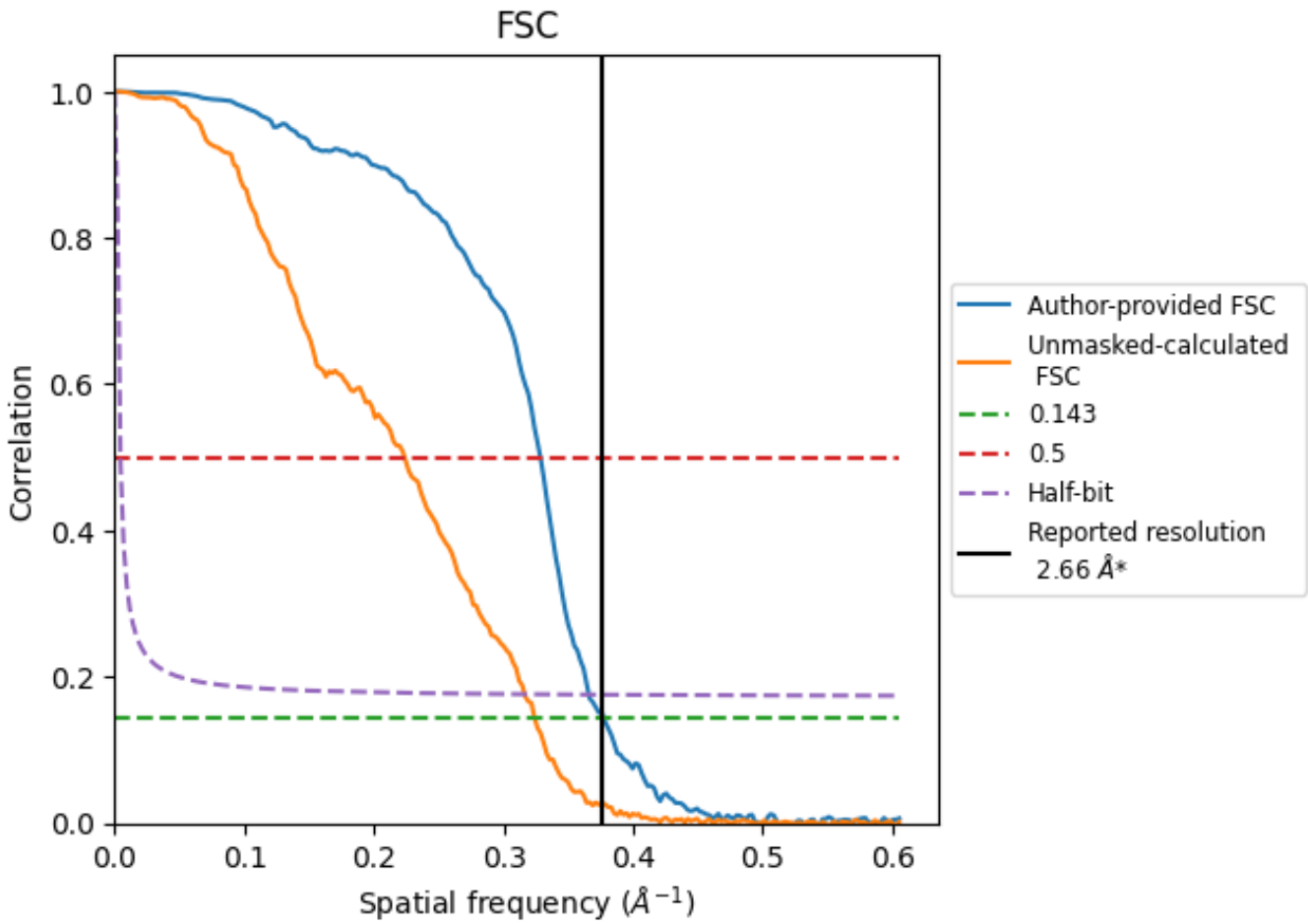


*Reported resolution corresponds to spatial frequency of 0.376 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.376 Å^{-1}

8.2 Resolution estimates (i)

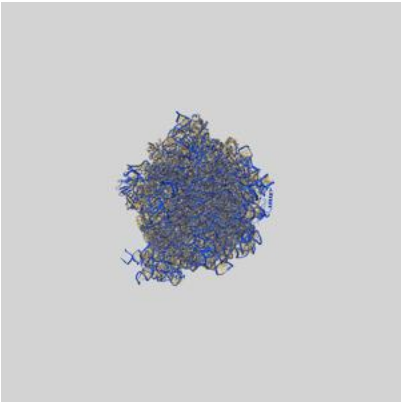
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.65	3.04	2.73
Unmasked-calculated*	3.08	4.47	3.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.08 differs from the reported value 2.66 by more than 10 %

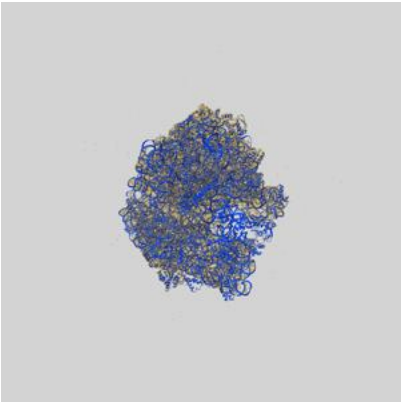
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24135 and PDB model 7N30. Per-residue inclusion information can be found in section 3 on page 17.

