



Full wwPDB EM Validation Report ⓘ

Oct 22, 2023 – 02:42 PM EDT

PDB ID : 8EVR
EMDB ID : EMD-28634
Title : Hypopseudouridylated yeast 80S bound with Taura syndrome virus (TSV) internal ribosome entry site (IRES), eEF2, GDP, and sordarin, Structure II
Authors : Zhao, Y.; Rai, J.; Li, H.
Deposited on : 2022-10-20
Resolution : 2.87 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 ⓘ symbol.

The types of validation reports are described at

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

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

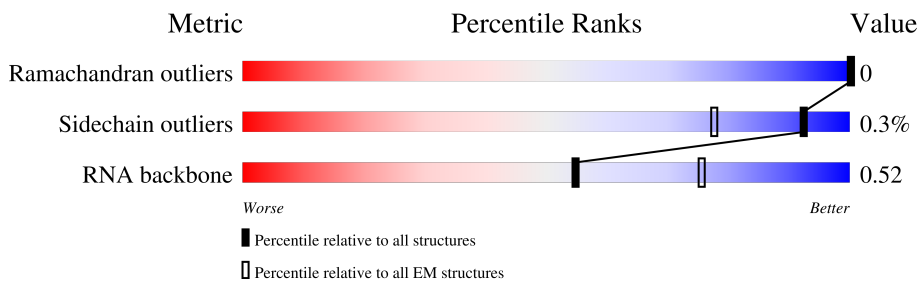
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.87 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	BA	252	 81% 18%
2	BB	255	 84% 16%
3	BC	254	 84% 15%
4	BE	261	 99%
5	BG	236	 96%
6	BH	190	 12% 96%
7	BI	200	 94% 6%
8	BJ	197	 94% 6%


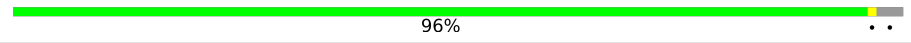
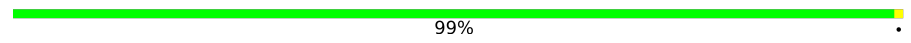
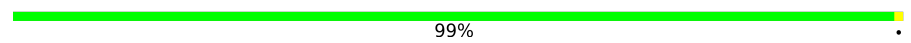



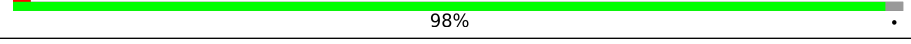



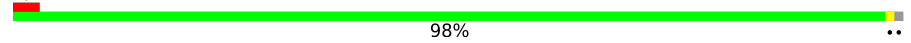
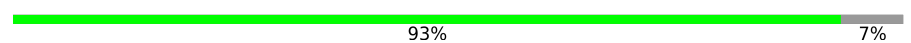
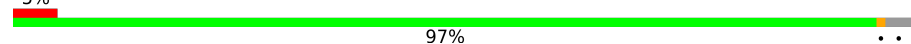
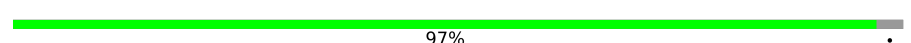
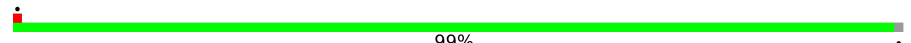
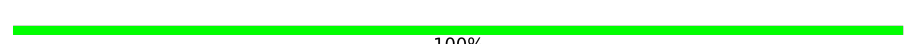

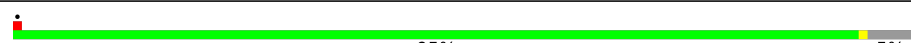




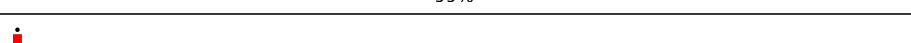

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Mol	Chain	Length	Quality of chain
9	BL	156	8% 97%
10	BN	151	99%
11	BO	137	92% 7%
12	BV	87	100%
13	BW	130	99%
14	BX	145	99%
15	BY	135	99%
16	Ba	119	81% 18%
17	Bb	82	9% 99%
18	Be	63	95% 5%
19	BD	240	5% 91% 7%
20	BF	225	13% 91% 8%
21	BK	105	12% 90% 9%
22	BP	142	15% 87% 13%
23	BQ	143	6% 98%
24	BR	136	18% 88% 11%
25	BS	146	5% 99%
26	BT	144	6% 97%
27	BU	121	9% 88% 12%
28	BZ	108	12% 63% 36%
29	Bc	67	15% 94% 6%
30	Bd	56	95% 5%
31	Bg	319	30% 98%
32	Bf	152	36% 49% 51%
33	BM	143	73% 86% 13%

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Mol	Chain	Length	Quality of chain
34	B5	1798	 73% 25% ..
35	AA	254	 96% ..
36	AB	387	 99% .
37	AC	362	 99% .
38	A1	3360	 76% 19% . 5%
39	A3	121	 89% 11%
40	A4	158	 80% 20%
41	AD	297	 98% .
42	AE	176	 88% . 11%
43	AF	244	 91% 9%
44	AG	256	 89% . 10%
45	AH	191	 98% ..
46	AI	221	 93% 7%
47	AJ	174	 5% 97% ..
48	AL	199	 97% .
49	AM	138	 99% .
50	AN	204	 100%
51	AO	199	 98% ..
52	AP	184	 95% . 5%
53	AQ	186	 99% ..
54	AR	189	 16% 99% ..
55	AS	178	 96% ..
56	AT	160	 99% .
57	AU	121	 81% . 17%
58	AV	137	 99% .

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Mol	Chain	Length	Quality of chain
59	AW	155	
60	AX	142	
61	AY	127	
62	AZ	136	
63	Aa	149	
64	Ab	59	
65	Ac	105	
66	Ad	113	
67	Ae	130	
68	Af	107	
69	Ag	121	
70	Ah	120	
71	Ai	100	
72	Aj	88	
73	Ak	78	
74	Al	51	
75	Am	128	
76	An	25	
77	Ao	106	
78	Ap	92	
79	E	217	
80	DC	842	
81	V	312	
82	EC	202	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	W9C	DC	902	X	-	-	-

2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 213962 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BA	206	1612	1034	285	291	2	0	0

- Molecule 2 is a protein called RPS1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BB	214	1709	1084	310	311	4	0	0

- Molecule 3 is a protein called RPS2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	BC	217	1635	1047	289	297	2	0	0

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	BE	260	2068	1316	389	360	3	0	0

- Molecule 5 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BG	226	1820	1142	350	325	3	0	0

- Molecule 6 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	BH	184	1481	951	265	265	0	0

- Molecule 7 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	BI	188	1489	925	298	264	2	0	0

- Molecule 8 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	BJ	185	1494	943	289	261	1	0	0

- Molecule 9 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BL	155	1244	798	235	208	3	0	0

- Molecule 10 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	BN	150	1192	759	224	207	2	0	0

- Molecule 11 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	BO	127	941	578	186	174	3	0	0

- Molecule 12 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BV	87	684	420	125	137	2	0	0

- Molecule 13 is a protein called RPS22A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BW	129	1021	650	188	180	3	0	0

- Molecule 14 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 15 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BY	134	Total	C	N	O	S	0	0
			1073	676	208	189			

- Molecule 16 is a protein called RPS26B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ba	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 17 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Bb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 18 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Be	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 19 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 20 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 21 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 22 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BP	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 23 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	BQ	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 24 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BR	121	Total	C	N	O	S	0	0
			975	611	183	179	2		

- Molecule 25 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 26 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BT	141	Total	C	N	O	S	0	0
			1095	685	206	202	2		

- Molecule 27 is a protein called RPS20 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 28 is a protein called RPS25A isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BZ	69	Total	C	N	O	0	0
			558	357	103	98		

- Molecule 29 is a protein called RPS28A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 30 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bd	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 31 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bg	312	Total	C	N	O	S	0	0
			2401	1522	410	461	8		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	75	Total	C	N	O	S	0	0
			605	386	116	99	4		

- Molecule 33 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BM	124	Total	C	N	O	S	0	0
			935	587	165	181	2		

- Molecule 34 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B5	1782	Total	C	N	O	P	1	0
			38004	17005	6718	12499	1782		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	1280	4AC	C	modified residue	GB 1329886537
B5	1773	4AC	C	modified residue	GB 1329886537

- Molecule 35 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	AA	247	1878	1170	381	326	1	0	0

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	AB	386	3081	1956	584	533	8	0	0

- Molecule 37 is a protein called RPL4A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	AC	361	2748	1729	522	494	3	0	0

- Molecule 38 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	A1	3198	68444	30595	12331	22320	3198	0	0

- Molecule 39 is a RNA chain called 5s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	A3	121	2579	1152	461	845	121	0	0

- Molecule 40 is a RNA chain called 5.8 S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
40	A4	158	3353	1500	586	1109	158	0	0

- Molecule 41 is a protein called RPL5 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AD	292	Total	C	N	O	S	0	0
			2341	1478	408	453	2		

- Molecule 42 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AE	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 43 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AF	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 44 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AG	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 45 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 46 is a protein called RPL10 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AI	205	Total	C	N	O	S	0	0
			1672	1063	316	288	5		

- Molecule 47 is a protein called RPL11A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 48 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	AL	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 49 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 50 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 51 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AO	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 52 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	AP	175	Total	C	N	O	0	0
			1388	862	277	249		

- Molecule 53 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 54 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	AR	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 55 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 56 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 57 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	AU	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 58 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 59 is a protein called RPL24A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AW	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 60 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AX	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 61 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	AY	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 62 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
62	AZ	135	1092	710	202	180	0	0

- Molecule 63 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	Aa	148	1173	749	231	190	3	0	0

- Molecule 64 is a protein called RPL29 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
64	Ab	58	462	289	100	73	0	0

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	Ac	97	743	479	124	139	1	0	0

- Molecule 66 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	Ad	109	890	565	168	156	1	0	0

- Molecule 67 is a protein called RPL32 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	Ae	127	1020	647	205	167	1	0	0

- Molecule 68 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Af	106	850	540	165	144	1	0	0

- Molecule 69 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ag	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 70 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ah	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 71 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ai	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 72 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 73 is a protein called RPL38 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	Ak	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 74 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Al	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 75 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Am	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 76 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 77 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ao	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 78 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ap	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 79 is a protein called RPL1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	E	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

- Molecule 80 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	DC	824	Total	C	N	O	S	0	0
			6419	4085	1096	1208	30		

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	V	189	Total	C	N	O	S	0	0
			1473	942	257	270	4		

- Molecule 82 is a RNA chain called TSV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	EC	191	Total	C	N	O	P	0	0
			4045	1806	718	1330	191		

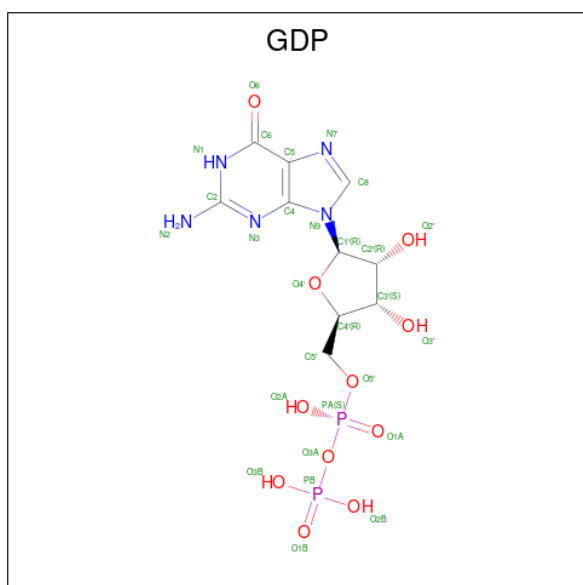
- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
83	Ba	1	Total Mg 1 1	0
83	B5	33	Total Mg 33 33	0
83	AB	1	Total Mg 1 1	0
83	A1	173	Total Mg 173 173	0
83	A3	2	Total Mg 2 2	0
83	A4	4	Total Mg 4 4	0
83	AL	1	Total Mg 1 1	0
83	AO	1	Total Mg 1 1	0
83	DC	1	Total Mg 1 1	0

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

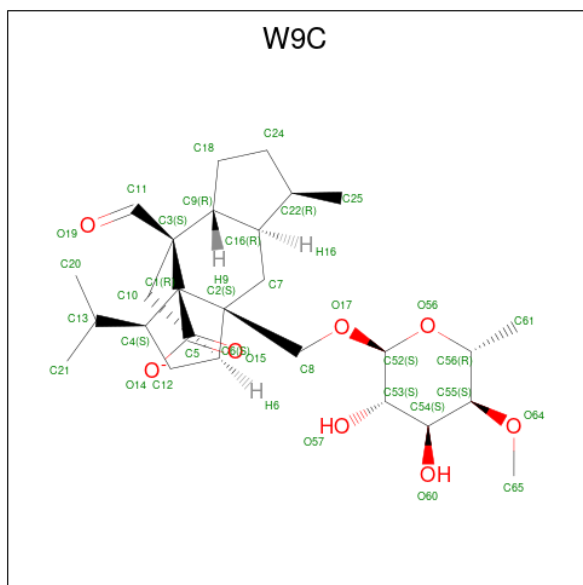
Mol	Chain	Residues	Atoms	AltConf
84	Ao	1	Total Zn 1 1	0

- Molecule 85 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

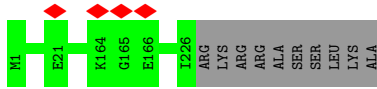


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
85	DC	1	28	10	5	11	2	0

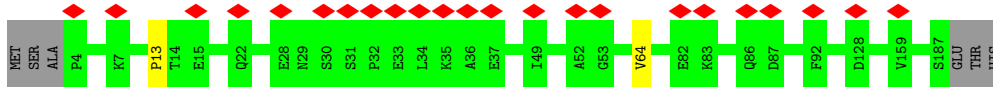
- Molecule 86 is (1S,3S,3aR,4S,4aR,7R,7aR,8aS)-8a-[[[(6-deoxy-4-O-methyl-alpha-D-altropyranosyl)oxy]methyl]-4-formyl-7-methyl-3-(propan-2-yl)decahydro-1,4-methano-s-indacene-3a(1H)-carboxylate (three-letter code: W9C) (formula: C₂₇H₄₁O₈).



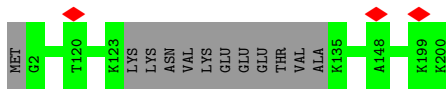
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
86	DC	1	35	27	8	0



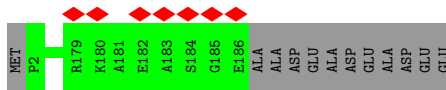
- Molecule 6: 40S ribosomal protein S7-A



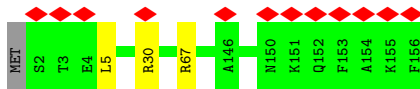
- Molecule 7: 40S ribosomal protein S8-A



- Molecule 8: 40S ribosomal protein S9-A



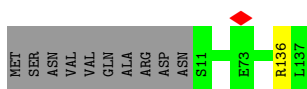
- Molecule 9: 40S ribosomal protein S11-A



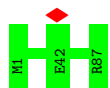
- Molecule 10: 40S ribosomal protein S13



- Molecule 11: 40S ribosomal protein S14-A



- Molecule 12: 40S ribosomal protein S21-A



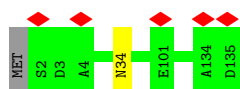
- Molecule 13: RPS22A isoform 1



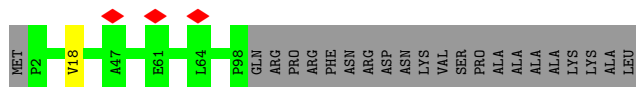
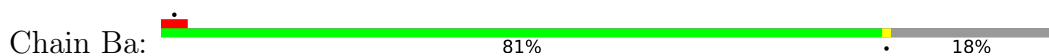
- Molecule 14: 40S ribosomal protein S23-A



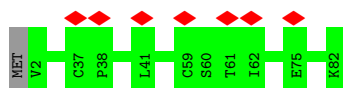
- Molecule 15: 40S ribosomal protein S24-A



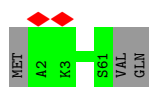
- Molecule 16: RPS26B isoform 1



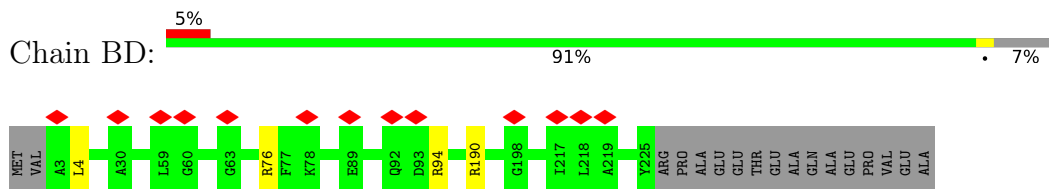
- Molecule 17: 40S ribosomal protein S27-A



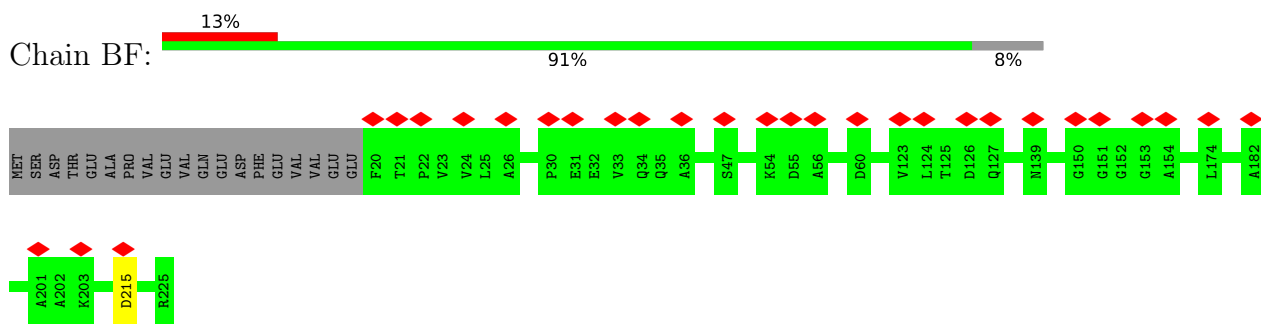
- Molecule 18: 40S ribosomal protein S30-A



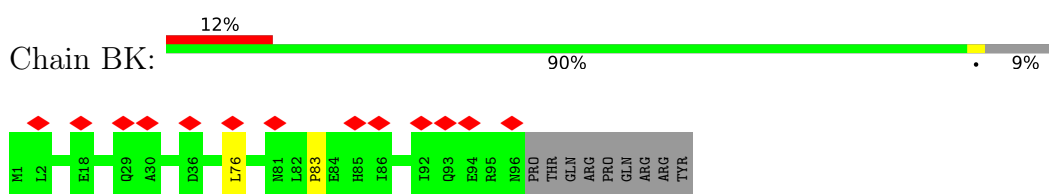
• Molecule 19: RPS3 isoform 1



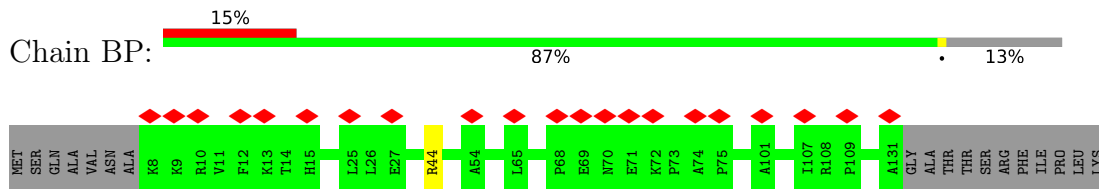
• Molecule 20: Rps5p



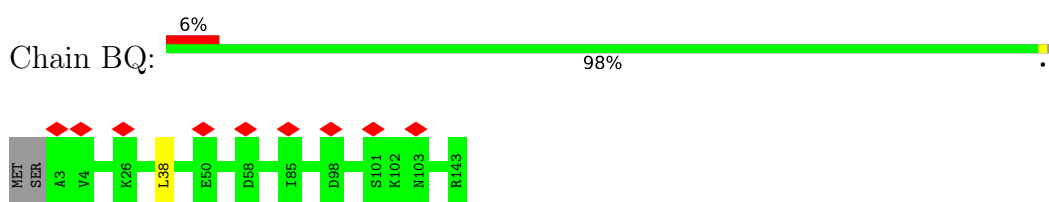
• Molecule 21: 40S ribosomal protein S10-A



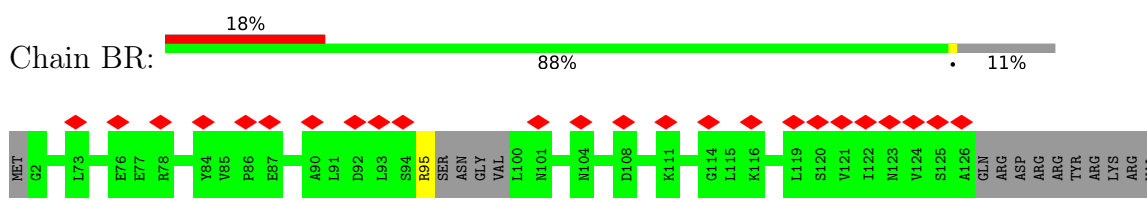
• Molecule 22: RPS15 isoform 1



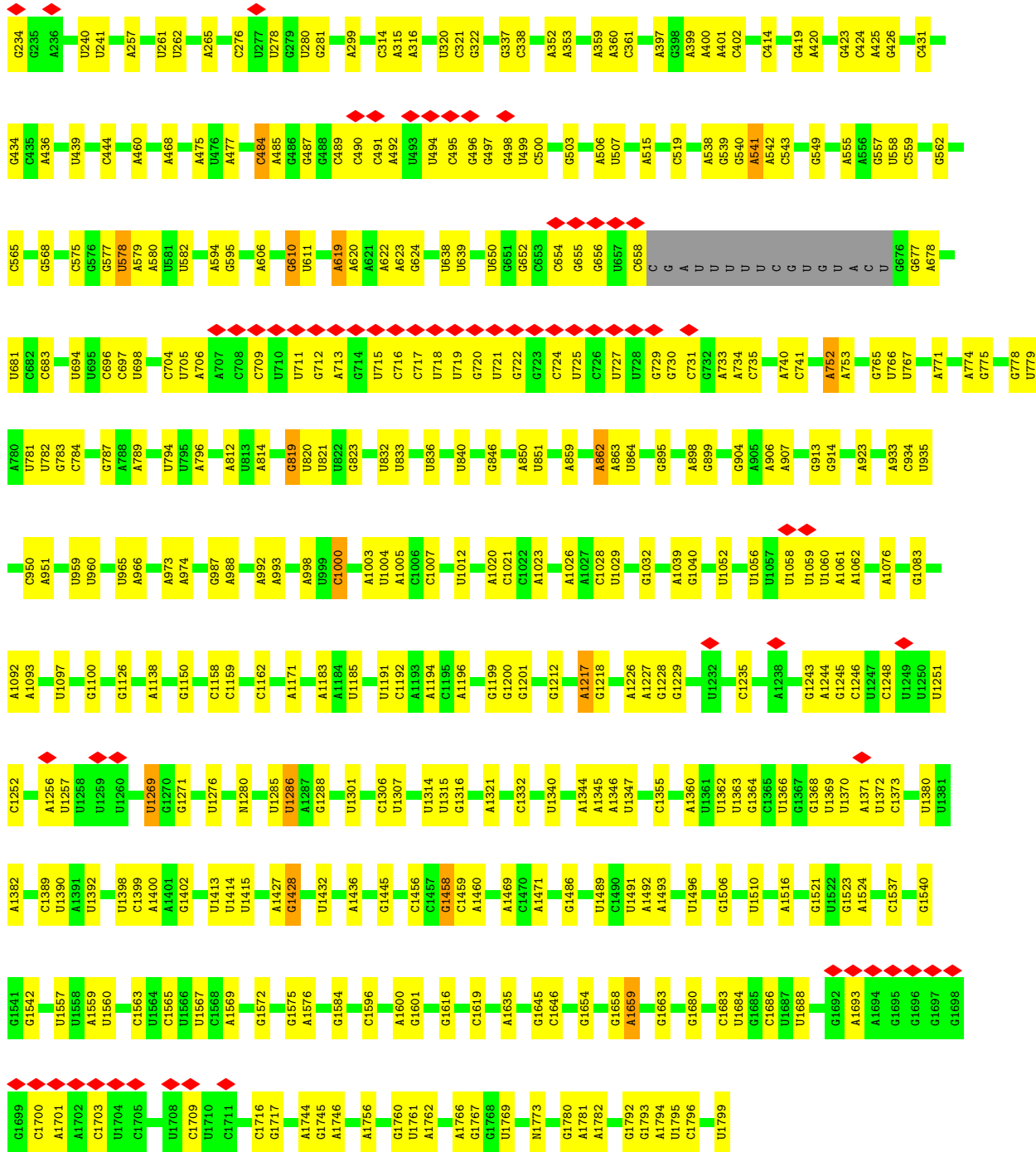
• Molecule 23: 40S ribosomal protein S16-A



• Molecule 24: 40S ribosomal protein S17-A



• Molecule 25: 40S ribosomal protein S18-A



• Molecule 35: 60S ribosomal protein L2-A



• Molecule 36: 60S ribosomal protein L3

Chain AB:  99%




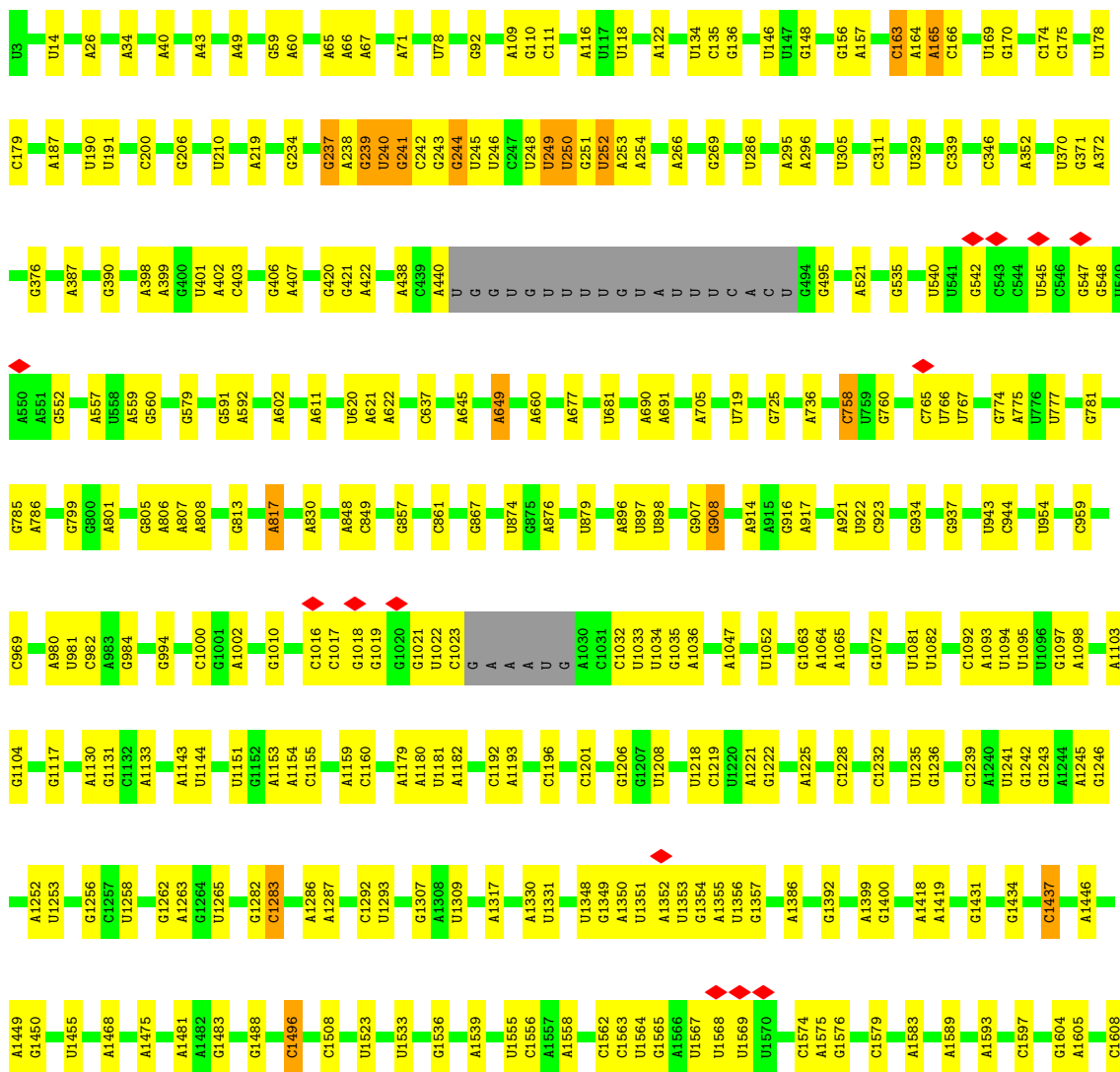
- Molecule 37: RPL4A isoform 1

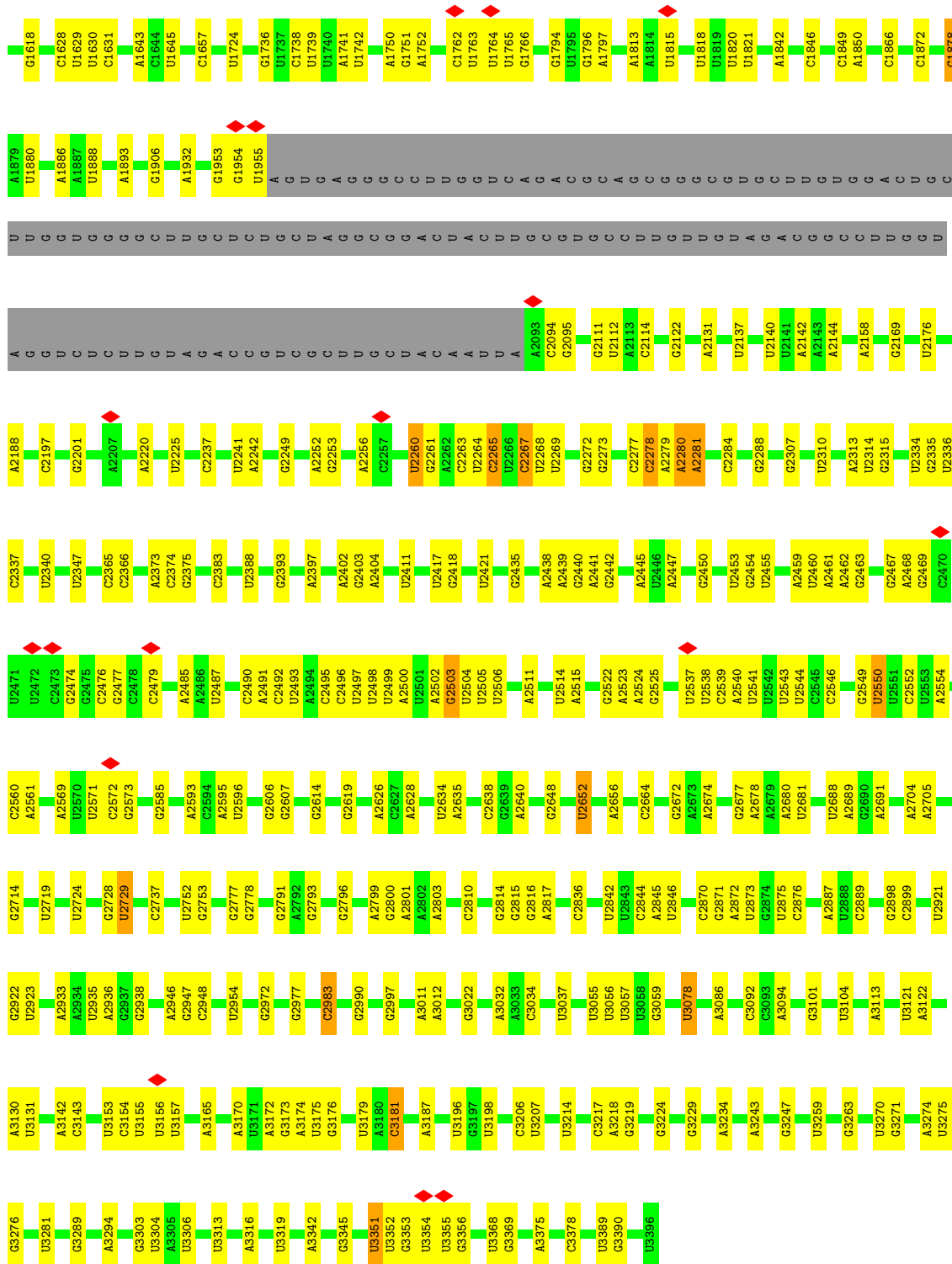
Chain AC:  99%



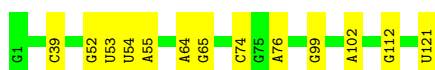
- Molecule 38: 25S rRNA

Chain A1:  76% 19% 5%

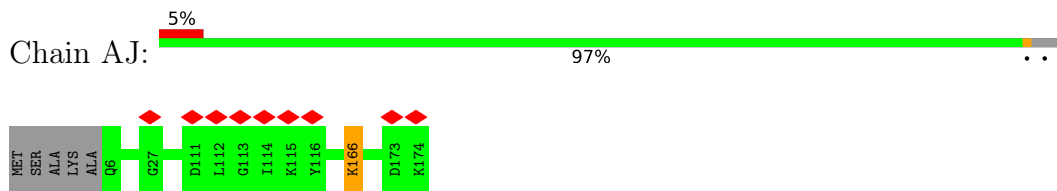




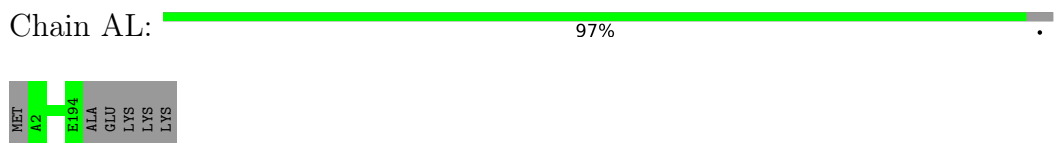
• Molecule 39: 5s rRNA



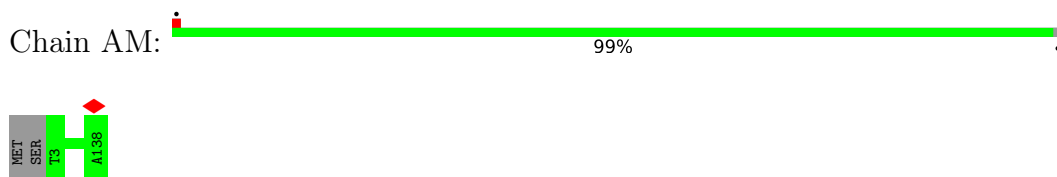
- Molecule 47: RPL11A isoform 1



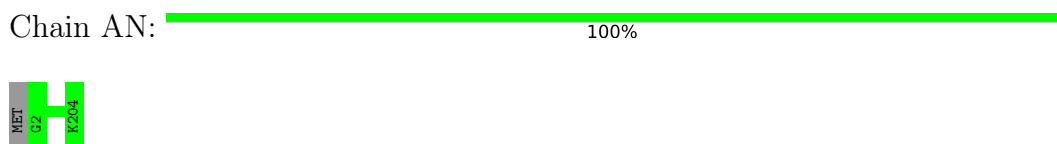
- Molecule 48: 60S ribosomal protein L13-A



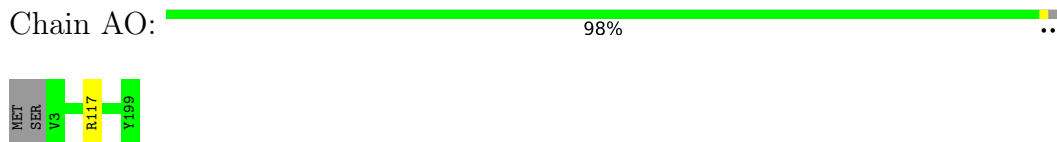
- Molecule 49: 60S ribosomal protein L14-A



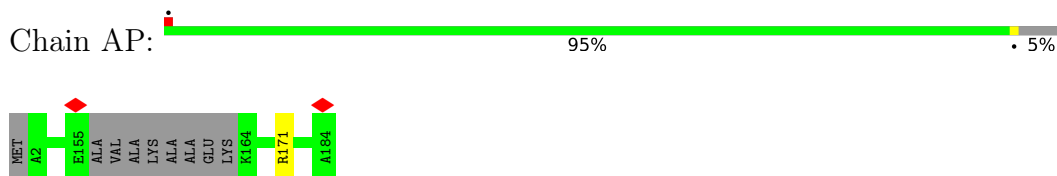
- Molecule 50: 60S ribosomal protein L15-A



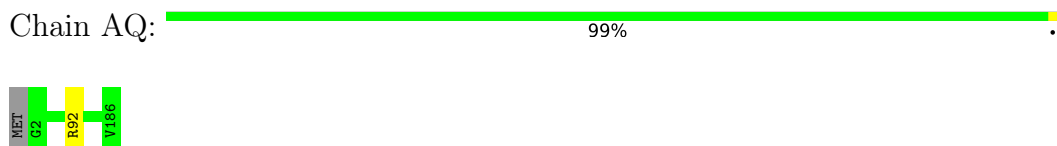
- Molecule 51: 60S ribosomal protein L16-A

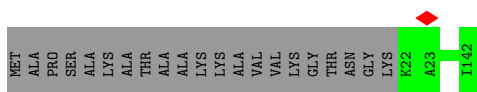


- Molecule 52: 60S ribosomal protein L17-A



- Molecule 53: 60S ribosomal protein L18-A





- Molecule 61: 60S ribosomal protein L26-A

Chain AY: 99%



- Molecule 62: 60S ribosomal protein L27-A

Chain AZ: 99%



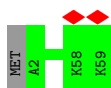
- Molecule 63: 60S ribosomal protein L28

Chain Aa: 99%



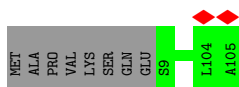
- Molecule 64: RPL29 isoform 1

Chain Ab: 98%



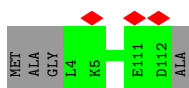
- Molecule 65: 60S ribosomal protein L30

Chain Ac: 92% 8%



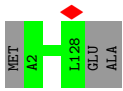
- Molecule 66: 60S ribosomal protein L31-A

Chain Ad: 96%



- Molecule 67: RPL32 isoform 1

Chain Ae:  98%



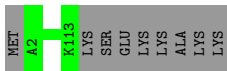
- Molecule 68: 60S ribosomal protein L33-A

Chain Af:  99%



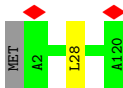
- Molecule 69: 60S ribosomal protein L34-A

Chain Ag:  93% 7%



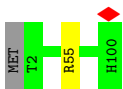
- Molecule 70: 60S ribosomal protein L35-A

Chain Ah:  98%



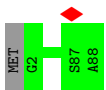
- Molecule 71: 60S ribosomal protein L36-A

Chain Ai:  98%



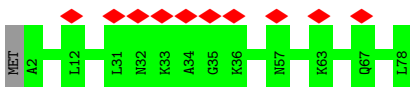
- Molecule 72: 60S ribosomal protein L37-A

Chain Aj:  99%



- Molecule 73: RPL38 isoform 1

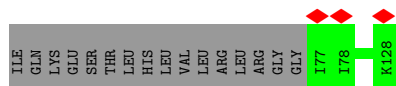
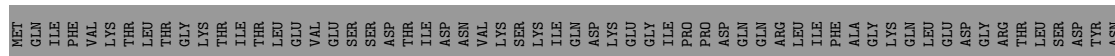
Chain Ak:  13% 99%



• Molecule 74: 60S ribosomal protein L39



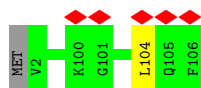
• Molecule 75: Ubiquitin-60S ribosomal protein L40



• Molecule 76: 60S ribosomal protein L41-A



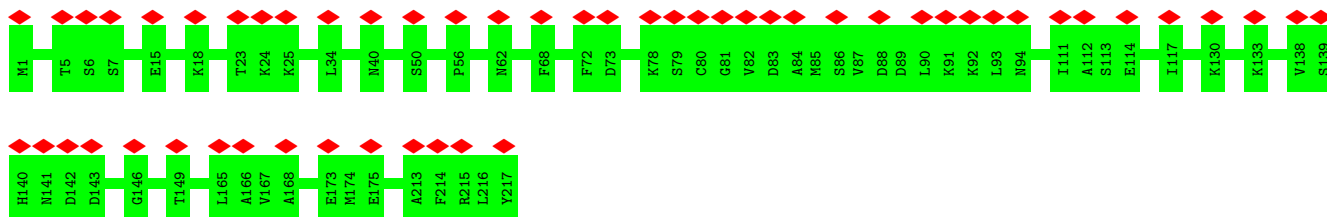
• Molecule 77: 60S ribosomal protein L42-A



• Molecule 78: 60S ribosomal protein L43-A



• Molecule 79: RPL1A isoform 1



U6902	U6903	U6904	G6905	G6906	G6907	C6908	A6909	A6910	A6911	G6912	U6913	A6914	G6915	A6916	G6917	A6918	G6919	C6920	C6921	G6922	C6923	G6924	C6925	U6926	U6927	G6928	C6929	G6930	U6931	G6935	G6936	G6937	A6938	C6939	U6940	U6941	A6942	A6943	U6944	U6945	A6946	A6947	U6948	G	C	C	U	U	G	C	C	U	A	A	C	C
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47514	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.410	Depositor
Minimum map value	-1.730	Depositor
Average map value	0.058	Depositor
Map value standard deviation	0.237	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, OMC, 5MC, XSX, GDP, 4AC, 1MA, HIC, ZN, OMG, A2M, MG, W9C, UR3, G7M, DDE, MA6

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	BA	0.46	2/1653 (0.1%)	0.85	5/2261 (0.2%)
2	BB	0.28	0/1735	0.61	1/2335 (0.0%)
3	BC	0.32	0/1665	0.57	1/2263 (0.0%)
4	BE	0.29	0/2109	0.63	2/2839 (0.1%)
5	BG	0.27	0/1844	0.58	0/2464
6	BH	0.29	0/1506	0.62	1/2028 (0.0%)
7	BI	0.27	0/1514	0.61	0/2021
8	BJ	0.26	0/1519	0.57	0/2035
9	BL	0.28	0/1272	0.60	1/1712 (0.1%)
10	BN	0.31	0/1215	0.60	0/1638
11	BO	0.29	0/952	0.67	0/1279
12	BV	0.29	0/693	0.69	0/935
13	BW	0.27	0/1038	0.58	0/1395
14	BX	0.26	0/1139	0.57	0/1518
15	BY	0.29	0/1087	0.61	0/1449
16	Ba	0.29	0/782	0.76	1/1047 (0.1%)
17	Bb	0.27	0/620	0.65	0/838
18	Be	0.25	0/483	0.66	0/643
19	BD	0.28	0/1759	0.63	1/2368 (0.0%)
20	BF	0.34	0/1629	0.62	1/2202 (0.0%)
21	BK	0.63	2/837 (0.2%)	1.10	6/1131 (0.5%)
22	BP	0.28	0/1012	0.60	0/1356
23	BQ	0.28	0/1125	0.58	1/1510 (0.1%)
24	BR	0.26	0/984	0.62	0/1318
25	BS	0.26	0/1211	0.61	1/1628 (0.1%)
26	BT	0.28	0/1113	0.56	0/1494
27	BU	0.27	0/865	0.56	0/1169
28	BZ	0.28	0/566	0.62	0/761
29	Bc	0.30	0/499	0.78	0/670
30	Bd	0.28	0/452	0.61	0/600
31	Bg	0.27	0/2454	0.60	0/3340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Bf	0.29	0/616	0.65	1/817 (0.1%)
33	BM	0.29	0/943	0.71	2/1274 (0.2%)
34	B5	0.31	0/41880	0.91	67/65248 (0.1%)
35	AA	0.31	0/1912	0.66	2/2569 (0.1%)
36	AB	0.29	0/3139	0.58	1/4219 (0.0%)
37	AC	0.28	0/2800	0.56	1/3790 (0.0%)
38	A1	0.39	0/75586	0.90	117/117845 (0.1%)
39	A3	0.35	0/2883	0.88	2/4491 (0.0%)
40	A4	0.36	0/3746	0.85	3/5832 (0.1%)
41	AD	0.29	0/2390	0.54	0/3225
42	AE	0.28	0/1260	0.54	0/1694
43	AF	0.29	0/1821	0.51	0/2451
44	AG	0.28	0/1830	0.53	0/2469
45	AH	0.34	0/1531	0.60	0/2062
46	AI	0.29	0/1708	0.56	0/2290
47	AJ	0.29	0/1374	0.65	0/1842
48	AL	0.28	0/1568	0.58	0/2106
49	AM	0.26	0/1068	0.53	0/1438
50	AN	0.29	0/1757	0.60	0/2354
51	AO	0.29	0/1585	0.53	0/2128
52	AP	0.30	0/1410	0.59	0/1893
53	AQ	0.28	0/1465	0.58	0/1965
54	AR	0.26	0/1538	0.58	0/2050
55	AS	0.32	0/1481	0.58	0/1990
56	AT	0.31	0/1300	0.55	0/1743
57	AU	0.30	0/812	0.62	2/1099 (0.2%)
58	AV	0.30	0/1018	0.60	0/1369
59	AW	0.32	0/533	0.59	0/707
60	AX	0.30	0/983	0.55	0/1325
61	AY	0.30	0/1004	0.62	0/1341
62	AZ	0.29	0/1118	0.54	0/1497
63	Aa	0.29	0/1204	0.58	0/1612
64	Ab	0.27	0/473	0.52	0/629
65	Ac	0.30	0/751	0.55	0/1008
66	Ad	0.28	0/904	0.57	0/1213
67	Ae	0.28	0/1041	0.55	0/1394
68	Af	0.31	0/868	0.59	0/1168
69	Ag	0.32	0/890	0.63	0/1189
70	Ah	0.26	0/978	0.53	1/1301 (0.1%)
71	Ai	0.29	0/778	0.62	0/1034
72	Aj	0.29	0/696	0.59	0/923
73	Ak	0.27	0/618	0.61	0/826
74	Al	0.29	0/443	0.67	1/588 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Am	0.30	0/423	0.61	0/562
76	An	0.26	0/234	0.72	0/300
77	Ao	0.32	0/860	0.68	1/1136 (0.1%)
78	Ap	0.30	0/701	0.57	0/934
79	E	0.26	0/1745	0.58	0/2342
80	DC	0.29	0/6521	0.61	3/8830 (0.0%)
81	V	0.28	0/1498	0.61	1/2025 (0.0%)
82	EC	0.33	1/4521 (0.0%)	0.97	12/7039 (0.2%)
All	All	0.33	5/227538 (0.0%)	0.80	239/333423 (0.1%)

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
3	BC	0	2
6	BH	0	1
15	BY	0	1
44	AG	0	2
47	AJ	0	1
76	An	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	97	PRO	CB-CG	-11.35	0.93	1.50
21	BK	83	PRO	CB-CG	-11.28	0.93	1.50
82	EC	6758	A	OP3-P	-10.56	1.48	1.61
21	BK	83	PRO	CG-CD	-10.02	1.17	1.50
1	BA	97	PRO	CG-CD	-8.93	1.21	1.50