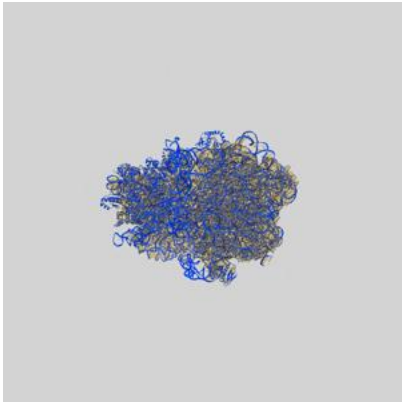
9.1 Map-model overlay (i)



X



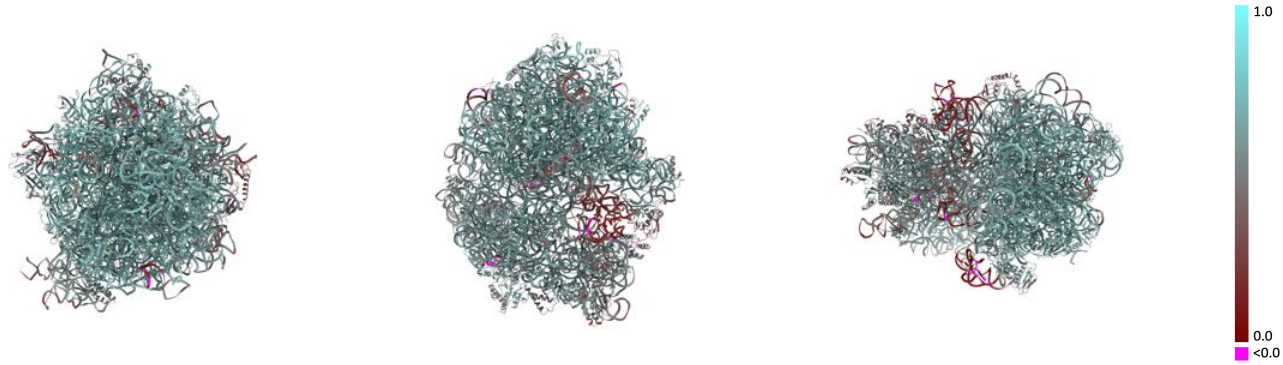
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0193 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.

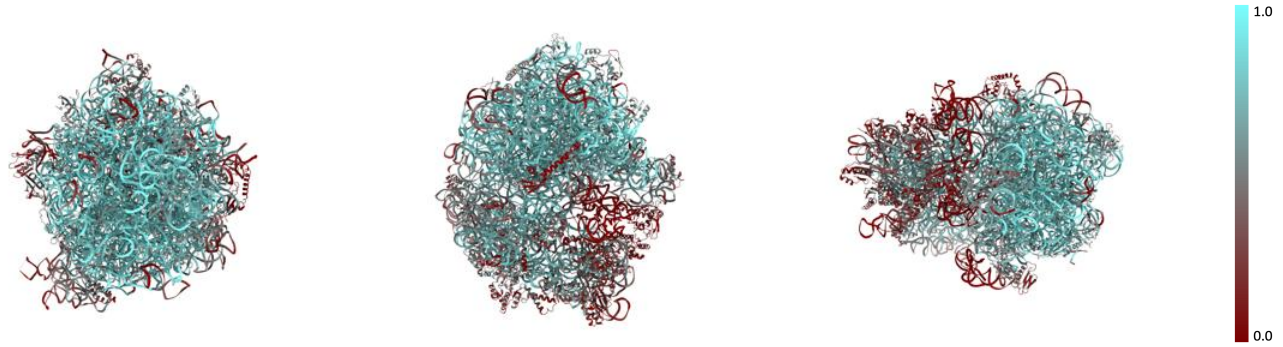
9.2 Q-score mapped to coordinate model (i)



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.