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	97	PRO	N-CD-CG	-18.30	75.76	103.20
21	BK	83	PRO	N-CD-CG	-17.68	76.67	103.20
1	BA	97	PRO	CA-CB-CG	-16.89	71.92	104.00
21	BK	83	PRO	CA-CB-CG	-16.53	72.59	104.00
21	BK	83	PRO	CB-CG-CD	14.33	162.40	106.50
80	DC	385	MET	CG-SD-CE	-10.00	84.20	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	250	U	N1-C2-O2	9.34	129.34	122.80
38	A1	237	G	C8-N9-C4	-9.19	102.72	106.40
38	A1	250	U	N3-C2-O2	-9.09	115.84	122.20
1	BA	97	PRO	CB-CG-CD	9.05	141.81	106.50
38	A1	250	U	C2-N1-C1'	8.78	128.23	117.70
33	BM	82	PRO	CA-N-CD	-8.73	99.28	111.50
9	BL	5	LEU	CA-CB-CG	8.60	135.07	115.30
38	A1	163	C	C2-N1-C1'	8.44	128.08	118.80
38	A1	2506	U	C2-N1-C1'	8.33	127.69	117.70
32	Bf	144	CYS	CA-CB-SG	8.31	128.95	114.00
34	B5	965	U	C2-N1-C1'	8.15	127.48	117.70
38	A1	922	U	C2-N1-C1'	8.10	127.42	117.70
34	B5	1000	C	N1-C2-O2	8.09	123.76	118.90
38	A1	3034	C	C2-N1-C1'	7.93	127.52	118.80
38	A1	163	C	C5-C6-N1	7.79	124.89	121.00
38	A1	3181	C	N1-C2-O2	7.77	123.56	118.90
38	A1	240	U	P-O3'-C3'	7.54	128.74	119.70
38	A1	922	U	N1-C2-O2	7.53	128.07	122.80
38	A1	2225	U	N3-C2-O2	-7.51	116.94	122.20
34	B5	1389	C	C2-N1-C1'	7.46	127.01	118.80
34	B5	1686	C	N1-C2-O2	7.45	123.37	118.90
34	B5	1000	C	N3-C2-O2	-7.36	116.75	121.90
38	A1	2260	U	N1-C2-O2	7.34	127.94	122.80
82	EC	6908	C	N1-C2-O2	7.25	123.25	118.90
34	B5	1286	U	N1-C2-O2	7.24	127.86	122.80
1	BA	97	PRO	CA-N-CD	-7.16	101.48	111.50
38	A1	163	C	C6-N1-C2	-7.15	117.44	120.30
21	BK	83	PRO	CA-N-CD	-7.06	101.62	111.50
38	A1	2506	U	N1-C2-O2	7.06	127.74	122.80
38	A1	3034	C	N1-C2-O2	7.02	123.11	118.90
38	A1	922	U	N3-C2-O2	-7.01	117.30	122.20
37	AC	182	LEU	CA-CB-CG	6.98	131.36	115.30
34	B5	1286	U	C2-N1-C1'	6.95	126.04	117.70
4	BE	87	MET	CA-CB-CG	6.94	125.10	113.30
38	A1	2260	U	N3-C2-O2	-6.92	117.36	122.20
80	DC	385	MET	CB-CG-SD	6.86	132.98	112.40
38	A1	163	C	N1-C2-O2	6.83	123.00	118.90
38	A1	3181	C	C2-N1-C1'	6.80	126.28	118.80
38	A1	2550	U	N3-C2-O2	-6.79	117.45	122.20
38	A1	406	G	O4'-C1'-N9	6.75	113.60	108.20
34	B5	1000	C	C2-N1-C1'	6.71	126.18	118.80
38	A1	2237	C	N3-C2-O2	-6.70	117.21	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1286	U	N3-C2-O2	-6.69	117.52	122.20
34	B5	610	G	N3-C4-C5	-6.66	125.27	128.60
34	B5	1686	C	C2-N1-C1'	6.64	126.10	118.80
38	A1	3034	C	N3-C2-O2	-6.63	117.25	121.90
38	A1	2225	U	N1-C2-O2	6.61	127.42	122.80
33	BM	82	PRO	N-CD-CG	-6.58	93.32	103.20
38	A1	3181	C	N3-C2-O2	-6.57	117.30	121.90
38	A1	239	G	P-O3'-C3'	6.55	127.56	119.70
82	EC	6796	C	N1-C2-O2	6.55	122.83	118.90
34	B5	1380	U	C2-N1-C1'	6.54	125.55	117.70
38	A1	2267	C	N1-C2-O2	6.51	122.81	118.90
40	A4	5	U	C2-N1-C1'	6.50	125.50	117.70
34	B5	864	U	C2-N1-C1'	6.49	125.49	117.70
34	B5	1162	C	N1-C2-O2	6.49	122.80	118.90
34	B5	959	U	N1-C2-O2	6.46	127.32	122.80
38	A1	2836	C	C2-N1-C1'	6.39	125.83	118.80
40	A4	5	U	N3-C2-O2	-6.37	117.74	122.20
34	B5	767	U	N3-C2-O2	-6.36	117.75	122.20
38	A1	2267	C	N3-C2-O2	-6.36	117.45	121.90
34	B5	1560	U	C2-N1-C1'	6.35	125.32	117.70
34	B5	1567	U	N1-C2-O2	6.34	127.24	122.80
34	B5	1389	C	C6-N1-C2	-6.33	117.77	120.30
80	DC	385	MET	CA-CB-CG	-6.33	102.54	113.30
38	A1	1222	G	O4'-C1'-N9	6.29	113.23	108.20
34	B5	1567	U	N3-C2-O2	-6.28	117.80	122.20
38	A1	237	G	N7-C8-N9	6.28	116.24	113.10
34	B5	1307	U	N1-C2-O2	6.24	127.17	122.80
38	A1	3078	U	N1-C2-O2	6.23	127.16	122.80
38	A1	2225	U	C2-N1-C1'	6.23	125.18	117.70
38	A1	2550	U	N1-C2-O2	6.22	127.15	122.80
34	B5	166	C	C2-N1-C1'	6.21	125.63	118.80
38	A1	2899	C	C2-N1-C1'	6.20	125.61	118.80
38	A1	237	G	N9-C4-C5	6.18	107.87	105.40
34	B5	959	U	C2-N1-C1'	6.18	125.11	117.70
34	B5	1458	G	N3-C4-C5	-6.16	125.52	128.60
38	A1	2983	C	C2-N1-C1'	6.16	125.58	118.80
38	A1	3078	U	C2-N1-C1'	6.15	125.08	117.70
19	BD	4	LEU	CA-CB-CG	6.12	129.39	115.30
38	A1	2260	U	C2-N1-C1'	6.12	125.04	117.70
38	A1	165	A	P-O3'-C3'	6.11	127.03	119.70
38	A1	982	C	C2-N1-C1'	6.10	125.51	118.80
4	BE	87	MET	CG-SD-CE	-6.10	90.44	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	1283	C	C5-C6-N1	6.06	124.03	121.00
82	EC	6943	A	P-O3'-C3'	6.03	126.93	119.70
38	A1	3078	U	N3-C2-O2	-6.02	117.99	122.20
34	B5	1659	A	N7-C8-N9	6.02	116.81	113.80
38	A1	252	U	C5-C6-N1	6.01	125.71	122.70
34	B5	166	C	N1-C2-O2	6.00	122.50	118.90
34	B5	1560	U	N3-C2-O2	-5.99	118.01	122.20
38	A1	237	G	N3-C2-N2	-5.99	115.71	119.90
38	A1	3214	U	C2-N1-C1'	5.98	124.88	117.70
38	A1	2264	U	C5-C6-N1	5.97	125.69	122.70
34	B5	965	U	N1-C2-O2	5.97	126.98	122.80
38	A1	1496	C	C2-N1-C1'	5.97	125.36	118.80
34	B5	864	U	N1-C2-O2	5.96	126.97	122.80
38	A1	2237	C	N1-C2-O2	5.96	122.48	118.90
38	A1	2550	U	C2-N1-C1'	5.96	124.86	117.70
57	AU	91	ASP	CB-CG-OD1	5.96	123.67	118.30
40	A4	100	U	C2-N1-C1'	5.95	124.84	117.70
1	BA	43	ASP	CB-CG-OD1	5.93	123.64	118.30
38	A1	2846	U	N3-C2-O2	-5.92	118.05	122.20
34	B5	1567	U	C2-N1-C1'	5.92	124.80	117.70
38	A1	240	U	C2-N1-C1'	5.91	124.79	117.70
38	A1	3037	U	N3-C2-O2	-5.90	118.07	122.20
82	EC	6908	C	C2-N1-C1'	5.90	125.29	118.80
34	B5	819	G	P-O3'-C3'	5.89	126.77	119.70
34	B5	959	U	N3-C2-O2	-5.89	118.08	122.20
6	BH	13	PRO	C-N-CA	5.89	136.42	121.70
34	B5	767	U	C2-N1-C1'	5.87	124.74	117.70
38	A1	2506	U	C6-N1-C1'	-5.87	112.99	121.20
38	A1	241	G	P-O3'-C3'	5.84	126.71	119.70
38	A1	169	U	N1-C2-O2	5.83	126.88	122.80
38	A1	2899	C	N1-C2-O2	5.83	122.39	118.90
38	A1	1604	G	C4-N9-C1'	5.82	134.07	126.50
2	BB	54	LEU	CA-CB-CG	5.81	128.67	115.30
38	A1	969	C	N1-C2-O2	5.81	122.39	118.90
34	B5	484	C	N1-C2-O2	5.81	122.39	118.90
34	B5	1162	C	C2-N1-C1'	5.80	125.18	118.80
34	B5	1307	U	C2-N1-C1'	5.80	124.67	117.70
38	A1	2846	U	C2-N1-C1'	5.79	124.65	117.70
35	AA	51	ASP	CB-CG-OD2	5.79	123.51	118.30
38	A1	239	G	OP2-P-O3'	5.78	117.92	105.20
34	B5	965	U	C6-N1-C1'	-5.78	113.11	121.20
34	B5	862	A	P-O3'-C3'	5.76	126.61	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	610	G	C2-N3-C4	5.75	114.78	111.90
34	B5	1744	A	C5-C6-N1	5.75	120.57	117.70
74	A1	13	MET	CG-SD-CE	-5.75	91.00	100.20
38	A1	2506	U	N3-C2-O2	-5.74	118.18	122.20
82	EC	6851	G	P-O3'-C3'	5.73	126.58	119.70
38	A1	3037	U	C2-N1-C1'	5.72	124.57	117.70
39	A3	39	C	N1-C2-O2	5.71	122.33	118.90
38	A1	1872	C	N1-C2-O2	5.71	122.33	118.90
82	EC	6859	U	O4'-C1'-N1	-5.71	103.63	108.20
38	A1	169	U	N3-C2-O2	-5.71	118.21	122.20
77	Ao	104	LEU	CA-CB-CG	5.68	128.36	115.30
34	B5	116	U	N3-C2-O2	-5.66	118.23	122.20
38	A1	954	U	C2-N1-C1'	5.66	124.49	117.70
34	B5	1458	G	C2-N3-C4	5.65	114.73	111.90
38	A1	3034	C	C6-N1-C2	-5.63	118.05	120.30
38	A1	2836	C	N3-C2-O2	-5.62	117.96	121.90
25	BS	51	ASP	CB-CG-OD2	5.62	123.36	118.30
57	AU	90	ARG	C-N-CA	5.62	135.76	121.70
34	B5	1654	G	N3-C2-N2	-5.61	115.97	119.90
34	B5	610	G	N3-C4-N9	5.61	129.37	126.00
38	A1	252	U	N1-C2-O2	5.61	126.72	122.80
82	EC	6796	C	C2-N1-C1'	5.60	124.96	118.80
82	EC	6908	C	N3-C2-O2	-5.60	117.98	121.90
38	A1	954	U	N3-C2-O2	-5.58	118.29	122.20
21	BK	76	LEU	CB-CG-CD1	-5.58	101.51	111.00
38	A1	2846	U	N1-C2-O2	5.57	126.70	122.80
38	A1	3181	C	C6-N1-C2	-5.57	118.07	120.30
34	B5	1456	C	C2-N1-C1'	5.55	124.91	118.80
16	Ba	18	VAL	C-N-CA	5.55	135.56	121.70
34	B5	87	C	C2-N1-C1'	5.54	124.90	118.80
38	A1	2546	C	C2-N1-C1'	5.54	124.90	118.80
38	A1	252	U	N3-C2-O2	-5.51	118.34	122.20
38	A1	1878	G	C4-N9-C1'	5.51	133.67	126.50
39	A3	39	C	C2-N1-C1'	5.51	124.86	118.80
34	B5	1307	U	N3-C2-O2	-5.50	118.35	122.20
38	A1	758	C	C2-N1-C1'	5.50	124.85	118.80
38	A1	240	U	N3-C2-O2	-5.48	118.37	122.20
34	B5	864	U	N3-C2-O2	-5.48	118.37	122.20
34	B5	1332	C	C2-N1-C1'	5.47	124.82	118.80
34	B5	1000	C	C6-N1-C2	-5.46	118.11	120.30
70	Ah	28	LEU	CA-CB-CG	5.45	127.84	115.30
3	BC	81	MET	CG-SD-CE	5.43	108.89	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BQ	38	LEU	CA-CB-CG	5.43	127.78	115.30
34	B5	1380	U	N1-C2-O2	5.42	126.59	122.80
38	A1	2137	U	C2-N1-C1'	5.42	124.20	117.70
38	A1	2546	C	C6-N1-C2	-5.42	118.13	120.30
82	EC	6799	C	C6-N1-C2	-5.41	118.14	120.30
34	B5	1745	G	O4'-C1'-N9	5.40	112.52	108.20
34	B5	1686	C	N3-C2-O2	-5.39	118.13	121.90
82	EC	6851	G	OP1-P-O3'	5.39	117.05	105.20
34	B5	1389	C	N1-C2-O2	5.39	122.13	118.90
38	A1	922	U	C6-N1-C1'	-5.38	113.67	121.20
38	A1	250	U	C6-N1-C1'	-5.36	113.69	121.20
38	A1	2503	G	C4-N9-C1'	5.36	133.47	126.50
38	A1	169	U	C2-N1-C1'	5.36	124.13	117.70
35	AA	32	LEU	CB-CG-CD2	-5.36	101.89	111.00
38	A1	969	C	N3-C2-O2	-5.34	118.16	121.90
38	A1	163	C	C6-N1-C1'	-5.33	114.40	120.80
34	B5	184	C	C2-N1-C1'	5.33	124.66	118.80
38	A1	1645	U	N3-C2-O2	-5.33	118.47	122.20
34	B5	1596	C	C2-N1-C1'	5.33	124.66	118.80
34	B5	1332	C	N1-C2-O2	5.32	122.09	118.90
38	A1	2873	U	C2-N1-C1'	5.31	124.07	117.70
38	A1	3034	C	C6-N1-C1'	-5.31	114.43	120.80
34	B5	1286	U	C5-C6-N1	5.30	125.35	122.70
38	A1	954	U	N1-C2-O2	5.30	126.51	122.80
38	A1	179	C	C5-C6-N1	5.29	123.65	121.00
38	A1	240	U	C6-N1-C2	-5.28	117.83	121.00
34	B5	1744	A	N3-C4-N9	5.27	131.62	127.40
38	A1	240	U	C5-C6-N1	5.27	125.33	122.70
38	A1	244	G	P-O3'-C3'	5.27	126.02	119.70
34	B5	1560	U	N1-C2-O2	5.26	126.48	122.80
38	A1	249	U	O5'-P-OP2	5.26	117.01	110.70
38	A1	2836	C	N1-C2-O2	5.26	122.05	118.90
21	BK	76	LEU	CB-CG-CD2	-5.24	102.10	111.00
38	A1	2265	C	C6-N1-C2	-5.24	118.20	120.30
38	A1	2652	U	N3-C2-O2	-5.23	118.54	122.20
38	A1	3214	U	N3-C2-O2	-5.22	118.54	122.20
20	BF	215	ASP	CB-CG-OD1	5.21	122.99	118.30
38	A1	252	U	C6-N1-C2	-5.21	117.88	121.00
34	B5	965	U	N3-C2-O2	-5.20	118.56	122.20
38	A1	2476	C	C6-N1-C2	-5.19	118.22	120.30
38	A1	78	U	N3-C2-O2	-5.19	118.57	122.20
38	A1	1608	C	C2-N1-C1'	5.14	124.45	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	1597	C	C5-C6-N1	5.13	123.56	121.00
38	A1	1283	C	C6-N1-C2	-5.12	118.25	120.30
38	A1	3057	U	N1-C2-O2	5.11	126.37	122.80
34	B5	752	A	P-O3'-C3'	5.10	125.82	119.70
36	AB	351	LEU	CA-CB-CG	5.10	127.04	115.30
34	B5	934	C	C2-N1-C1'	5.10	124.41	118.80
34	B5	1162	C	N3-C2-O2	-5.10	118.33	121.90
38	A1	3306	U	C2-N1-C1'	5.10	123.82	117.70
34	B5	1217	A	P-O3'-C3'	5.10	125.82	119.70
34	B5	543	C	N1-C2-O2	5.09	121.96	118.90
38	A1	2522	G	N3-C4-C5	-5.08	126.06	128.60
82	EC	6779	C	N1-C2-O2	5.08	121.95	118.90
38	A1	1604	G	N3-C4-C5	-5.06	126.07	128.60
38	A1	2267	C	C6-N1-C2	-5.06	118.28	120.30
38	A1	3037	U	N1-C2-O2	5.06	126.34	122.80
38	A1	2836	C	C6-N1-C2	-5.06	118.28	120.30
82	EC	6796	C	N3-C2-O2	-5.05	118.37	121.90
38	A1	3351	U	N1-C2-O2	5.05	126.33	122.80
81	V	77	LEU	CA-CB-CG	5.05	126.91	115.30
38	A1	1604	G	N3-C4-N9	5.04	129.02	126.00
38	A1	3057	U	N3-C2-O2	-5.02	118.68	122.20
38	A1	2899	C	N3-C2-O2	-5.01	118.39	121.90
34	B5	1012	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	AG	121	SER	Peptide
44	AG	30	THR	Peptide
47	AJ	166	LYS	Peptide
76	An	23	ARG	Sidechain
3	BC	144	TRP	Peptide
3	BC	145	GLY	Peptide
6	BH	64	VAL	Peptide
15	BY	34	ASN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	204/252 (81%)	182 (89%)	22 (11%)	0	100	100
2	BB	212/255 (83%)	184 (87%)	28 (13%)	0	100	100
3	BC	215/254 (85%)	204 (95%)	11 (5%)	0	100	100
4	BE	258/261 (99%)	233 (90%)	25 (10%)	0	100	100
5	BG	224/236 (95%)	215 (96%)	9 (4%)	0	100	100
6	BH	182/190 (96%)	170 (93%)	12 (7%)	0	100	100
7	BI	184/200 (92%)	167 (91%)	17 (9%)	0	100	100
8	BJ	183/197 (93%)	172 (94%)	11 (6%)	0	100	100
9	BL	153/156 (98%)	138 (90%)	15 (10%)	0	100	100
10	BN	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
11	BO	125/137 (91%)	111 (89%)	14 (11%)	0	100	100
12	BV	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
13	BW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
14	BX	142/145 (98%)	126 (89%)	16 (11%)	0	100	100
15	BY	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
16	Ba	95/119 (80%)	80 (84%)	15 (16%)	0	100	100
17	Bb	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
18	Be	58/63 (92%)	51 (88%)	7 (12%)	0	100	100
19	BD	221/240 (92%)	206 (93%)	15 (7%)	0	100	100
20	BF	204/225 (91%)	186 (91%)	18 (9%)	0	100	100
21	BK	94/105 (90%)	82 (87%)	12 (13%)	0	100	100
22	BP	122/142 (86%)	112 (92%)	10 (8%)	0	100	100
23	BQ	139/143 (97%)	134 (96%)	5 (4%)	0	100	100
24	BR	117/136 (86%)	109 (93%)	8 (7%)	0	100	100
25	BS	143/146 (98%)	126 (88%)	17 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BT	139/144 (96%)	126 (91%)	13 (9%)	0	100	100
27	BU	105/121 (87%)	97 (92%)	8 (8%)	0	100	100
28	BZ	67/108 (62%)	63 (94%)	4 (6%)	0	100	100
29	Bc	61/67 (91%)	56 (92%)	5 (8%)	0	100	100
30	Bd	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
31	Bg	310/319 (97%)	278 (90%)	32 (10%)	0	100	100
32	Bf	73/152 (48%)	64 (88%)	9 (12%)	0	100	100
33	BM	122/143 (85%)	115 (94%)	7 (6%)	0	100	100
35	AA	245/254 (96%)	228 (93%)	17 (7%)	0	100	100
36	AB	383/387 (99%)	361 (94%)	22 (6%)	0	100	100
37	AC	359/362 (99%)	337 (94%)	22 (6%)	0	100	100
41	AD	290/297 (98%)	274 (94%)	16 (6%)	0	100	100
42	AE	152/176 (86%)	141 (93%)	11 (7%)	0	100	100
43	AF	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
44	AG	228/256 (89%)	210 (92%)	18 (8%)	0	100	100
45	AH	188/191 (98%)	171 (91%)	17 (9%)	0	100	100
46	AI	201/221 (91%)	195 (97%)	6 (3%)	0	100	100
47	AJ	167/174 (96%)	150 (90%)	17 (10%)	0	100	100
48	AL	191/199 (96%)	178 (93%)	13 (7%)	0	100	100
49	AM	134/138 (97%)	127 (95%)	7 (5%)	0	100	100
50	AN	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
51	AO	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
52	AP	171/184 (93%)	163 (95%)	8 (5%)	0	100	100
53	AQ	183/186 (98%)	177 (97%)	6 (3%)	0	100	100
54	AR	186/189 (98%)	178 (96%)	8 (4%)	0	100	100
55	AS	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
56	AT	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
57	AU	98/121 (81%)	92 (94%)	6 (6%)	0	100	100
58	AV	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
59	AW	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
60	AX	119/142 (84%)	114 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AY	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
62	AZ	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
63	Aa	146/149 (98%)	133 (91%)	13 (9%)	0	100	100
64	Ab	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
65	Ac	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
66	Ad	107/113 (95%)	100 (94%)	7 (6%)	0	100	100
67	Ae	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
68	Af	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
69	Ag	110/121 (91%)	105 (96%)	5 (4%)	0	100	100
70	Ah	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
71	Ai	97/100 (97%)	89 (92%)	8 (8%)	0	100	100
72	Aj	85/88 (97%)	81 (95%)	4 (5%)	0	100	100
73	Ak	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
74	Al	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
75	Am	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	91 (88%)	12 (12%)	0	100	100
78	Ap	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
79	E	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
80	DC	819/842 (97%)	759 (93%)	60 (7%)	0	100	100
81	V	187/312 (60%)	176 (94%)	11 (6%)	0	100	100
All	All	12115/13257 (91%)	11288 (93%)	827 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	173/210 (82%)	173 (100%)	0	100	100
2	BB	191/224 (85%)	191 (100%)	0	100	100
3	BC	176/205 (86%)	175 (99%)	1 (1%)	86	95
4	BE	221/222 (100%)	221 (100%)	0	100	100
5	BG	193/201 (96%)	193 (100%)	0	100	100
6	BH	165/170 (97%)	165 (100%)	0	100	100
7	BI	150/161 (93%)	150 (100%)	0	100	100
8	BJ	158/166 (95%)	158 (100%)	0	100	100
9	BL	136/137 (99%)	134 (98%)	2 (2%)	65	86
10	BN	127/128 (99%)	127 (100%)	0	100	100
11	BO	96/105 (91%)	95 (99%)	1 (1%)	76	91
12	BV	74/74 (100%)	74 (100%)	0	100	100
13	BW	110/111 (99%)	110 (100%)	0	100	100
14	BX	119/120 (99%)	119 (100%)	0	100	100
15	BY	112/113 (99%)	112 (100%)	0	100	100
16	Ba	83/100 (83%)	83 (100%)	0	100	100
17	Bb	70/71 (99%)	70 (100%)	0	100	100
18	Be	51/54 (94%)	51 (100%)	0	100	100
19	BD	182/195 (93%)	179 (98%)	3 (2%)	62	85
20	BF	173/191 (91%)	173 (100%)	0	100	100
21	BK	89/98 (91%)	89 (100%)	0	100	100
22	BP	104/118 (88%)	103 (99%)	1 (1%)	76	91
23	BQ	117/119 (98%)	117 (100%)	0	100	100
24	BR	110/124 (89%)	109 (99%)	1 (1%)	78	92
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	112 (99%)	1 (1%)	78	92
27	BU	100/114 (88%)	100 (100%)	0	100	100
28	BZ	61/89 (68%)	60 (98%)	1 (2%)	62	85
29	Bc	56/60 (93%)	56 (100%)	0	100	100
30	Bd	47/49 (96%)	47 (100%)	0	100	100
31	Bg	256/262 (98%)	256 (100%)	0	100	100
32	Bf	66/135 (49%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BM	100/119 (84%)	100 (100%)	0	100	100
35	AA	189/196 (96%)	188 (100%)	1 (0%)	88	96
36	AB	321/322 (100%)	319 (99%)	2 (1%)	86	95
37	AC	288/289 (100%)	286 (99%)	2 (1%)	84	94
41	AD	241/245 (98%)	241 (100%)	0	100	100
42	AE	134/153 (88%)	133 (99%)	1 (1%)	84	94
43	AF	186/205 (91%)	186 (100%)	0	100	100
44	AG	189/208 (91%)	189 (100%)	0	100	100
45	AH	170/171 (99%)	168 (99%)	2 (1%)	71	89
46	AI	176/187 (94%)	176 (100%)	0	100	100
47	AJ	147/150 (98%)	146 (99%)	1 (1%)	84	94
48	AL	154/159 (97%)	154 (100%)	0	100	100
49	AM	107/109 (98%)	107 (100%)	0	100	100
50	AN	175/176 (99%)	175 (100%)	0	100	100
51	AO	160/162 (99%)	159 (99%)	1 (1%)	86	95
52	AP	141/146 (97%)	140 (99%)	1 (1%)	84	94
53	AQ	150/151 (99%)	149 (99%)	1 (1%)	84	94
54	AR	153/154 (99%)	152 (99%)	1 (1%)	84	94
55	AS	156/162 (96%)	155 (99%)	1 (1%)	86	95
56	AT	136/137 (99%)	136 (100%)	0	100	100
57	AU	87/107 (81%)	87 (100%)	0	100	100
58	AV	104/105 (99%)	104 (100%)	0	100	100
59	AW	55/129 (43%)	55 (100%)	0	100	100
60	AX	105/118 (89%)	105 (100%)	0	100	100
61	AY	109/110 (99%)	109 (100%)	0	100	100
62	AZ	115/116 (99%)	115 (100%)	0	100	100
63	Aa	118/119 (99%)	118 (100%)	0	100	100
64	Ab	46/47 (98%)	46 (100%)	0	100	100
65	Ac	81/88 (92%)	81 (100%)	0	100	100
66	Ad	96/97 (99%)	96 (100%)	0	100	100
67	Ae	109/111 (98%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Af	90/91 (99%)	90 (100%)	0	100	100
69	Ag	95/103 (92%)	95 (100%)	0	100	100
70	Ah	104/105 (99%)	104 (100%)	0	100	100
71	Ai	81/82 (99%)	80 (99%)	1 (1%)	71	89
72	Aj	70/71 (99%)	70 (100%)	0	100	100
73	Ak	68/69 (99%)	68 (100%)	0	100	100
74	Al	45/46 (98%)	45 (100%)	0	100	100
75	Am	47/116 (40%)	47 (100%)	0	100	100
76	An	23/23 (100%)	23 (100%)	0	100	100
77	Ao	90/91 (99%)	90 (100%)	0	100	100
78	Ap	71/72 (99%)	71 (100%)	0	100	100
79	E	198/198 (100%)	198 (100%)	0	100	100
80	DC	699/714 (98%)	698 (100%)	1 (0%)	93	98
81	V	160/254 (63%)	160 (100%)	0	100	100
All	All	10346/11154 (93%)	10319 (100%)	27 (0%)	92	97

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	BC	43	ARG
9	BL	30	ARG
9	BL	67	ARG
11	BO	136	ARG
19	BD	76	ARG
19	BD	94	ARG
19	BD	190	ARG
22	BP	44	ARG
24	BR	95	ARG
26	BT	134	ARG
28	BZ	58	ARG
35	AA	149	ARG
36	AB	332	ARG
36	AB	369	ARG
37	AC	138	ARG
37	AC	300	ARG
42	AE	77	ARG
45	AH	23	ARG

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Mol	Chain	Res	Type
45	AH	166	ARG
47	AJ	166	LYS
51	AO	117[A]	ARG
52	AP	171	ARG
53	AQ	92	ARG
54	AR	20	ARG
55	AS	26	ARG
71	Ai	55	ARG
80	DC	87	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	15	GLN
2	BB	124	ASN
2	BB	149	GLN
2	BB	160	HIS
2	BB	209	ASN
3	BC	110	HIS
4	BE	36	HIS
4	BE	130	GLN
4	BE	142	HIS
4	BE	157	ASN
5	BG	65	GLN
5	BG	176	GLN
6	BH	161	GLN
8	BJ	123	HIS
12	BV	35	ASN
14	BX	22	ASN
15	BY	15	ASN
18	Be	17	GLN
20	BF	100	ASN
21	BK	12	HIS
21	BK	28	ASN
21	BK	93	GLN
23	BQ	8	GLN
23	BQ	94	GLN
23	BQ	100	GLN
24	BR	31	ASN
25	BS	55	HIS
25	BS	104	ASN
26	BT	16	ASN

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Mol	Chain	Res	Type
27	BU	47	GLN
27	BU	48	HIS
36	AB	280	HIS
37	AC	237	GLN
42	AE	57	HIS
42	AE	97	ASN
44	AG	77	GLN
45	AH	9	GLN
45	AH	102	ASN
45	AH	157	ASN
45	AH	163	GLN
47	AJ	20	ASN
47	AJ	39	GLN
52	AP	179	GLN
54	AR	7	GLN
54	AR	66	HIS
54	AR	134	HIS
54	AR	144	GLN
58	AV	98	ASN
61	AY	81	GLN
64	Ab	48	HIS
66	Ad	87	ASN
69	Ag	98	GLN
70	Ah	59	ASN
70	Ah	104	GLN
72	Aj	20	ASN
73	Ak	10	GLN
73	Ak	40	GLN
73	Ak	67	GLN
79	E	94	ASN
79	E	108	ASN
79	E	127	GLN
80	DC	18	ASN
80	DC	27	HIS
80	DC	108	HIS
80	DC	145	GLN
80	DC	355	GLN
80	DC	414	GLN
80	DC	603	ASN
80	DC	791	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1775/1798 (98%)	415 (23%)	11 (0%)
38	A1	3194/3360 (95%)	595 (18%)	21 (0%)
39	A3	120/121 (99%)	11 (9%)	1 (0%)
40	A4	157/158 (99%)	30 (19%)	0
82	EC	188/202 (93%)	101 (53%)	7 (3%)
All	All	5434/5639 (96%)	1152 (21%)	40 (0%)

All (1152) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	2	A
34	B5	4	C
34	B5	9	U
34	B5	10	G
34	B5	11	A
34	B5	13	C
34	B5	17	C
34	B5	22	A
34	B5	25	C
34	B5	26	A
34	B5	34	G
34	B5	42	G
34	B5	47	A
34	B5	50	C
34	B5	57	G
34	B5	60	U
34	B5	67	A
34	B5	68	A
34	B5	72	A
34	B5	73	U
34	B5	74	U
34	B5	75	U
34	B5	77	U
34	B5	81	G
34	B5	104	A
34	B5	111	U
34	B5	114	C
34	B5	115	G
34	B5	116	U
34	B5	127	G
34	B5	130	C
34	B5	131	C
34	B5	132	U

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Mol	Chain	Res	Type
34	B5	133	U
34	B5	134	U
34	B5	135	A
34	B5	136	C
34	B5	137	U
34	B5	138	A
34	B5	141	U
34	B5	145	A
34	B5	154	G
34	B5	159	U
34	B5	162	A
34	B5	163	G
34	B5	164	A
34	B5	166	C
34	B5	167	U
34	B5	169	A
34	B5	178	U
34	B5	179	A
34	B5	181	A
34	B5	182	A
34	B5	185	U
34	B5	188	A
34	B5	190	C
34	B5	191	C
34	B5	192	U
34	B5	193	U
34	B5	194	U
34	B5	195	G
34	B5	196	G
34	B5	198	A
34	B5	217	A
34	B5	218	A
34	B5	223	U
34	B5	224	C
34	B5	225	A
34	B5	227	U
34	B5	228	G
34	B5	229	U
34	B5	230	C
34	B5	231	U
34	B5	233	C
34	B5	234	G

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Mol	Chain	Res	Type
34	B5	240	U
34	B5	241	U
34	B5	257	A
34	B5	261	U
34	B5	262	U
34	B5	265	A
34	B5	276	C
34	B5	278	U
34	B5	280	U
34	B5	281	G
34	B5	299	A
34	B5	314	C
34	B5	315	A
34	B5	316	A
34	B5	320	U
34	B5	321	C
34	B5	322	G
34	B5	337	G
34	B5	338	C
34	B5	352	A
34	B5	353	A
34	B5	359	A
34	B5	360	A
34	B5	361	C
34	B5	397	A
34	B5	399	A
34	B5	400	A
34	B5	401	A
34	B5	402	C
34	B5	419	G
34	B5	423	G
34	B5	424	C
34	B5	425	A
34	B5	426	G
34	B5	431	C
34	B5	434	G
34	B5	439	U
34	B5	444	C
34	B5	460	A
34	B5	468	A
34	B5	475	A
34	B5	477	A

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Mol	Chain	Res	Type
34	B5	484	C
34	B5	485	A
34	B5	487	G
34	B5	489	C
34	B5	490	C
34	B5	491	C
34	B5	492	A
34	B5	494	U
34	B5	495	C
34	B5	496	G
34	B5	497	G
34	B5	498	G
34	B5	499	U
34	B5	500	C
34	B5	503	G
34	B5	506	A
34	B5	507	U
34	B5	515	A
34	B5	519	C
34	B5	538	A
34	B5	539	G
34	B5	540	G
34	B5	541	A2M
34	B5	542	A
34	B5	549	G
34	B5	555	A
34	B5	557	G
34	B5	558	U
34	B5	559	C
34	B5	565	C
34	B5	568	G
34	B5	575	C
34	B5	577	G
34	B5	578	OMU
34	B5	579	A
34	B5	580	A
34	B5	582	U
34	B5	594	A
34	B5	595	G
34	B5	606	A
34	B5	610	G
34	B5	611	U

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Mol	Chain	Res	Type
34	B5	619	A2M
34	B5	620	A
34	B5	622	A
34	B5	623	A
34	B5	624	G
34	B5	638	U
34	B5	639	U
34	B5	650	U
34	B5	652	G
34	B5	654	C
34	B5	655	G
34	B5	656	G
34	B5	658	C
34	B5	677	G
34	B5	678	A
34	B5	681	U
34	B5	683	C
34	B5	694	U
34	B5	696	C
34	B5	697	C
34	B5	698	U
34	B5	704	C
34	B5	705	U
34	B5	706	A
34	B5	709	C
34	B5	711	U
34	B5	712	G
34	B5	713	A
34	B5	715	U
34	B5	716	C
34	B5	717	C
34	B5	718	U
34	B5	719	U
34	B5	720	G
34	B5	721	U
34	B5	722	G
34	B5	724	C
34	B5	725	U
34	B5	727	U
34	B5	729	G
34	B5	730	G
34	B5	731	C

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Mol	Chain	Res	Type
34	B5	733	A
34	B5	734	A
34	B5	735	C
34	B5	740	A
34	B5	741	C
34	B5	753	A
34	B5	765	G
34	B5	766	U
34	B5	771	A
34	B5	774	A
34	B5	775	G
34	B5	778	G
34	B5	779	U
34	B5	781	U
34	B5	782	U
34	B5	783	G
34	B5	784	C
34	B5	787	G
34	B5	789	A
34	B5	794	U
34	B5	812	A
34	B5	814	A
34	B5	819	G
34	B5	820	U
34	B5	821	U
34	B5	823	G
34	B5	832	U
34	B5	833	U
34	B5	836	U
34	B5	840	U
34	B5	846	G
34	B5	850	A
34	B5	851	U
34	B5	859	A
34	B5	862	A
34	B5	863	A
34	B5	895	G
34	B5	898	A
34	B5	899	G
34	B5	904	G
34	B5	906	A
34	B5	907	A

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Mol	Chain	Res	Type
34	B5	913	G
34	B5	914	G
34	B5	923	A
34	B5	933	A
34	B5	935	U
34	B5	951	A
34	B5	960	U
34	B5	966	A
34	B5	973	A
34	B5	987	G
34	B5	988	A
34	B5	992	A
34	B5	993	A
34	B5	998	A
34	B5	1000	C
34	B5	1003	A
34	B5	1004	U
34	B5	1005	A
34	B5	1020	A
34	B5	1021	C
34	B5	1023	A
34	B5	1026	A
34	B5	1028	C
34	B5	1029	U
34	B5	1032	G
34	B5	1039	A
34	B5	1040	G
34	B5	1052	U
34	B5	1056	U
34	B5	1058	U
34	B5	1059	U
34	B5	1060	U
34	B5	1061	A
34	B5	1062	A
34	B5	1076	A
34	B5	1083	G
34	B5	1092	A
34	B5	1093	A
34	B5	1097	U
34	B5	1100	G
34	B5	1138	A
34	B5	1150	G

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Mol	Chain	Res	Type
34	B5	1158	C
34	B5	1159	C
34	B5	1171	A
34	B5	1183	A
34	B5	1185	U
34	B5	1192	C
34	B5	1194	A
34	B5	1196	A
34	B5	1199	G
34	B5	1200	G
34	B5	1201	G
34	B5	1212	G
34	B5	1217	A
34	B5	1218	G
34	B5	1226	A
34	B5	1227	A
34	B5	1228	G
34	B5	1229	G
34	B5	1235	C
34	B5	1243	G
34	B5	1244	A
34	B5	1245	G
34	B5	1246	C
34	B5	1248	C
34	B5	1251	U
34	B5	1252	C
34	B5	1256	A
34	B5	1257	U
34	B5	1269	OMU
34	B5	1276	U
34	B5	1286	U
34	B5	1288	G
34	B5	1301	U
34	B5	1306	C
34	B5	1314	U
34	B5	1315	U
34	B5	1316	G
34	B5	1321	A
34	B5	1340	U
34	B5	1344	A
34	B5	1345	A
34	B5	1346	A

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Mol	Chain	Res	Type
34	B5	1347	U
34	B5	1355	C
34	B5	1360	A
34	B5	1362	U
34	B5	1363	U
34	B5	1364	G
34	B5	1366	U
34	B5	1368	G
34	B5	1370	U
34	B5	1371	A
34	B5	1372	U
34	B5	1373	C
34	B5	1382	A
34	B5	1390	U
34	B5	1392	U
34	B5	1398	U
34	B5	1399	C
34	B5	1400	A
34	B5	1402	G
34	B5	1413	U
34	B5	1414	U
34	B5	1415	U
34	B5	1427	A
34	B5	1428	OMG
34	B5	1432	U
34	B5	1436	A
34	B5	1445	G
34	B5	1459	C
34	B5	1460	A
34	B5	1469	A
34	B5	1471	A
34	B5	1486	G
34	B5	1489	U
34	B5	1491	U
34	B5	1492	A
34	B5	1493	A
34	B5	1496	U
34	B5	1506	G
34	B5	1510	U
34	B5	1516	A
34	B5	1521	G
34	B5	1523	G

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Mol	Chain	Res	Type
34	B5	1524	A
34	B5	1537	C
34	B5	1540	G
34	B5	1542	G
34	B5	1557	U
34	B5	1559	A
34	B5	1563	C
34	B5	1565	C
34	B5	1569	A
34	B5	1576	A
34	B5	1584	G
34	B5	1600	A
34	B5	1601	G
34	B5	1616	G
34	B5	1619	C
34	B5	1635	A
34	B5	1646	C
34	B5	1658	G
34	B5	1659	A
34	B5	1663	G
34	B5	1680	G
34	B5	1683	C
34	B5	1684	U
34	B5	1688	U
34	B5	1693	A
34	B5	1700	C
34	B5	1701	A
34	B5	1703	C
34	B5	1709	C
34	B5	1716	C
34	B5	1717	G
34	B5	1746	A
34	B5	1756[A]	A
34	B5	1760	G
34	B5	1761	U
34	B5	1762	A
34	B5	1766	A
34	B5	1767	G
34	B5	1769	U
34	B5	1780	G
34	B5	1792	G
34	B5	1793	G

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Mol	Chain	Res	Type
34	B5	1794	A
34	B5	1795	U
34	B5	1796	C
34	B5	1799	U
38	A1	14	U
38	A1	26	A
38	A1	34	A
38	A1	40	A
38	A1	43	A
38	A1	49	A
38	A1	59	G
38	A1	60	A
38	A1	65	A
38	A1	66	A
38	A1	67	A
38	A1	71	A
38	A1	92	G
38	A1	109	A
38	A1	110	G
38	A1	111	C
38	A1	116	A
38	A1	118	U
38	A1	122	A
38	A1	134	U
38	A1	135	C
38	A1	136	G
38	A1	146	U
38	A1	148	G
38	A1	156	G
38	A1	157	A
38	A1	163	C
38	A1	164	A
38	A1	165	A
38	A1	166	C
38	A1	170	G
38	A1	174	C
38	A1	175	C
38	A1	178	U
38	A1	187	A
38	A1	190	U
38	A1	191	U
38	A1	200	C

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Mol	Chain	Res	Type
38	A1	206	G
38	A1	210	U
38	A1	219	A
38	A1	234	G
38	A1	237	G
38	A1	238	A
38	A1	239	G
38	A1	240	U
38	A1	241	G
38	A1	242	C
38	A1	243	G
38	A1	244	G
38	A1	245	U
38	A1	246	U
38	A1	248	U
38	A1	249	U
38	A1	250	U
38	A1	251	G
38	A1	252	U
38	A1	253	A
38	A1	254	A
38	A1	266	A
38	A1	269	G
38	A1	286	U
38	A1	295	A
38	A1	296	A
38	A1	305	U
38	A1	311	C
38	A1	329	U
38	A1	339	C
38	A1	346	C
38	A1	352	A
38	A1	370	U
38	A1	371	G
38	A1	372	A
38	A1	376	G
38	A1	387	A
38	A1	390	G
38	A1	398	A
38	A1	399	A
38	A1	401	U
38	A1	402	A

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Mol	Chain	Res	Type
38	A1	403	C
38	A1	407	A
38	A1	420	G
38	A1	421	G
38	A1	422	A
38	A1	438	A
38	A1	440	A
38	A1	495	G
38	A1	521	A
38	A1	535	G
38	A1	540	U
38	A1	542	G
38	A1	545	U
38	A1	547	G
38	A1	548	G
38	A1	552	G
38	A1	557	A
38	A1	559	A
38	A1	560	G
38	A1	579	G
38	A1	591	G
38	A1	592	A
38	A1	602	A
38	A1	611	A
38	A1	620	U
38	A1	621	A
38	A1	622	A
38	A1	637	C
38	A1	649	A2M
38	A1	660	A
38	A1	677	A
38	A1	681	U
38	A1	690	A
38	A1	691	A
38	A1	705	A
38	A1	719	U
38	A1	725	G
38	A1	736	A
38	A1	758	C
38	A1	760	G
38	A1	765	C
38	A1	766	U

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Mol	Chain	Res	Type
38	A1	767	U
38	A1	774	G
38	A1	775	A
38	A1	777	U
38	A1	781	G
38	A1	785	G
38	A1	786	A
38	A1	799	G
38	A1	801	A
38	A1	806	A
38	A1	808	A
38	A1	813	G
38	A1	817	A2M
38	A1	830	A
38	A1	848	A
38	A1	849	C
38	A1	857	G
38	A1	861	C
38	A1	874	U
38	A1	879	U
38	A1	896	A
38	A1	897	U
38	A1	907	G
38	A1	908	OMG
38	A1	914	A
38	A1	916	G
38	A1	917	A
38	A1	921	A
38	A1	923	C
38	A1	934	G
38	A1	937	G
38	A1	943	U
38	A1	944	C
38	A1	959	C
38	A1	980	A
38	A1	981	U
38	A1	984	G
38	A1	994	G
38	A1	1000	C
38	A1	1002	A
38	A1	1010	G
38	A1	1016	C

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Mol	Chain	Res	Type
38	A1	1017	C
38	A1	1018	G
38	A1	1019	G
38	A1	1021	G
38	A1	1022	U
38	A1	1023	C
38	A1	1032	C
38	A1	1033	U
38	A1	1034	U
38	A1	1035	G
38	A1	1036	A
38	A1	1047	A
38	A1	1052	U
38	A1	1063	G
38	A1	1064	A
38	A1	1065	A
38	A1	1072	G
38	A1	1081	U
38	A1	1082	U
38	A1	1093	A
38	A1	1094	U
38	A1	1095	U
38	A1	1097	G
38	A1	1098	A
38	A1	1103	A
38	A1	1104	G
38	A1	1117	G
38	A1	1130	A
38	A1	1131	G
38	A1	1143	A
38	A1	1144	U
38	A1	1151	U
38	A1	1153	A
38	A1	1154	A
38	A1	1155	C
38	A1	1159	A
38	A1	1160	C
38	A1	1179	A
38	A1	1180	A
38	A1	1181	U
38	A1	1182	A
38	A1	1192	C

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Mol	Chain	Res	Type
38	A1	1193	A
38	A1	1196	C
38	A1	1201	C
38	A1	1206	G
38	A1	1208	U
38	A1	1219	C
38	A1	1221	A
38	A1	1225	A
38	A1	1228	C
38	A1	1232	C
38	A1	1235	U
38	A1	1236	G
38	A1	1239	C
38	A1	1241	U
38	A1	1242	G
38	A1	1243	G
38	A1	1245	A
38	A1	1246	G
38	A1	1252	A
38	A1	1253	U
38	A1	1256	G
38	A1	1258	U
38	A1	1262	G
38	A1	1263	A
38	A1	1265	U
38	A1	1282	G
38	A1	1283	C
38	A1	1286	A
38	A1	1287	A
38	A1	1293	U
38	A1	1307	G
38	A1	1309	U
38	A1	1317	A
38	A1	1330	A
38	A1	1331	U
38	A1	1348	U
38	A1	1349	G
38	A1	1350	A
38	A1	1351	U
38	A1	1352	A
38	A1	1353	U
38	A1	1354	G

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Mol	Chain	Res	Type
38	A1	1355	A
38	A1	1356	U
38	A1	1357	G
38	A1	1386	A
38	A1	1392	G
38	A1	1399	A
38	A1	1400	G
38	A1	1418	A
38	A1	1419	A
38	A1	1431	G
38	A1	1434	G
38	A1	1437	OMC
38	A1	1446	A
38	A1	1455	U
38	A1	1468	A
38	A1	1475	A
38	A1	1481	A
38	A1	1483	G
38	A1	1488	G
38	A1	1496	C
38	A1	1508	C
38	A1	1523	U
38	A1	1533	U
38	A1	1536	G
38	A1	1539	A
38	A1	1555	U
38	A1	1556	C
38	A1	1558	A
38	A1	1562	C
38	A1	1563	C
38	A1	1564	U
38	A1	1565	G
38	A1	1567	U
38	A1	1568	U
38	A1	1569	U
38	A1	1574	C
38	A1	1575	A
38	A1	1576	G
38	A1	1579	C
38	A1	1583	A
38	A1	1589	A
38	A1	1593	A

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Mol	Chain	Res	Type
38	A1	1605	A
38	A1	1618	G
38	A1	1628	C
38	A1	1629	U
38	A1	1630	U
38	A1	1631	C
38	A1	1643	A
38	A1	1657	C
38	A1	1724	U
38	A1	1736	G
38	A1	1738	C
38	A1	1739	U
38	A1	1741	A
38	A1	1742	U
38	A1	1750	A
38	A1	1751	G
38	A1	1752	A
38	A1	1762	C
38	A1	1763	U
38	A1	1764	U
38	A1	1765	U
38	A1	1766	G
38	A1	1794	G
38	A1	1796	G
38	A1	1797	A
38	A1	1813	A
38	A1	1815	U
38	A1	1818	U
38	A1	1820	U
38	A1	1821	U
38	A1	1842	A
38	A1	1846	C
38	A1	1849	C
38	A1	1850	A
38	A1	1866	C
38	A1	1878	G
38	A1	1880	U
38	A1	1886	A
38	A1	1893	A
38	A1	1906	G
38	A1	1932	A
38	A1	1953	G

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Mol	Chain	Res	Type
38	A1	1954	G
38	A1	1955	U
38	A1	2094	C
38	A1	2095	G
38	A1	2111	G
38	A1	2112	U
38	A1	2114	C
38	A1	2122	G
38	A1	2131	A
38	A1	2140	U
38	A1	2144	A
38	A1	2158	A
38	A1	2169	G
38	A1	2176	U
38	A1	2188	A
38	A1	2197	OMC
38	A1	2201	G
38	A1	2242	A
38	A1	2249	G
38	A1	2252	A
38	A1	2253	G
38	A1	2256	A
38	A1	2260	U
38	A1	2261	G
38	A1	2263	C
38	A1	2265	C
38	A1	2267	C
38	A1	2268	U
38	A1	2269	U
38	A1	2272	G
38	A1	2273	G
38	A1	2277	C
38	A1	2278	5MC
38	A1	2279	A
38	A1	2280	A2M
38	A1	2281	A2M
38	A1	2284	C
38	A1	2307	G
38	A1	2310	U
38	A1	2313	A
38	A1	2314	U
38	A1	2315	G