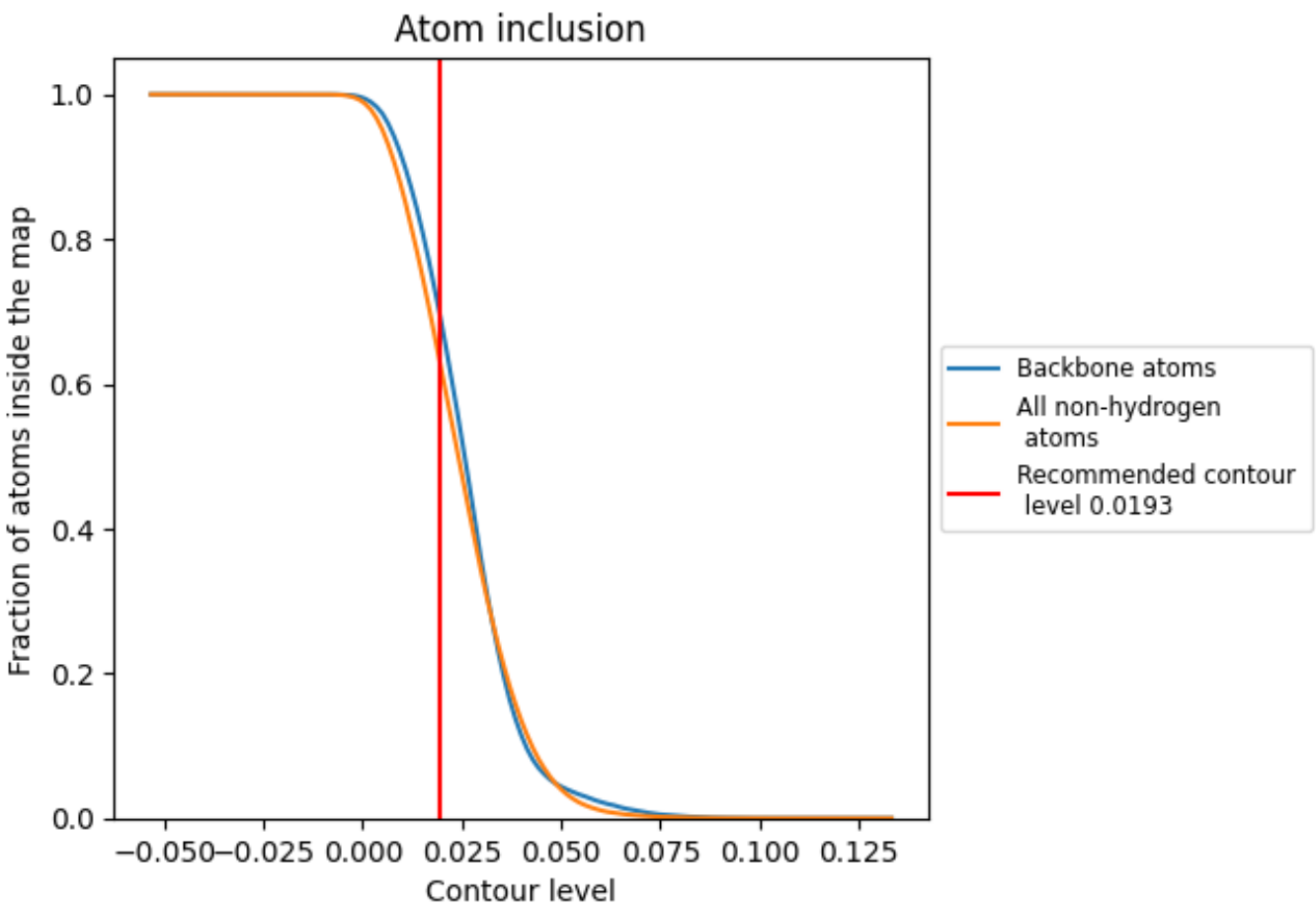
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0193).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.5920
16	0.6324	0.5900
23	0.7644	0.6100
5	0.6418	0.5960
Dt	0.2682	0.4110
LB	0.7113	0.6610
LC	0.7024	0.6500
LD	0.6259	0.6240
LE	0.1173	0.4470
LF	0.3608	0.5510
LI	0.0757	0.3770
LM	0.7118	0.6510
LN	0.6747	0.6540
LO	0.6641	0.6420
LP	0.6692	0.6460
LQ	0.7495	0.6640
LR	0.4408	0.5610
LS	0.6216	0.6310
LT	0.7522	0.6700
LU	0.6386	0.6250
LV	0.6914	0.6540
LW	0.5589	0.6010
LX	0.5286	0.6090
LY	0.5495	0.6070
La	0.6726	0.6480
Lb	0.6383	0.6410
Lc	0.5092	0.5710
Ld	0.6751	0.6260
Le	0.0391	0.2800
Lf	0.6916	0.6420
Lg	0.5131	0.6220
Lh	0.7690	0.6760
Li	0.7475	0.6670
Lj	0.6370	0.6390
Pp	0.2857	0.6310

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Pt	0.2268	0.4610
SB	0.3256	0.5240
SC	0.4262	0.5700
SD	0.3125	0.5490
SE	0.5638	0.6080
SF	0.3032	0.5190
SG	0.1486	0.4500
SH	0.5409	0.6160
SI	0.2533	0.5180
SJ	0.2416	0.4980
SK	0.4103	0.5760
SL	0.5834	0.6260
SM	0.1892	0.4880
SN	0.3372	0.5490
SO	0.4978	0.5880
SP	0.4696	0.5760
SQ	0.4446	0.5800
SR	0.4207	0.5780
SS	0.1763	0.5000
ST	0.3802	0.5660
SU	0.2732	0.5110
mR	0.6538	0.6060