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Mol	Chain	Res	Type
38	A1	2334	U
38	A1	2335	G
38	A1	2336	U
38	A1	2340	U
38	A1	2365	C
38	A1	2366	C
38	A1	2373	A
38	A1	2374	C
38	A1	2375	G
38	A1	2383	C
38	A1	2388	U
38	A1	2393	G
38	A1	2397	A
38	A1	2402	A
38	A1	2403	G
38	A1	2404	A
38	A1	2411	U
38	A1	2418	G
38	A1	2435	G
38	A1	2438	A
38	A1	2439	A
38	A1	2440	G
38	A1	2441	A
38	A1	2442	G
38	A1	2445	A
38	A1	2447	A
38	A1	2450	G
38	A1	2453	U
38	A1	2454	G
38	A1	2455	U
38	A1	2459	A
38	A1	2460	U
38	A1	2461	A
38	A1	2462	A
38	A1	2463	G
38	A1	2467	G
38	A1	2468	A
38	A1	2469	G
38	A1	2474	G
38	A1	2477	G
38	A1	2479	C
38	A1	2485	A

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Mol	Chain	Res	Type
38	A1	2487	U
38	A1	2490	C
38	A1	2491	A
38	A1	2492	C
38	A1	2493	U
38	A1	2495	C
38	A1	2496	C
38	A1	2497	U
38	A1	2498	U
38	A1	2499	U
38	A1	2500	A
38	A1	2502	A
38	A1	2503	G
38	A1	2504	U
38	A1	2505	U
38	A1	2511	A
38	A1	2514	U
38	A1	2515	A
38	A1	2523	A
38	A1	2524	A
38	A1	2525	G
38	A1	2537	U
38	A1	2538	U
38	A1	2539	C
38	A1	2540	A
38	A1	2541	U
38	A1	2543	U
38	A1	2544	U
38	A1	2549	G
38	A1	2550	U
38	A1	2552	C
38	A1	2554	A
38	A1	2560	C
38	A1	2561	A
38	A1	2569	A
38	A1	2571	U
38	A1	2572	C
38	A1	2573	G
38	A1	2585	G
38	A1	2593	A
38	A1	2595	A
38	A1	2596	U

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Mol	Chain	Res	Type
38	A1	2606	G
38	A1	2607	G
38	A1	2614	G
38	A1	2626	A
38	A1	2628	A
38	A1	2635	A
38	A1	2638	C
38	A1	2648	G
38	A1	2652	U
38	A1	2656	A
38	A1	2664	C
38	A1	2672	G
38	A1	2674	A
38	A1	2677	G
38	A1	2678	A
38	A1	2680	A
38	A1	2681	U
38	A1	2688	U
38	A1	2689	A
38	A1	2691	A
38	A1	2704	A
38	A1	2705	A
38	A1	2714	G
38	A1	2719	U
38	A1	2728	G
38	A1	2729	OMU
38	A1	2737	C
38	A1	2752	U
38	A1	2753	G
38	A1	2777	G
38	A1	2778	G
38	A1	2796	G
38	A1	2799	A
38	A1	2800	G
38	A1	2801	A
38	A1	2803	A
38	A1	2810	C
38	A1	2814	G
38	A1	2816	G
38	A1	2817	A
38	A1	2842	U
38	A1	2844	C

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Mol	Chain	Res	Type
38	A1	2845	A
38	A1	2871	G
38	A1	2872	A
38	A1	2875	U
38	A1	2876	C
38	A1	2887	A
38	A1	2889	C
38	A1	2898	G
38	A1	2923	U
38	A1	2933	A
38	A1	2935	U
38	A1	2936	A
38	A1	2938	G
38	A1	2947	G
38	A1	2954	U
38	A1	2972	G
38	A1	2977	G
38	A1	2983	C
38	A1	2990	G
38	A1	2997	G
38	A1	3011	A
38	A1	3012	A
38	A1	3022	G
38	A1	3032	A
38	A1	3055	U
38	A1	3056	U
38	A1	3059	G
38	A1	3078	U
38	A1	3086	A
38	A1	3092	C
38	A1	3094	A
38	A1	3101	G
38	A1	3104	U
38	A1	3113	A
38	A1	3122	A
38	A1	3130	A
38	A1	3131	U
38	A1	3142	A
38	A1	3143	C
38	A1	3153	U
38	A1	3154	C
38	A1	3155	U

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Mol	Chain	Res	Type
38	A1	3156	U
38	A1	3157	U
38	A1	3165	A
38	A1	3170	A
38	A1	3172	A
38	A1	3173	G
38	A1	3174	A
38	A1	3175	U
38	A1	3176	G
38	A1	3179	U
38	A1	3181	C
38	A1	3187	A
38	A1	3196	U
38	A1	3198	U
38	A1	3206	C
38	A1	3207	U
38	A1	3217	C
38	A1	3218	A
38	A1	3219	G
38	A1	3224	G
38	A1	3229	G
38	A1	3234	A
38	A1	3243	A
38	A1	3247	G
38	A1	3259	U
38	A1	3263	G
38	A1	3270	U
38	A1	3271	G
38	A1	3274	A
38	A1	3275	U
38	A1	3276	G
38	A1	3281	U
38	A1	3289	G
38	A1	3294	A
38	A1	3303	G
38	A1	3304	U
38	A1	3313	U
38	A1	3316	A
38	A1	3319	U
38	A1	3342	A
38	A1	3345	G
38	A1	3351	U

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Mol	Chain	Res	Type
38	A1	3352	U
38	A1	3353	G
38	A1	3354	U
38	A1	3355	U
38	A1	3356	G
38	A1	3368	U
38	A1	3369	G
38	A1	3375	A
38	A1	3378	C
38	A1	3389	U
38	A1	3390	G
39	A3	53	U
39	A3	54	U
39	A3	55	A
39	A3	64	A
39	A3	65	G
39	A3	74	C
39	A3	76	A
39	A3	99	G
39	A3	102	A
39	A3	112	G
39	A3	121	U
40	A4	33	A
40	A4	34	U
40	A4	35	C
40	A4	39	G
40	A4	51	G
40	A4	52	A
40	A4	53	A
40	A4	59	A
40	A4	62	C
40	A4	63	G
40	A4	76	C
40	A4	81	U
40	A4	82	U
40	A4	83	C
40	A4	85	G
40	A4	86	U
40	A4	87	G
40	A4	88	A
40	A4	90	U
40	A4	95	G

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Mol	Chain	Res	Type
40	A4	104	A
40	A4	106	C
40	A4	107	G
40	A4	111	A
40	A4	113	U
40	A4	116	G
40	A4	125	U
40	A4	152	G
40	A4	157	U
40	A4	158	U
82	EC	6762	U
82	EC	6768	U
82	EC	6769	A
82	EC	6770	U
82	EC	6771	U
82	EC	6772	G
82	EC	6773	G
82	EC	6774	U
82	EC	6775	U
82	EC	6776	A
82	EC	6777	C
82	EC	6778	C
82	EC	6779	C
82	EC	6780	A
82	EC	6782	C
82	EC	6788	C
82	EC	6789	G
82	EC	6790	A
82	EC	6791	A
82	EC	6792	A
82	EC	6793	A
82	EC	6794	C
82	EC	6800	G
82	EC	6801	A
82	EC	6802	A
82	EC	6803	C
82	EC	6804	A
82	EC	6811	G
82	EC	6816	A
82	EC	6817	A
82	EC	6818	G
82	EC	6819	G

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Mol	Chain	Res	Type
82	EC	6820	C
82	EC	6821	U
82	EC	6822	U
82	EC	6823	U
82	EC	6824	C
82	EC	6831	U
82	EC	6832	G
82	EC	6835	U
82	EC	6837	G
82	EC	6840	A
82	EC	6841	U
82	EC	6842	U
82	EC	6843	U
82	EC	6845	G
82	EC	6847	G
82	EC	6848	U
82	EC	6849	A
82	EC	6850	C
82	EC	6852	U
82	EC	6855	A
82	EC	6856	C
82	EC	6857	C
82	EC	6859	U
82	EC	6860	A
82	EC	6861	G
82	EC	6864	A
82	EC	6866	C
82	EC	6867	C
82	EC	6869	C
82	EC	6870	A
82	EC	6871	A
82	EC	6872	A
82	EC	6873	A
82	EC	6874	A
82	EC	6875	C
82	EC	6877	C
82	EC	6880	G
82	EC	6881	U
82	EC	6882	G
82	EC	6884	G
82	EC	6886	A
82	EC	6887	G

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Mol	Chain	Res	Type
82	EC	6889	A
82	EC	6890	A
82	EC	6895	C
82	EC	6896	A
82	EC	6897	G
82	EC	6902	U
82	EC	6903	U
82	EC	6908	C
82	EC	6910	A
82	EC	6911	A
82	EC	6915	G
82	EC	6916	A
82	EC	6918	A
82	EC	6919	G
82	EC	6925	C
82	EC	6928	G
82	EC	6929	C
82	EC	6935	G
82	EC	6938	A
82	EC	6940	U
82	EC	6941	U
82	EC	6942	A
82	EC	6943	A
82	EC	6944	U
82	EC	6945	U
82	EC	6946	A
82	EC	6948	U

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	B5	10	G
34	B5	752	A
34	B5	819	G
34	B5	862	A
34	B5	950	C
34	B5	1285	U
34	B5	1344	A
34	B5	1369	U
34	B5	1458	G
34	B5	1600	A
34	B5	1645	G

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Mol	Chain	Res	Type
38	A1	165	A
38	A1	237	G
38	A1	239	G
38	A1	240	U
38	A1	241	G
38	A1	244	G
38	A1	248	U
38	A1	249	U
38	A1	252	U
38	A1	253	A
38	A1	916	G
38	A1	1092	C
38	A1	1218	U
38	A1	1242	G
38	A1	1292	C
38	A1	1354	G
38	A1	1629	U
38	A1	2241	U
38	A1	2280	A2M
38	A1	2875	U
38	A1	3121	U
39	A3	52	G
82	EC	6789	G
82	EC	6831	U
82	EC	6844	A
82	EC	6851	G
82	EC	6876	A
82	EC	6889	A
82	EC	6943	A

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

67 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
38	OMU	A1	1888	38	19,22,23	1.26	3 (15%)	26,31,34	1.75	4 (15%)
38	OMC	A1	2337	38	19,22,23	0.83	0	26,31,34	0.88	1 (3%)
38	A2M	A1	2281	38	18,25,26	0.92	1 (5%)	18,36,39	1.26	2 (11%)
38	UR3	A1	2634	38	19,22,23	0.97	0	26,32,35	1.40	1 (3%)
38	OMU	A1	2729	38	19,22,23	1.27	3 (15%)	26,31,34	1.63	5 (19%)
38	OMG	A1	2793	38	18,26,27	0.93	1 (5%)	19,38,41	1.02	2 (10%)
38	1MA	A1	645	83,38	16,25,26	1.50	2 (12%)	18,37,40	1.07	3 (16%)
38	A2M	A1	2220	38	18,25,26	0.96	1 (5%)	18,36,39	1.38	3 (16%)
38	OMU	A1	2421	38	19,22,23	1.24	3 (15%)	26,31,34	1.73	5 (19%)
38	OMG	A1	2922	38	18,26,27	0.93	1 (5%)	19,38,41	1.05	2 (10%)
38	A2M	A1	2946	83,38	18,25,26	0.98	1 (5%)	18,36,39	1.33	2 (11%)
36	HIC	AB	243	36	8,11,12	1.60	2 (25%)	6,14,16	0.86	0
38	A2M	A1	817	83,38	18,25,26	1.00	1 (5%)	18,36,39	1.37	3 (16%)
34	OMU	B5	578	34	19,22,23	1.16	2 (10%)	26,31,34	1.70	5 (19%)
34	4AC	B5	1773	34	21,24,25	1.08	2 (9%)	29,34,37	1.32	4 (13%)
34	OMU	B5	1269	34	19,22,23	1.27	4 (21%)	26,31,34	1.80	7 (26%)
38	A2M	A1	1133	38	18,25,26	0.96	1 (5%)	18,36,39	1.31	2 (11%)
34	A2M	B5	28	34,83	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
34	OMG	B5	562	34	18,26,27	0.93	1 (5%)	19,38,41	1.05	2 (10%)
38	OMG	A1	805	38	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
38	A2M	A1	876	38	18,25,26	0.99	1 (5%)	18,36,39	1.22	2 (11%)
34	OMC	B5	414	34	19,22,23	0.83	0	26,31,34	0.80	1 (3%)
38	OMC	A1	2948	38	19,22,23	0.85	0	26,31,34	1.07	2 (7%)
38	OMU	A1	2921	38	19,22,23	1.22	3 (15%)	26,31,34	1.74	5 (19%)
38	OMU	A1	898	38	19,22,23	1.23	3 (15%)	26,31,34	1.68	5 (19%)
34	A2M	B5	420	34	18,25,26	0.99	1 (5%)	18,36,39	1.17	2 (11%)
38	OMU	A1	2347	38	19,22,23	1.29	4 (21%)	26,31,34	1.72	6 (23%)
34	A2M	B5	100	34,83	18,25,26	1.01	1 (5%)	18,36,39	1.21	2 (11%)
34	OMC	B5	1007	34	19,22,23	0.83	0	26,31,34	0.91	1 (3%)
38	OMG	A1	1450	83,38	18,26,27	0.91	1 (5%)	19,38,41	1.05	2 (10%)
34	MA6	B5	1781	34	19,26,27	0.99	1 (5%)	18,38,41	1.31	2 (11%)
38	OMG	A1	2791	38	18,26,27	0.93	1 (5%)	19,38,41	1.05	2 (10%)
38	5MC	A1	2870	83,38	18,22,23	1.02	2 (11%)	26,32,35	1.29	3 (11%)
34	OMG	B5	1572	34	18,26,27	0.93	1 (5%)	19,38,41	1.16	2 (10%)
38	OMC	A1	663	38	19,22,23	0.83	0	26,31,34	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	OMC	A1	2197	38	19,22,23	0.80	0	26,31,34	0.78	0
38	OMG	A1	2619	38	18,26,27	0.93	1 (5%)	19,38,41	1.02	2 (10%)
38	A2M	A1	1449	83,38	18,25,26	1.03	1 (5%)	18,36,39	1.19	2 (11%)
38	OMG	A1	2815	38	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
34	MA6	B5	1782	34	19,26,27	0.92	1 (5%)	18,38,41	1.40	3 (16%)
38	OMU	A1	2417	38	19,22,23	1.23	3 (15%)	26,31,34	1.66	4 (15%)
38	A2M	A1	807	38	18,25,26	0.97	1 (5%)	18,36,39	1.20	2 (11%)
38	OMC	A1	2959	38	19,22,23	0.82	0	26,31,34	0.81	0
38	A2M	A1	2280	38	18,25,26	0.98	1 (5%)	18,36,39	1.36	2 (11%)
38	OMC	A1	650	83,38	19,22,23	0.82	0	26,31,34	0.78	0
34	A2M	B5	796	34	18,25,26	1.05	1 (5%)	18,36,39	1.35	2 (11%)
34	4AC	B5	1280	34	21,24,25	1.07	1 (4%)	29,34,37	1.06	2 (6%)
34	A2M	B5	436	34	18,25,26	1.02	1 (5%)	18,36,39	1.27	2 (11%)
38	5MC	A1	2278	83,38	18,22,23	0.96	2 (11%)	26,32,35	1.27	3 (11%)
38	OMG	A1	2288	38	18,26,27	0.94	1 (5%)	19,38,41	1.04	2 (10%)
38	A2M	A1	2640	38	18,25,26	1.00	1 (5%)	18,36,39	1.23	2 (11%)
34	OMG	B5	1271	34	18,26,27	0.92	1 (5%)	19,38,41	1.03	2 (10%)
34	OMG	B5	1428	34	18,26,27	0.91	1 (5%)	19,38,41	1.07	2 (10%)
38	1MA	A1	2142	83,38	16,25,26	1.51	2 (12%)	18,37,40	1.06	3 (16%)
34	A2M	B5	974	34	18,25,26	1.00	1 (5%)	18,36,39	1.24	2 (11%)
80	DDE	DC	699	82,80	14,20,21	1.02	1 (7%)	14,28,30	1.16	1 (7%)
38	OMG	A1	867	38	18,26,27	0.91	1 (5%)	19,38,41	1.08	2 (10%)
34	A2M	B5	619	34,83	18,25,26	0.95	1 (5%)	18,36,39	1.30	2 (11%)
38	A2M	A1	649	38	18,25,26	0.96	1 (5%)	18,36,39	1.24	2 (11%)
38	OMU	A1	2724	38	19,22,23	1.21	3 (15%)	26,31,34	1.71	5 (19%)
34	G7M	B5	1575	34	20,26,27	2.89	6 (30%)	17,39,42	1.78	4 (23%)
34	XSX	B5	1191	34	24,28,29	0.99	1 (4%)	33,40,43	1.94	7 (21%)
38	OMC	A1	1437	83,38	19,22,23	0.86	0	26,31,34	1.20	3 (11%)
38	OMG	A1	908	38	18,26,27	0.95	1 (5%)	19,38,41	1.12	2 (10%)
34	OMG	B5	1126	34	18,26,27	0.91	1 (5%)	19,38,41	1.07	2 (10%)
34	OMC	B5	1639	34	19,22,23	0.81	0	26,31,34	0.78	0
34	A2M	B5	541	34	18,25,26	1.05	1 (5%)	18,36,39	1.24	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	OMU	A1	1888	38	-	0/9/27/28	0/2/2/2
38	OMC	A1	2337	38	-	1/9/27/28	0/2/2/2
38	A2M	A1	2281	38	-	1/5/27/28	0/3/3/3
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
38	OMU	A1	2729	38	-	3/9/27/28	0/2/2/2
38	OMG	A1	2793	38	-	0/5/27/28	0/3/3/3
38	1MA	A1	645	83,38	-	0/3/25/26	0/3/3/3
38	A2M	A1	2220	38	-	0/5/27/28	0/3/3/3
38	OMU	A1	2421	38	-	1/9/27/28	0/2/2/2
38	OMG	A1	2922	38	-	0/5/27/28	0/3/3/3
38	A2M	A1	2946	83,38	-	1/5/27/28	0/3/3/3
36	HIC	AB	243	36	-	0/5/6/8	0/1/1/1
38	A2M	A1	817	83,38	-	2/5/27/28	0/3/3/3
34	OMU	B5	578	34	-	4/9/27/28	0/2/2/2
34	4AC	B5	1773	34	-	4/11/29/30	0/2/2/2
34	OMU	B5	1269	34	-	5/9/27/28	0/2/2/2
38	A2M	A1	1133	38	-	0/5/27/28	0/3/3/3
34	A2M	B5	28	34,83	-	0/5/27/28	0/3/3/3
34	OMG	B5	562	34	-	0/5/27/28	0/3/3/3
38	OMG	A1	805	38	-	0/5/27/28	0/3/3/3
38	A2M	A1	876	38	-	1/5/27/28	0/3/3/3
34	OMC	B5	414	34	-	1/9/27/28	0/2/2/2
38	OMC	A1	2948	38	-	2/9/27/28	0/2/2/2
38	OMU	A1	2921	38	-	0/9/27/28	0/2/2/2
38	OMU	A1	898	38	-	1/9/27/28	0/2/2/2
34	A2M	B5	420	34	-	1/5/27/28	0/3/3/3
38	OMU	A1	2347	38	-	0/9/27/28	0/2/2/2
34	A2M	B5	100	34,83	-	2/5/27/28	0/3/3/3
34	OMC	B5	1007	34	-	1/9/27/28	0/2/2/2
38	OMG	A1	1450	83,38	-	1/5/27/28	0/3/3/3
34	MA6	B5	1781	34	-	2/7/29/30	0/3/3/3
38	OMG	A1	2791	38	-	1/5/27/28	0/3/3/3
38	5MC	A1	2870	83,38	-	4/7/25/26	0/2/2/2
34	OMG	B5	1572	34	-	0/5/27/28	0/3/3/3
38	OMC	A1	663	38	-	1/9/27/28	0/2/2/2
38	OMC	A1	2197	38	-	6/9/27/28	0/2/2/2
38	OMG	A1	2619	38	-	1/5/27/28	0/3/3/3
38	A2M	A1	1449	83,38	-	0/5/27/28	0/3/3/3
38	OMG	A1	2815	38	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	MA6	B5	1782	34	-	5/7/29/30	0/3/3/3
38	OMU	A1	2417	38	-	1/9/27/28	0/2/2/2
38	A2M	A1	807	38	-	0/5/27/28	0/3/3/3
38	OMC	A1	2959	38	-	0/9/27/28	0/2/2/2
38	A2M	A1	2280	38	-	2/5/27/28	0/3/3/3
38	OMC	A1	650	83,38	-	0/9/27/28	0/2/2/2
34	A2M	B5	796	34	-	0/5/27/28	0/3/3/3
34	4AC	B5	1280	34	-	2/11/29/30	0/2/2/2
34	A2M	B5	436	34	-	1/5/27/28	0/3/3/3
38	5MC	A1	2278	83,38	-	0/7/25/26	0/2/2/2
38	OMG	A1	2288	38	-	0/5/27/28	0/3/3/3
38	A2M	A1	2640	38	-	1/5/27/28	0/3/3/3
34	OMG	B5	1271	34	-	1/5/27/28	0/3/3/3
34	OMG	B5	1428	34	-	4/5/27/28	0/3/3/3
38	1MA	A1	2142	83,38	-	0/3/25/26	0/3/3/3
34	A2M	B5	974	34	-	0/5/27/28	0/3/3/3
80	DDE	DC	699	82,80	-	6/20/21/23	0/1/1/1
38	OMG	A1	867	38	-	1/5/27/28	0/3/3/3
34	A2M	B5	619	34,83	-	2/5/27/28	0/3/3/3
38	A2M	A1	649	38	-	1/5/27/28	0/3/3/3
38	OMU	A1	2724	38	-	1/9/27/28	0/2/2/2
34	G7M	B5	1575	34	-	0/3/25/26	0/3/3/3
34	XSX	B5	1191	34	-	4/16/34/35	0/2/2/2
38	OMC	A1	1437	83,38	-	3/9/27/28	0/2/2/2
38	OMG	A1	908	38	-	0/5/27/28	0/3/3/3
34	OMG	B5	1126	34	-	2/5/27/28	0/3/3/3
34	OMC	B5	1639	34	-	0/9/27/28	0/2/2/2
34	A2M	B5	541	34	-	3/5/27/28	0/3/3/3

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	C8-N9	7.44	1.46	1.33
34	B5	1575	G7M	C8-N7	7.41	1.46	1.33
38	A1	2142	1MA	C2-N3	4.74	1.34	1.29
38	A1	645	1MA	C2-N3	4.57	1.34	1.29
34	B5	1575	G7M	C5-C4	4.01	1.47	1.39
34	B5	1575	G7M	C2'-C1'	-3.90	1.47	1.53
36	AB	243	HIC	CD2-CG	3.40	1.41	1.36
38	A1	645	1MA	C6-N6	3.11	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2142	1MA	C6-N6	3.01	1.35	1.27
34	B5	1280	4AC	C4-N4	-2.90	1.35	1.39
38	A1	2870	5MC	C6-C5	2.85	1.39	1.34
34	B5	1773	4AC	C4-N4	-2.79	1.35	1.39
38	A1	2347	OMU	C4-N3	-2.76	1.33	1.38
38	A1	2729	OMU	C4-N3	-2.74	1.33	1.38
38	A1	2421	OMU	C4-N3	-2.72	1.33	1.38
38	A1	1888	OMU	C4-N3	-2.71	1.33	1.38
38	A1	2815	OMG	C6-N1	-2.70	1.33	1.37
38	A1	2921	OMU	C4-N3	-2.69	1.33	1.38
38	A1	898	OMU	C4-N3	-2.66	1.33	1.38
38	A1	2288	OMG	C6-N1	-2.64	1.33	1.37
38	A1	2417	OMU	C4-N3	-2.63	1.33	1.38
38	A1	2793	OMG	C6-N1	-2.63	1.34	1.37
38	A1	2278	5MC	C6-C5	2.63	1.38	1.34
38	A1	2724	OMU	C4-N3	-2.62	1.33	1.38
38	A1	2619	OMG	C6-N1	-2.61	1.34	1.37
34	B5	1126	OMG	C6-N1	-2.60	1.34	1.37
34	B5	541	A2M	C5-C4	2.58	1.47	1.40
34	B5	1781	MA6	C5-C4	2.57	1.47	1.40
38	A1	805	OMG	C6-N1	-2.56	1.34	1.37
38	A1	908	OMG	C6-N1	-2.55	1.34	1.37
38	A1	2922	OMG	C6-N1	-2.55	1.34	1.37
38	A1	2791	OMG	C6-N1	-2.54	1.34	1.37
34	B5	1269	OMU	C2-N1	2.54	1.42	1.38
34	B5	1269	OMU	C4-N3	-2.54	1.34	1.38
34	B5	562	OMG	C6-N1	-2.52	1.34	1.37
34	B5	1271	OMG	C6-N1	-2.50	1.34	1.37
38	A1	1450	OMG	C6-N1	-2.49	1.34	1.37
38	A1	867	OMG	C6-N1	-2.48	1.34	1.37
34	B5	436	A2M	C5-C4	2.45	1.47	1.40
34	B5	578	OMU	C4-N3	-2.43	1.34	1.38
38	A1	2220	A2M	C5-C4	2.43	1.47	1.40
34	B5	1572	OMG	C6-N1	-2.42	1.34	1.37
38	A1	1449	A2M	C5-C4	2.41	1.47	1.40
38	A1	2870	5MC	C6-N1	-2.41	1.33	1.38
34	B5	796	A2M	C5-C4	2.40	1.47	1.40
38	A1	2921	OMU	C2-N3	-2.40	1.33	1.38
34	B5	1428	OMG	C6-N1	-2.40	1.34	1.37
34	B5	974	A2M	C5-C4	2.38	1.47	1.40
34	B5	28	A2M	C5-C4	2.38	1.47	1.40
38	A1	2640	A2M	C5-C4	2.37	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	876	A2M	C5-C4	2.37	1.47	1.40
34	B5	420	A2M	C5-C4	2.36	1.47	1.40
38	A1	2421	OMU	C2-N3	-2.35	1.33	1.38
38	A1	2280	A2M	C5-C4	2.35	1.47	1.40
38	A1	898	OMU	C2-N3	-2.35	1.33	1.38
34	B5	1191	XSX	C2-N1	2.35	1.41	1.38
38	A1	807	A2M	C5-C4	2.34	1.47	1.40
34	B5	619	A2M	C5-C4	2.32	1.47	1.40
34	B5	100	A2M	C5-C4	2.32	1.47	1.40
38	A1	649	A2M	C5-C4	2.32	1.47	1.40
38	A1	2729	OMU	C2-N3	-2.31	1.33	1.38
34	B5	1575	G7M	C2'-C3'	-2.31	1.47	1.53
38	A1	2278	5MC	C6-N1	-2.31	1.34	1.38
34	B5	1782	MA6	C5-C4	2.28	1.47	1.40
38	A1	2724	OMU	C2-N3	-2.27	1.33	1.38
38	A1	2946	A2M	C5-C4	2.27	1.46	1.40
38	A1	817	A2M	C5-C4	2.27	1.46	1.40
38	A1	1888	OMU	C2-N3	-2.27	1.33	1.38
38	A1	1133	A2M	C5-C4	2.25	1.46	1.40
38	A1	2417	OMU	C2-N3	-2.25	1.34	1.38
38	A1	2347	OMU	C2-N3	-2.24	1.34	1.38
34	B5	1773	4AC	C7-N4	-2.23	1.33	1.37
38	A1	2417	OMU	C5-C4	-2.21	1.38	1.43
38	A1	2281	A2M	C5-C4	2.21	1.46	1.40
38	A1	2729	OMU	C5-C4	-2.19	1.38	1.43
38	A1	2347	OMU	C2-N1	2.18	1.42	1.38
38	A1	898	OMU	C5-C4	-2.18	1.38	1.43
34	B5	578	OMU	C2-N3	-2.18	1.34	1.38
38	A1	2347	OMU	C5-C4	-2.15	1.38	1.43
34	B5	1575	G7M	C6-N1	-2.15	1.34	1.37
38	A1	2724	OMU	C5-C4	-2.15	1.38	1.43
80	DC	699	DDE	CD2-NE2	2.13	1.39	1.36
38	A1	2421	OMU	C5-C4	-2.12	1.38	1.43
38	A1	1888	OMU	C5-C4	-2.12	1.38	1.43
34	B5	1269	OMU	C2-N3	-2.10	1.34	1.38
36	AB	243	HIC	CZ-NE2	-2.10	1.42	1.48
38	A1	2921	OMU	C5-C4	-2.04	1.39	1.43
34	B5	1269	OMU	C5-C4	-2.02	1.39	1.43

All (165) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2634	UR3	C4-N3-C2	-5.76	119.14	124.56
34	B5	1191	XSX	C3-C1-N3	-5.14	102.37	112.00
34	B5	1191	XSX	C4-N3-C2	-4.96	118.41	124.63
34	B5	1773	4AC	N4-C4-N3	4.83	121.96	113.85
38	A1	2921	OMU	C4-N3-C2	-4.59	120.53	126.58
38	A1	2421	OMU	C4-N3-C2	-4.58	120.54	126.58
38	A1	2870	5MC	C5-C6-N1	-4.47	118.74	123.34
38	A1	2724	OMU	C4-N3-C2	-4.46	120.69	126.58
34	B5	578	OMU	C4-N3-C2	-4.46	120.70	126.58
38	A1	1888	OMU	C4-N3-C2	-4.44	120.72	126.58
38	A1	2921	OMU	N3-C2-N1	4.39	120.72	114.89
38	A1	898	OMU	C4-N3-C2	-4.34	120.85	126.58
38	A1	2421	OMU	N3-C2-N1	4.33	120.64	114.89
38	A1	2724	OMU	N3-C2-N1	4.31	120.61	114.89
38	A1	1888	OMU	N3-C2-N1	4.27	120.56	114.89
38	A1	2417	OMU	C4-N3-C2	-4.24	120.99	126.58
38	A1	898	OMU	N3-C2-N1	4.23	120.51	114.89
38	A1	2417	OMU	N3-C2-N1	4.13	120.38	114.89
34	B5	1191	XSX	C1'-N1-C2	4.07	123.86	116.99
38	A1	2347	OMU	N3-C2-N1	4.06	120.28	114.89
34	B5	578	OMU	N3-C2-N1	4.02	120.23	114.89
38	A1	2347	OMU	C4-N3-C2	-4.02	121.28	126.58
38	A1	2729	OMU	C4-N3-C2	-4.01	121.28	126.58
34	B5	1269	OMU	C4-N3-C2	-4.00	121.30	126.58
34	B5	1269	OMU	N3-C2-N1	3.93	120.11	114.89
38	A1	2729	OMU	N3-C2-N1	3.88	120.04	114.89
38	A1	2220	A2M	N3-C2-N1	-3.70	122.89	128.68
38	A1	2921	OMU	C5-C4-N3	3.66	120.31	114.84
38	A1	2421	OMU	C5-C4-N3	3.64	120.29	114.84
34	B5	1781	MA6	C4-C5-N7	-3.64	105.60	109.40
34	B5	1782	MA6	N3-C2-N1	-3.62	123.02	128.68
34	B5	578	OMU	C5-C4-N3	3.61	120.24	114.84
38	A1	2724	OMU	C5-C4-N3	3.58	120.19	114.84
38	A1	2729	OMU	C5-C4-N3	3.56	120.17	114.84
34	B5	1191	XSX	C6-N1-C2	-3.55	118.61	121.79
38	A1	898	OMU	C5-C4-N3	3.54	120.13	114.84
38	A1	1888	OMU	C5-C4-N3	3.53	120.12	114.84
34	B5	1191	XSX	O2-C2-N3	-3.50	117.12	121.99
38	A1	1437	OMC	O2-C2-N3	-3.47	116.69	122.33
34	B5	1575	G7M	O3'-C3'-C4'	3.46	121.05	111.05
34	B5	1575	G7M	O2'-C2'-C3'	3.46	123.01	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2417	OMU	C5-C4-N3	3.45	120.00	114.84
34	B5	1269	OMU	C5-C4-N3	3.44	119.98	114.84
34	B5	1280	4AC	N4-C4-N3	3.43	119.60	113.85
38	A1	2946	A2M	N3-C2-N1	-3.40	123.36	128.68
34	B5	1191	XSX	C1-N3-C4	3.40	123.85	117.14
34	B5	1269	OMU	C1'-N1-C2	3.39	123.72	117.57
34	B5	796	A2M	N3-C2-N1	-3.36	123.42	128.68
38	A1	2347	OMU	C5-C4-N3	3.35	119.85	114.84
38	A1	817	A2M	N3-C2-N1	-3.34	123.46	128.68
34	B5	1781	MA6	N3-C2-N1	-3.33	123.47	128.68
34	B5	974	A2M	N3-C2-N1	-3.31	123.50	128.68
38	A1	2347	OMU	C1'-N1-C2	3.28	123.52	117.57
38	A1	649	A2M	N3-C2-N1	-3.26	123.58	128.68
38	A1	1133	A2M	N3-C2-N1	-3.24	123.61	128.68
38	A1	876	A2M	N3-C2-N1	-3.21	123.66	128.68
34	B5	100	A2M	N3-C2-N1	-3.19	123.69	128.68
34	B5	420	A2M	N3-C2-N1	-3.18	123.70	128.68
34	B5	436	A2M	N3-C2-N1	-3.18	123.72	128.68
34	B5	541	A2M	N3-C2-N1	-3.15	123.76	128.68
38	A1	2281	A2M	N3-C2-N1	-3.14	123.78	128.68
34	B5	28	A2M	N3-C2-N1	-3.13	123.78	128.68
38	A1	1449	A2M	N3-C2-N1	-3.13	123.79	128.68
38	A1	2640	A2M	N3-C2-N1	-3.10	123.83	128.68
34	B5	619	A2M	N3-C2-N1	-3.06	123.89	128.68
38	A1	2417	OMU	O4-C4-C5	-3.06	119.79	125.16
38	A1	898	OMU	O4-C4-C5	-3.04	119.82	125.16
38	A1	2280	A2M	N3-C2-N1	-3.03	123.94	128.68
38	A1	2948	OMC	O2-C2-N3	-3.03	117.40	122.33
38	A1	2724	OMU	O4-C4-C5	-3.03	119.83	125.16
38	A1	2278	5MC	O2-C2-N3	-3.03	117.41	122.33
38	A1	2421	OMU	O4-C4-C5	-3.00	119.89	125.16
38	A1	1888	OMU	O4-C4-C5	-2.98	119.92	125.16
38	A1	1437	OMC	C1'-N1-C2	2.94	124.97	118.42
38	A1	2729	OMU	O4-C4-C5	-2.93	120.00	125.16
38	A1	2278	5MC	C5-C6-N1	-2.93	120.32	123.34
38	A1	2640	A2M	C4-C5-N7	-2.91	106.37	109.40
34	B5	1269	OMU	O4-C4-C5	-2.90	120.06	125.16
34	B5	578	OMU	O4-C4-C5	-2.90	120.07	125.16
34	B5	1575	G7M	C3'-C2'-C1'	2.89	105.33	100.98
38	A1	2921	OMU	O4-C4-C5	-2.89	120.08	125.16
34	B5	1782	MA6	C4-C5-N7	-2.84	106.44	109.40
34	B5	28	A2M	C4-C5-N7	-2.83	106.45	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1191	XSX	C5-C4-N3	2.82	119.22	115.50
38	A1	1133	A2M	C4-C5-N7	-2.82	106.47	109.40
38	A1	2347	OMU	O4-C4-C5	-2.81	120.21	125.16
38	A1	817	A2M	C4-C5-N7	-2.80	106.48	109.40
34	B5	1782	MA6	N1-C6-N6	2.79	119.99	117.06
34	B5	619	A2M	C4-C5-N7	-2.79	106.49	109.40
34	B5	436	A2M	C4-C5-N7	-2.77	106.51	109.40
38	A1	807	A2M	C4-C5-N7	-2.77	106.51	109.40
38	A1	807	A2M	N3-C2-N1	-2.74	124.40	128.68
38	A1	2870	5MC	C5-C4-N3	-2.73	118.72	121.67
38	A1	876	A2M	C4-C5-N7	-2.73	106.55	109.40
38	A1	2278	5MC	C5-C4-N3	-2.72	118.74	121.67
34	B5	1575	G7M	CN7-N7-C8	-2.70	112.43	125.43
38	A1	2220	A2M	C2-N1-C6	2.67	123.32	118.75
34	B5	974	A2M	C4-C5-N7	-2.65	106.64	109.40
34	B5	420	A2M	C4-C5-N7	-2.62	106.67	109.40
38	A1	2280	A2M	C4-C5-N7	-2.58	106.71	109.40
38	A1	649	A2M	C4-C5-N7	-2.57	106.72	109.40
34	B5	100	A2M	C4-C5-N7	-2.57	106.72	109.40
34	B5	796	A2M	C4-C5-N7	-2.56	106.73	109.40
34	B5	1007	OMC	O2-C2-N3	-2.56	118.17	122.33
34	B5	541	A2M	C4-C5-N7	-2.56	106.73	109.40
38	A1	2142	1MA	C5-C6-N1	2.54	117.68	113.90
38	A1	1449	A2M	C4-C5-N7	-2.54	106.76	109.40
80	DC	699	DDE	CAU-CBW-CBI	-2.53	106.18	111.20
38	A1	2946	A2M	C4-C5-N7	-2.49	106.80	109.40
38	A1	2337	OMC	O2-C2-N3	-2.47	118.31	122.33
38	A1	2948	OMC	C1'-N1-C2	2.45	123.88	118.42
34	B5	1773	4AC	C5-C4-N4	-2.43	118.69	122.92
34	B5	1572	OMG	C8-N7-C5	2.43	107.61	102.99
38	A1	2791	OMG	C8-N7-C5	2.39	107.55	102.99
34	B5	1773	4AC	C6-C5-C4	2.38	119.88	116.96
34	B5	578	OMU	O2-C2-N1	-2.36	119.65	122.79
38	A1	805	OMG	C8-N7-C5	2.36	107.48	102.99
38	A1	2815	OMG	C5-C6-N1	2.36	118.11	113.95
38	A1	867	OMG	C5-C6-N1	2.34	118.09	113.95
34	B5	562	OMG	C8-N7-C5	2.32	107.41	102.99
38	A1	645	1MA	C5-C6-N1	2.32	117.36	113.90
34	B5	1126	OMG	C8-N7-C5	2.32	107.40	102.99
38	A1	645	1MA	C8-N7-C5	2.31	107.40	102.99
34	B5	1280	4AC	C6-C5-C4	2.31	119.79	116.96
38	A1	2619	OMG	C5-C6-N1	2.31	118.02	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	867	OMG	C8-N7-C5	2.30	107.38	102.99
38	A1	2288	OMG	C5-C6-N1	2.29	118.00	113.95
34	B5	562	OMG	C5-C6-N1	2.28	117.98	113.95
38	A1	2220	A2M	C4-C5-N7	-2.28	107.03	109.40
38	A1	2619	OMG	C8-N7-C5	2.27	107.31	102.99
38	A1	908	OMG	C5-C6-N1	2.27	117.96	113.95
34	B5	1126	OMG	C5-C6-N1	2.27	117.95	113.95
34	B5	1271	OMG	C5-C6-N1	2.26	117.95	113.95
38	A1	2815	OMG	C8-N7-C5	2.26	107.30	102.99
38	A1	2922	OMG	C8-N7-C5	2.24	107.25	102.99
38	A1	2793	OMG	C8-N7-C5	2.24	107.25	102.99
34	B5	1428	OMG	C5-C6-N1	2.24	117.90	113.95
34	B5	1572	OMG	C5-C6-N1	2.23	117.89	113.95
38	A1	2791	OMG	C5-C6-N1	2.23	117.88	113.95
38	A1	805	OMG	C5-C6-N1	2.22	117.88	113.95
38	A1	2921	OMU	O2-C2-N1	-2.22	119.84	122.79
38	A1	2922	OMG	C5-C6-N1	2.20	117.84	113.95
38	A1	2288	OMG	C8-N7-C5	2.20	107.18	102.99
38	A1	1450	OMG	C5-C6-N1	2.20	117.83	113.95
38	A1	2724	OMU	O2-C2-N1	-2.19	119.88	122.79
38	A1	2281	A2M	C4-C5-N7	-2.19	107.12	109.40
38	A1	2421	OMU	O2-C2-N1	-2.19	119.88	122.79
34	B5	1271	OMG	C8-N7-C5	2.18	107.15	102.99
38	A1	2793	OMG	C5-C6-N1	2.18	117.80	113.95
38	A1	2729	OMU	C1'-N1-C2	2.18	121.51	117.57
34	B5	1269	OMU	O2-C2-N3	-2.15	117.49	121.50
38	A1	1437	OMC	O2-C2-N1	2.14	123.32	118.89
38	A1	2142	1MA	N1-C2-N3	-2.12	123.55	126.02
34	B5	414	OMC	O2-C2-N3	-2.10	118.91	122.33
38	A1	908	OMG	C8-N7-C5	2.10	106.99	102.99
34	B5	1428	OMG	C8-N7-C5	2.10	106.99	102.99
38	A1	817	A2M	O3'-C3'-C4'	-2.09	105.02	111.05
38	A1	1450	OMG	C8-N7-C5	2.08	106.96	102.99
38	A1	645	1MA	N1-C2-N3	-2.08	123.59	126.02
34	B5	1269	OMU	CM2-O2'-C2'	-2.08	109.06	114.52
38	A1	2347	OMU	O2-C2-N3	-2.05	117.68	121.50
38	A1	2142	1MA	C8-N7-C5	2.05	106.89	102.99
34	B5	1773	4AC	C5-C4-N3	-2.04	119.31	122.59
38	A1	2870	5MC	O2-C2-N3	-2.02	119.05	122.33
38	A1	898	OMU	O2-C2-N1	-2.02	120.10	122.79

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B5	100	A2M	C1'-C2'-O2'-CM'
34	B5	414	OMC	C1'-C2'-O2'-CM2
34	B5	420	A2M	C1'-C2'-O2'-CM'
34	B5	436	A2M	C1'-C2'-O2'-CM'
34	B5	619	A2M	O4'-C4'-C5'-O5'
34	B5	1007	OMC	C1'-C2'-O2'-CM2
34	B5	1191	XSX	O4'-C1'-N1-C2
34	B5	1271	OMG	C1'-C2'-O2'-CM2
34	B5	1428	OMG	C1'-C2'-O2'-CM2
34	B5	1782	MA6	C5-C6-N6-C9
34	B5	1782	MA6	C5-C6-N6-C10
34	B5	1280	4AC	N3-C4-N4-C7
34	B5	1280	4AC	C5-C4-N4-C7
34	B5	1773	4AC	N3-C4-N4-C7
34	B5	1773	4AC	C5-C4-N4-C7
34	B5	1773	4AC	O7-C7-N4-C4
34	B5	1773	4AC	CM7-C7-N4-C4
38	A1	663	OMC	C1'-C2'-O2'-CM2
38	A1	876	A2M	C1'-C2'-O2'-CM'
38	A1	1437	OMC	C1'-C2'-O2'-CM2
38	A1	2197	OMC	C2'-C1'-N1-C2
38	A1	2197	OMC	C2'-C1'-N1-C6
38	A1	2337	OMC	C1'-C2'-O2'-CM2
38	A1	2417	OMU	C1'-C2'-O2'-CM2
38	A1	2421	OMU	C1'-C2'-O2'-CM2
38	A1	2619	OMG	C1'-C2'-O2'-CM2
38	A1	2640	A2M	C1'-C2'-O2'-CM'
38	A1	2724	OMU	C1'-C2'-O2'-CM2
38	A1	2729	OMU	C1'-C2'-O2'-CM2
38	A1	2791	OMG	C1'-C2'-O2'-CM2
38	A1	2946	A2M	C1'-C2'-O2'-CM'
38	A1	2948	OMC	C1'-C2'-O2'-CM2
34	B5	541	A2M	O4'-C4'-C5'-O5'
34	B5	541	A2M	C3'-C4'-C5'-O5'
38	A1	2197	OMC	O4'-C4'-C5'-O5'
38	A1	2280	A2M	O4'-C4'-C5'-O5'
38	A1	2729	OMU	C3'-C4'-C5'-O5'
38	A1	2729	OMU	O4'-C4'-C5'-O5'
34	B5	1191	XSX	O4'-C1'-N1-C6
34	B5	619	A2M	C3'-C4'-C5'-O5'
34	B5	1428	OMG	O4'-C4'-C5'-O5'
34	B5	1428	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
34	B5	1782	MA6	O4'-C4'-C5'-O5'
38	A1	2280	A2M	C3'-C4'-C5'-O5'
34	B5	1782	MA6	N1-C6-N6-C9
34	B5	1191	XSX	N4-C7-C9-O10
34	B5	1781	MA6	C5-C6-N6-C9
34	B5	1781	MA6	C5-C6-N6-C10
38	A1	2197	OMC	C3'-C4'-C5'-O5'
38	A1	817	A2M	C4'-C5'-O5'-P
34	B5	1126	OMG	C3'-C4'-C5'-O5'
80	DC	699	DDE	CBI-CBW-NCB-CAB
80	DC	699	DDE	CBI-CBW-NCB-CAC
38	A1	2870	5MC	C2'-C1'-N1-C6
38	A1	898	OMU	C1'-C2'-O2'-CM2
80	DC	699	DDE	CE1-CAT-CAU-CBW
80	DC	699	DDE	CAU-CBW-NCB-CAB
80	DC	699	DDE	CAU-CBW-NCB-CAC
34	B5	1269	OMU	O4'-C1'-N1-C6
34	B5	541	A2M	C4'-C5'-O5'-P
34	B5	1428	OMG	C4'-C5'-O5'-P
34	B5	1782	MA6	C3'-C4'-C5'-O5'
38	A1	2870	5MC	O4'-C1'-N1-C6
34	B5	578	OMU	C2'-C1'-N1-C6
34	B5	1269	OMU	O4'-C1'-N1-C2
38	A1	2197	OMC	O4'-C1'-N1-C6
34	B5	1269	OMU	C4'-C5'-O5'-P
38	A1	649	A2M	C4'-C5'-O5'-P
38	A1	2197	OMC	O4'-C1'-N1-C2
38	A1	1450	OMG	C4'-C5'-O5'-P
38	A1	2281	A2M	O4'-C4'-C5'-O5'
38	A1	2870	5MC	O4'-C1'-N1-C2
38	A1	1437	OMC	O4'-C4'-C5'-O5'
34	B5	1191	XSX	N4-C7-C9-O11
34	B5	578	OMU	O4'-C1'-N1-C6
34	B5	1126	OMG	C1'-C2'-O2'-CM2
38	A1	867	OMG	C1'-C2'-O2'-CM2
38	A1	1437	OMC	C2'-C1'-N1-C2
38	A1	2870	5MC	C2'-C1'-N1-C2
34	B5	100	A2M	C4'-C5'-O5'-P
34	B5	578	OMU	O4'-C1'-N1-C2
38	A1	817	A2M	O4'-C4'-C5'-O5'
34	B5	578	OMU	C2'-C1'-N1-C2
34	B5	1269	OMU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
34	B5	1269	OMU	O4'-C4'-C5'-O5'
80	DC	699	DDE	CAT-CAU-CBW-CBI
38	A1	2948	OMC	C2'-C1'-N1-C2

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 220 ligands modelled in this entry, 218 are monoatomic - leaving 2 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
85	GDP	DC	901	83	24,30,30	0.93	1 (4%)	30,47,47	1.21	4 (13%)
86	W9C	DC	902	-	35,39,39	0.66	2 (5%)	39,64,64	1.09	4 (10%)

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
85	GDP	DC	901	83	-	4/12/32/32	0/3/3/3
86	W9C	DC	902	-	1/1/15/16	3/21/104/104	0/7/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	DC	902	W9C	O14-C5	-2.75	1.20	1.30
85	DC	901	GDP	C6-N1	-2.68	1.33	1.37
86	DC	902	W9C	C1-C5	2.03	1.55	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	DC	902	W9C	C12-C6-C2	-4.23	98.40	105.11
85	DC	901	GDP	PA-O3A-PB	-3.16	121.98	132.83
86	DC	902	W9C	C20-C13-C4	2.94	120.27	112.42
85	DC	901	GDP	O6-C6-C5	-2.17	120.14	124.37
86	DC	902	W9C	C18-C9-C16	-2.10	100.63	103.64
85	DC	901	GDP	C5-C6-N1	2.03	117.54	113.95
86	DC	902	W9C	C7-C2-C6	2.02	116.00	112.17
85	DC	901	GDP	C8-N7-C5	2.00	106.81	102.99

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
86	DC	902	W9C	C52

All (7) torsion outliers are listed below:

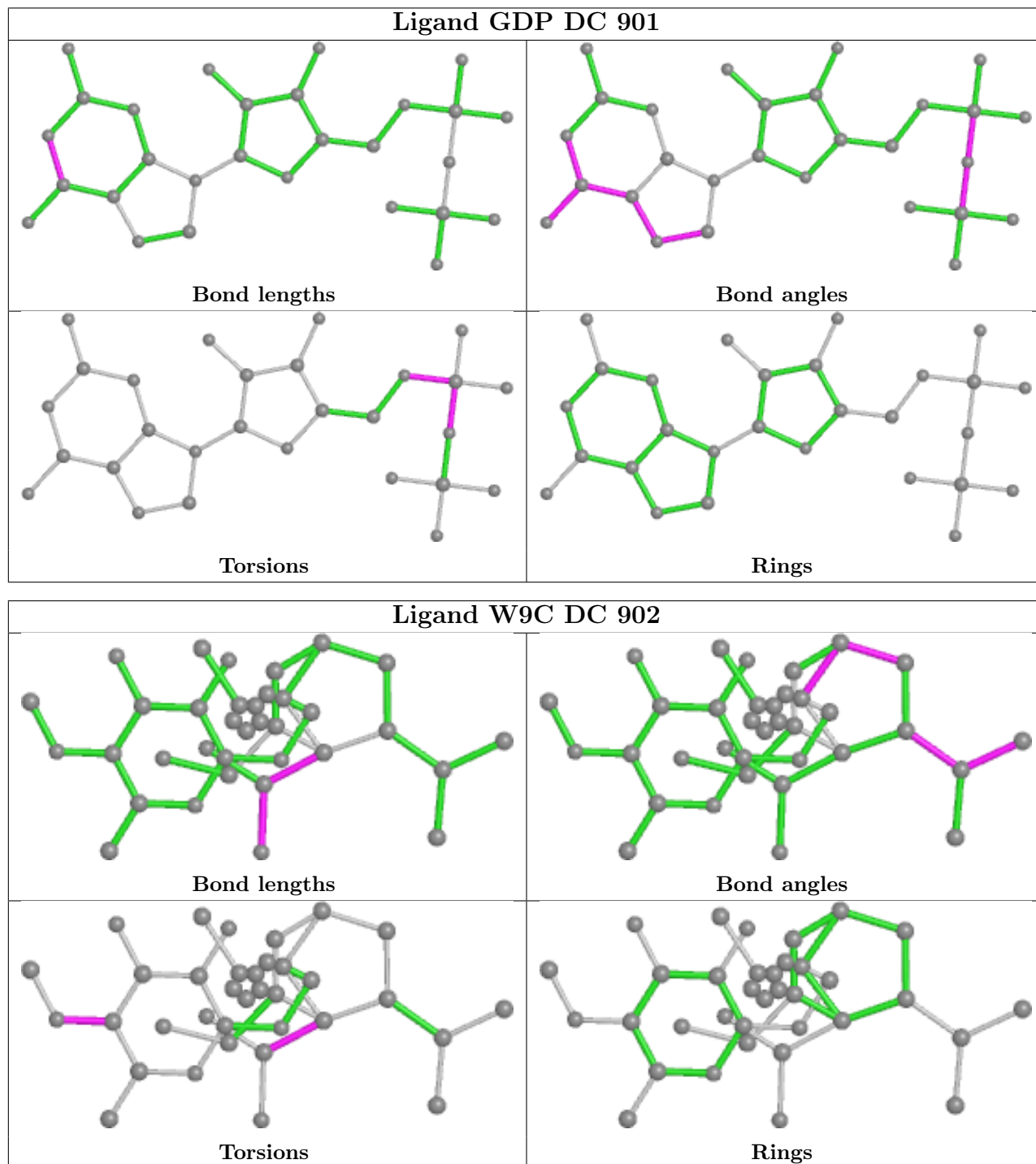
Mol	Chain	Res	Type	Atoms
85	DC	901	GDP	C5'-O5'-PA-O3A
86	DC	902	W9C	C2-C1-C5-O14
86	DC	902	W9C	C2-C1-C5-O15
86	DC	902	W9C	C54-C55-O64-C65
85	DC	901	GDP	C5'-O5'-PA-O2A
85	DC	901	GDP	PB-O3A-PA-O2A
85	DC	901	GDP	PB-O3A-PA-O1A

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

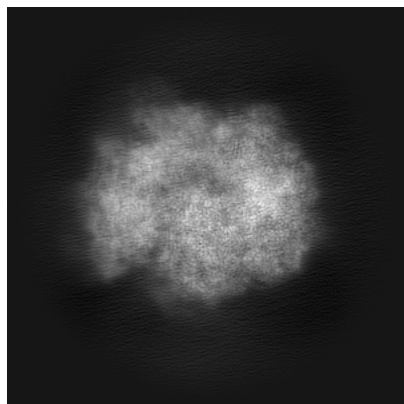
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28634. These allow visual inspection of the internal detail of the map and identification of artifacts.

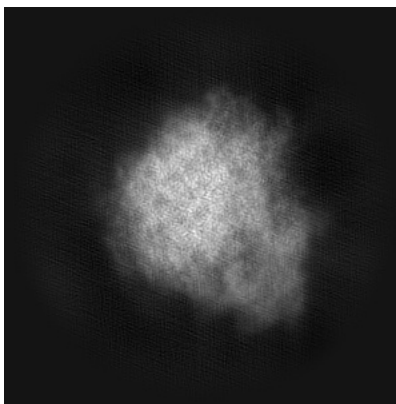
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

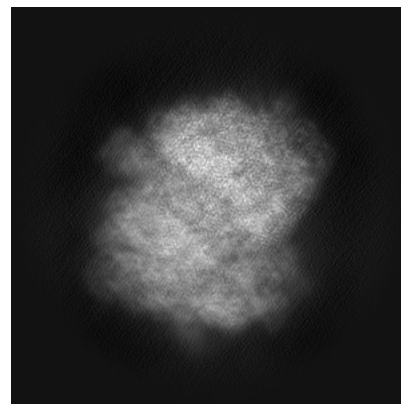
6.1.1 Primary map



X

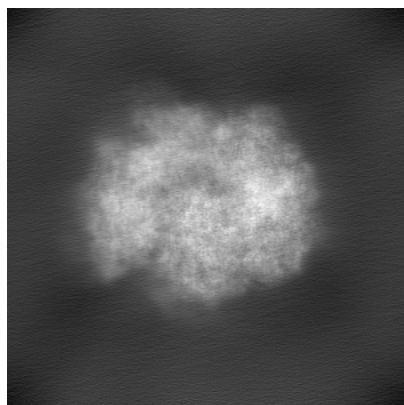


Y

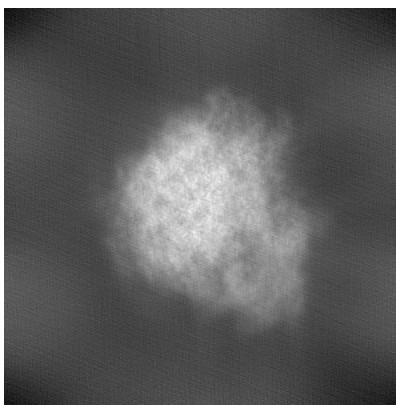


Z

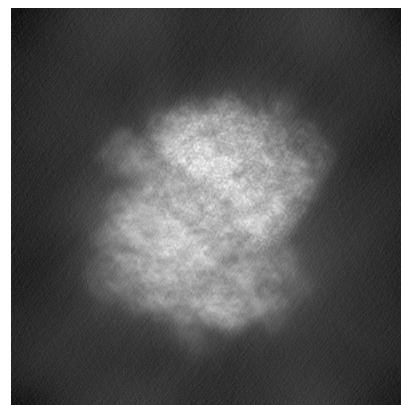
6.1.2 Raw map



X



Y

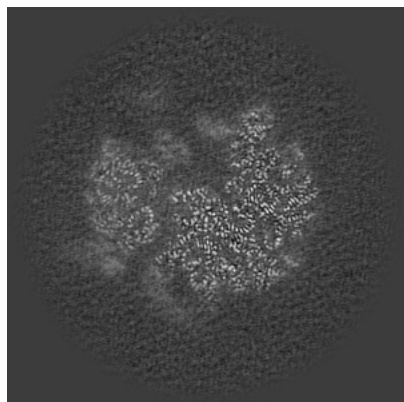


Z

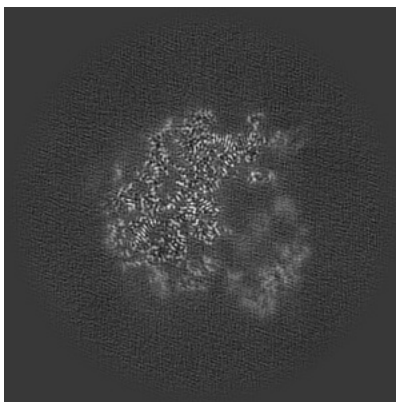
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

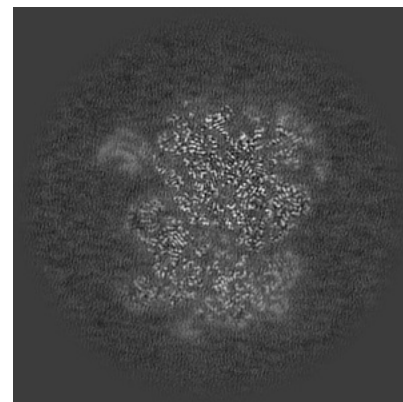
6.2.1 Primary map



X Index: 200

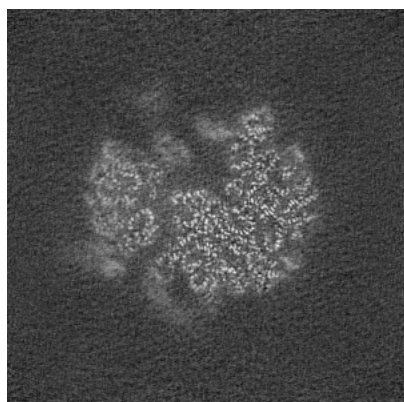


Y Index: 200

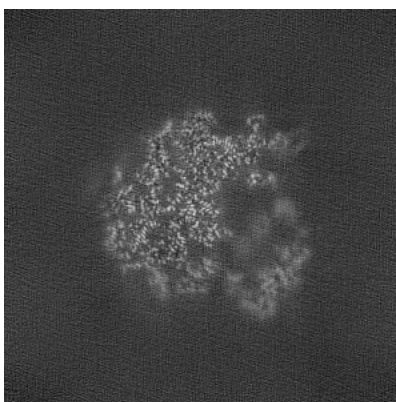


Z Index: 200

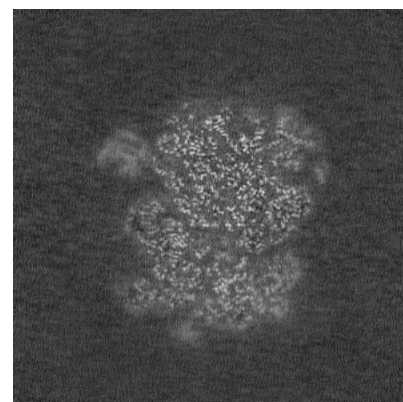
6.2.2 Raw map



X Index: 200



Y Index: 200

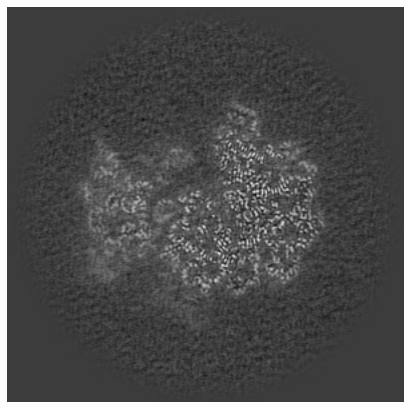


Z Index: 200

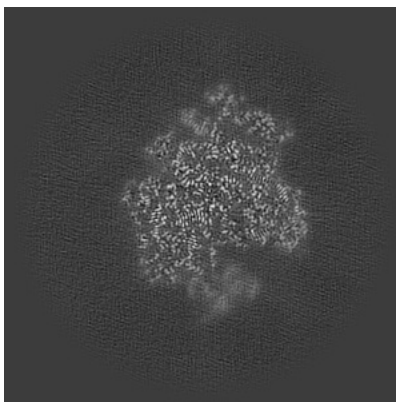
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

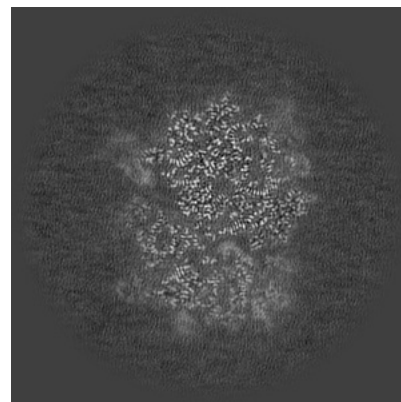
6.3.1 Primary map



X Index: 215

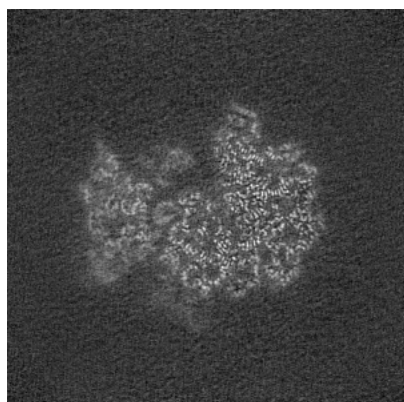


Y Index: 245

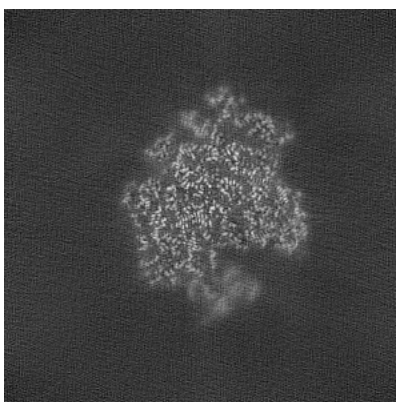


Z Index: 190

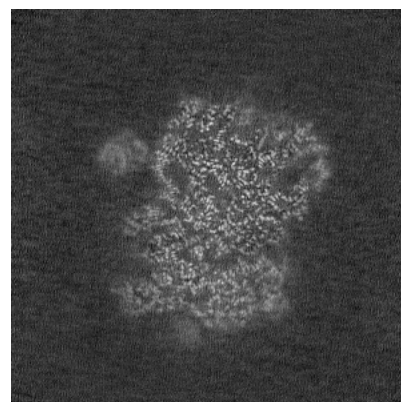
6.3.2 Raw map



X Index: 215



Y Index: 245

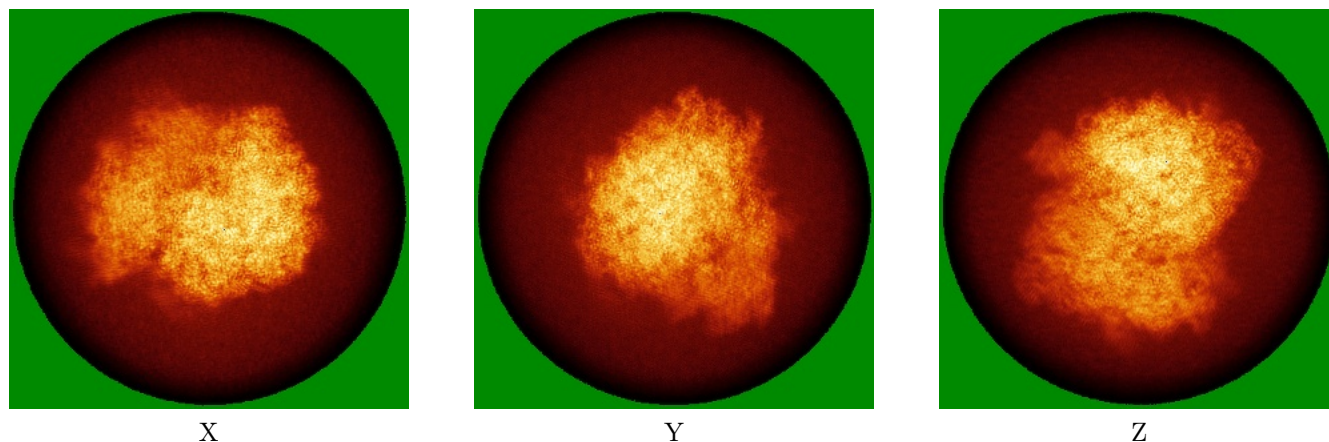


Z Index: 206

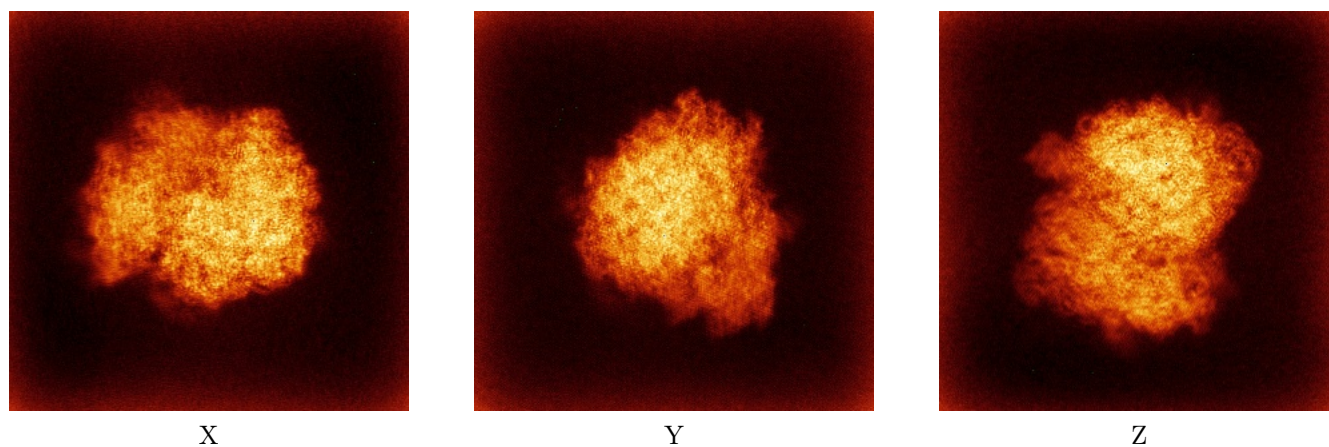
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



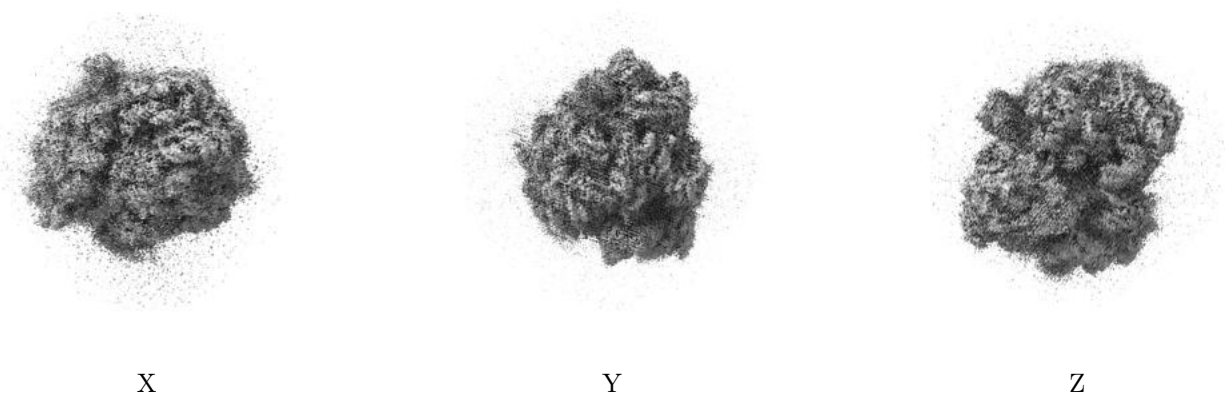
6.4.2 Raw map



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

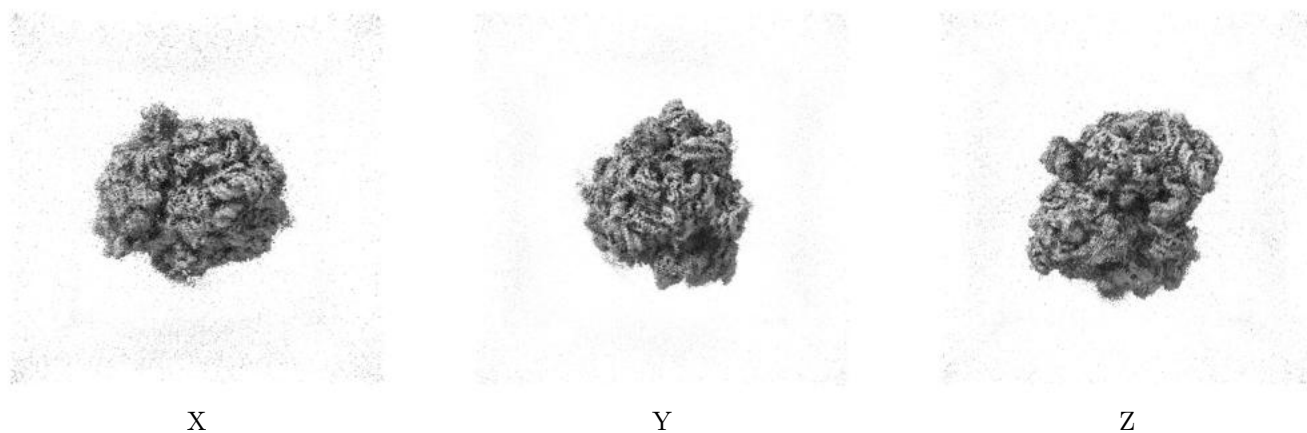
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

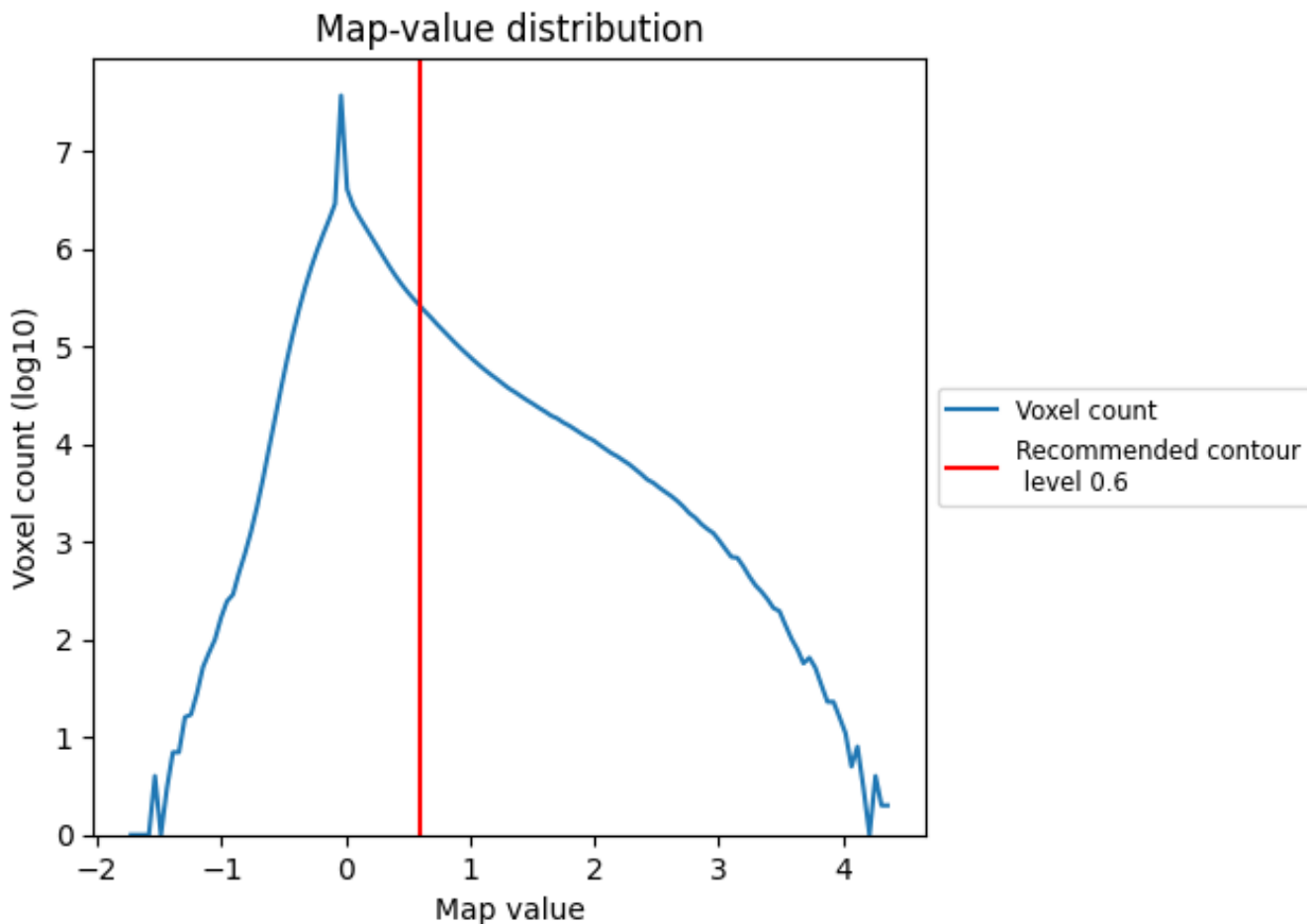
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

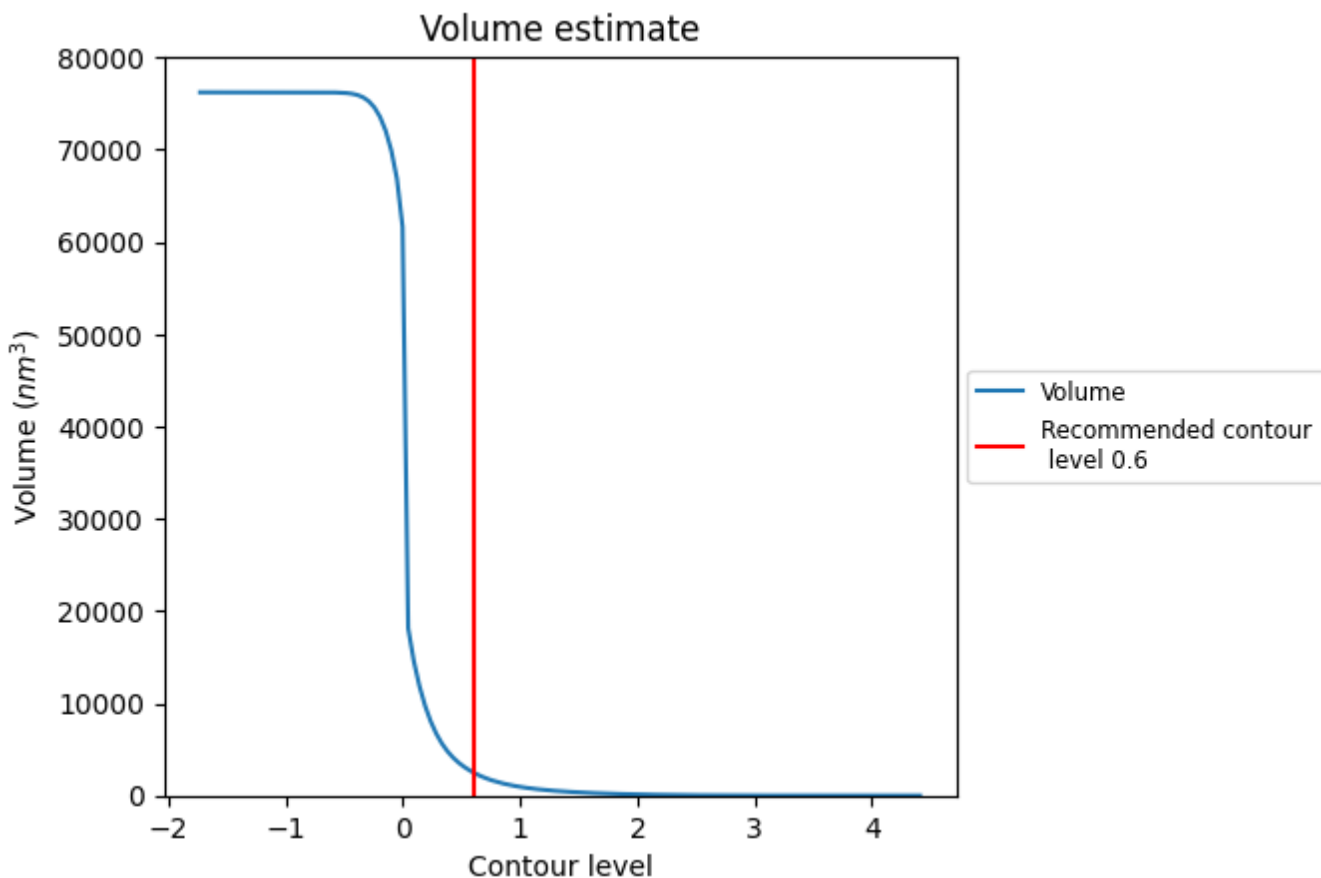
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

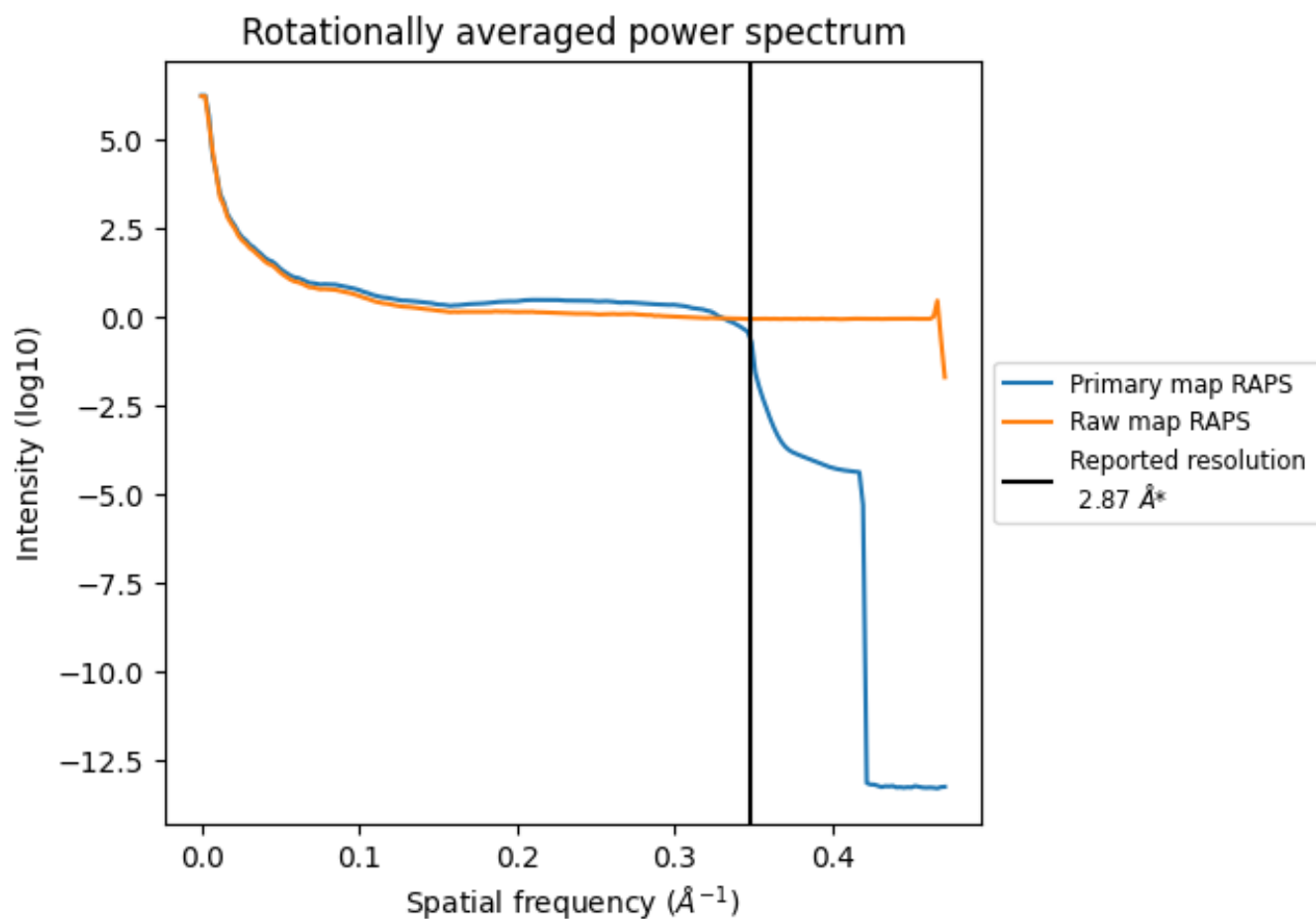
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2515 nm³; this corresponds to an approximate mass of 2272 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

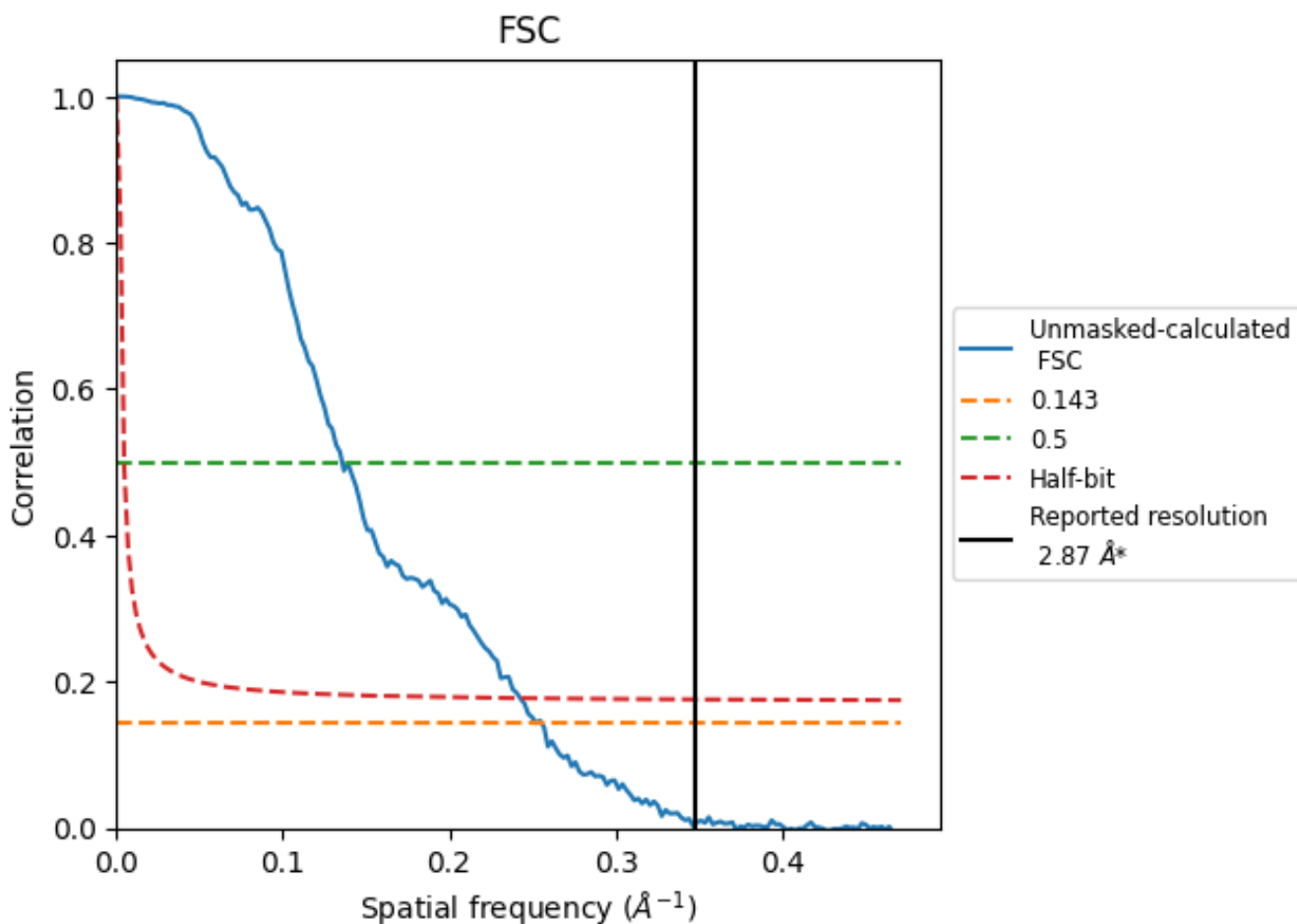


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

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 0.348 \AA^{-1}

8.2 Resolution estimates [i](#)

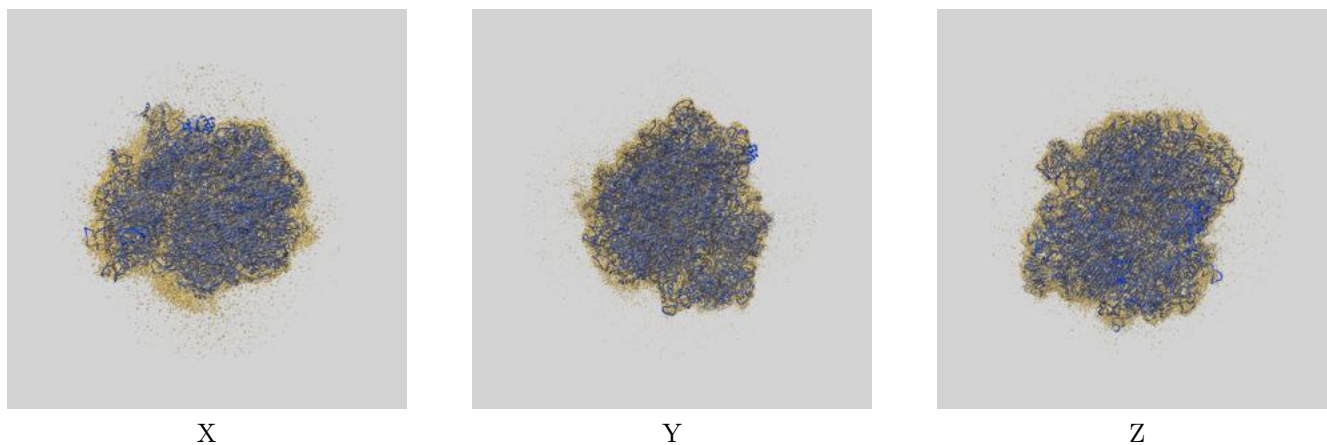
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	7.37	4.12

*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 3.96 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

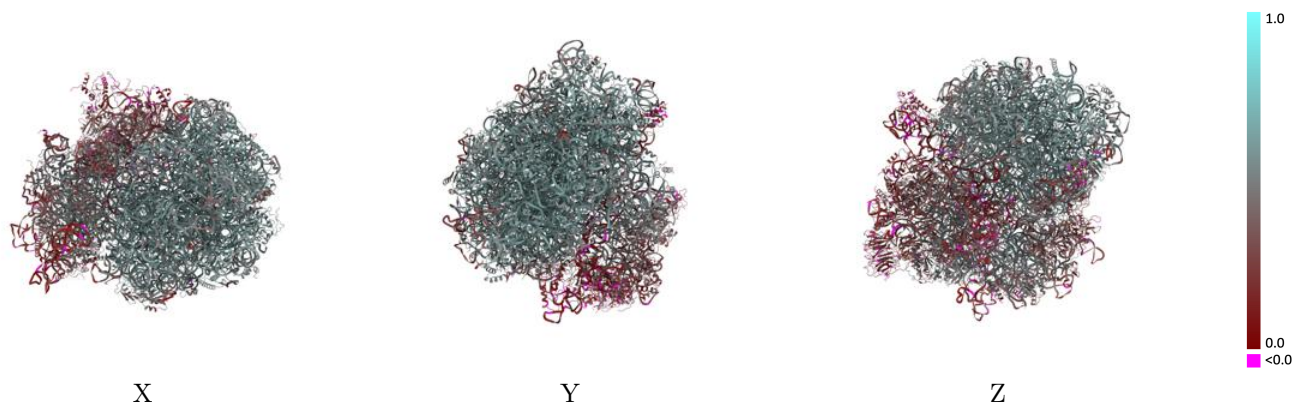
This section contains information regarding the fit between EMDB map EMD-28634 and PDB model 8EVR. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



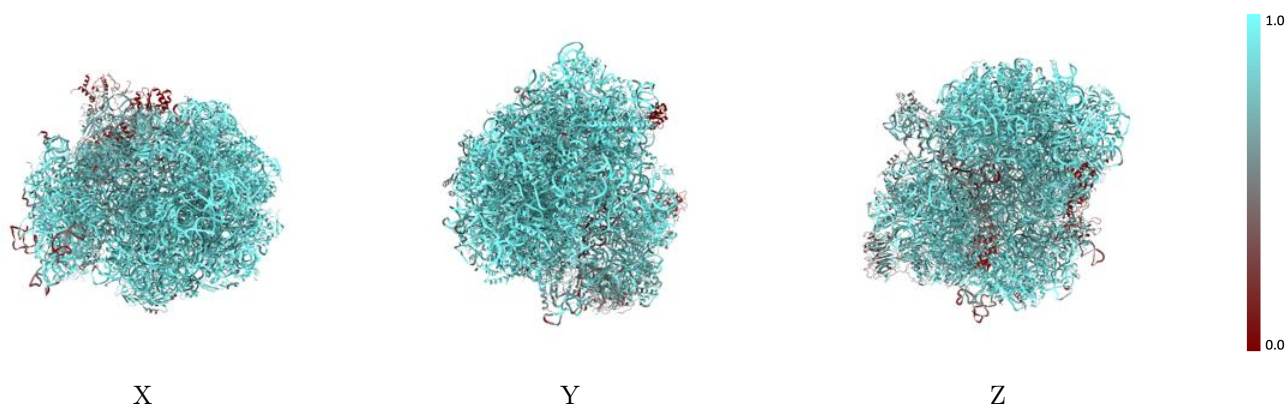
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



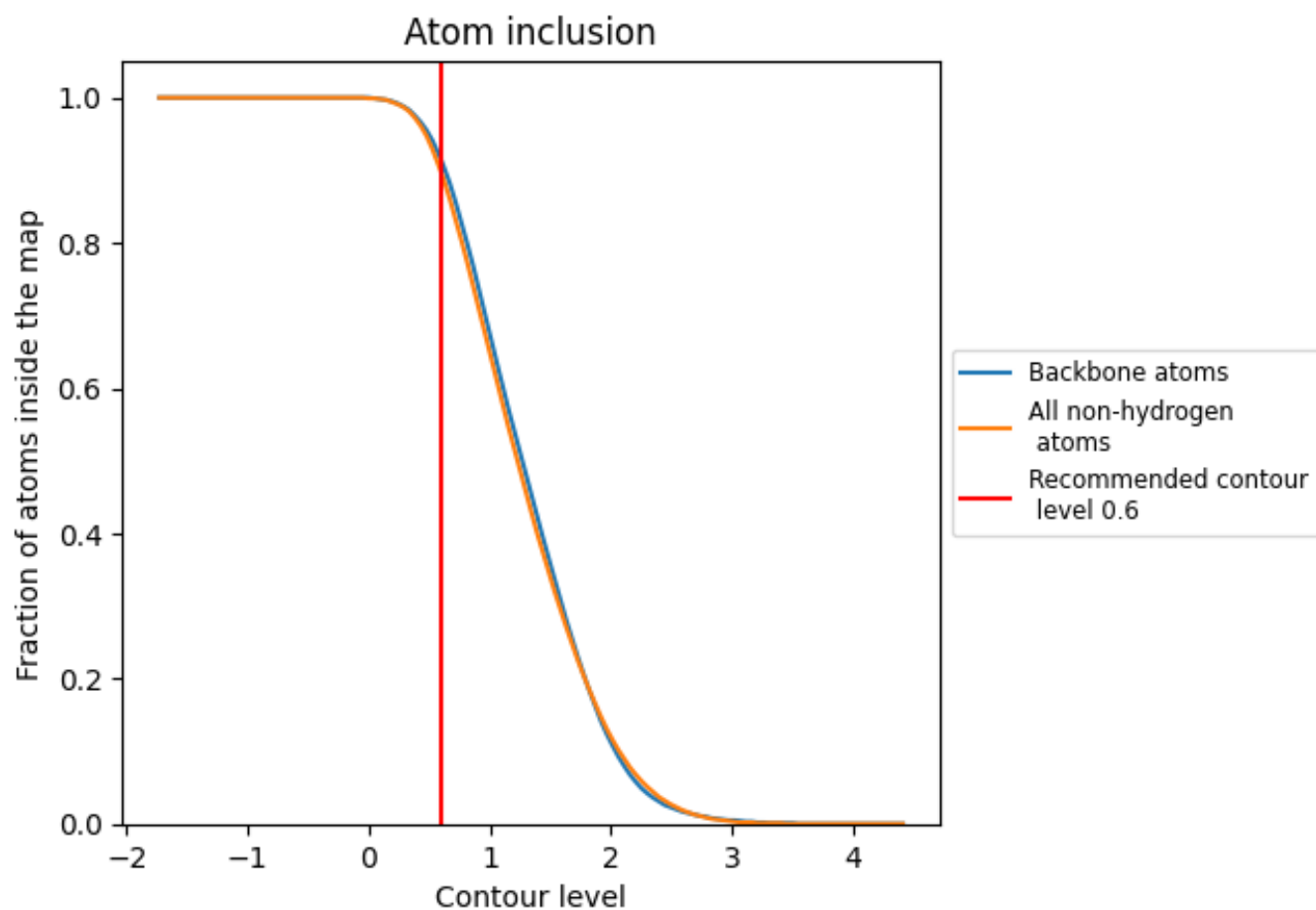
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.4700
A1	 0.9690	 0.5450
A3	 0.9880	 0.5370
A4	 0.9820	 0.5650
AA	 0.9650	 0.5960
AB	 0.9610	 0.5570
AC	 0.9600	 0.5680
AD	 0.9000	 0.4750
AE	 0.9400	 0.5160
AF	 0.9770	 0.5790
AG	 0.9170	 0.5240
AH	 0.9140	 0.5420
AI	 0.9570	 0.5560
AJ	 0.8430	 0.4180
AL	 0.9560	 0.5620
AM	 0.9560	 0.5510
AN	 0.9900	 0.6000
AO	 0.9620	 0.5680
AP	 0.9530	 0.5520
AQ	 0.9790	 0.5920
AR	 0.8140	 0.4660
AS	 0.9640	 0.5660
AT	 0.9600	 0.5490
AU	 0.8950	 0.4500
AV	 0.9550	 0.5720
AW	 0.9720	 0.5570
AX	 0.9420	 0.5390
AY	 0.9600	 0.5440
AZ	 0.9270	 0.5260
Aa	 0.9740	 0.5860
Ab	 0.9430	 0.5270
Ac	 0.9000	 0.5310
Ad	 0.9360	 0.5170
Ae	 0.9740	 0.5850
Af	 0.9820	 0.5850















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Chain	Atom inclusion	Q-score
Ag	 0.9400	 0.5430
Ah	 0.9640	 0.5500
Ai	 0.9600	 0.5280
Aj	 0.9860	 0.5960
Ak	 0.6730	 0.4290
Al	 0.9810	 0.5680
Am	 0.9230	 0.5480
An	 0.9580	 0.5180
Ao	 0.9050	 0.5520
Ap	 0.9700	 0.5790
B5	 0.9140	 0.4120
BA	 0.8380	 0.4370
BB	 0.8270	 0.4460
BC	 0.9330	 0.4880
BD	 0.7970	 0.3130
BE	 0.9220	 0.4430
BF	 0.6910	 0.2870
BG	 0.8690	 0.3610
BH	 0.7220	 0.3960
BI	 0.9090	 0.4430
BJ	 0.9200	 0.4600
BK	 0.7000	 0.2420
BL	 0.8850	 0.4680
BM	 0.1780	 0.1670
BN	 0.8830	 0.4760
BO	 0.8790	 0.4640
BP	 0.6790	 0.2990
BQ	 0.7860	 0.3070
BR	 0.6850	 0.3240
BS	 0.7510	 0.3010
BT	 0.8030	 0.3040
BU	 0.7410	 0.2740
BV	 0.9050	 0.4640
BW	 0.9740	 0.5400
BX	 0.9580	 0.5260
BY	 0.8900	 0.4040
BZ	 0.6720	 0.1990
Ba	 0.9040	 0.4920
Bb	 0.8000	 0.4400
Bc	 0.6500	 0.3000
Bd	 0.9030	 0.3510
Be	 0.8840	 0.4130

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Chain	Atom inclusion	Q-score
Bf	 0.2720	 0.1740
Bg	 0.5550	 0.2140
DC	 0.7140	 0.2960
E	 0.5730	 0.1810
EC	 0.5020	 0.1100
V	 0.1250	 0.2160