



Full wwPDB EM Validation Report ⓘ

Dec 18, 2024 – 09:06 AM EST

PDB ID : 8EVQ
EMDB ID : EMD-28633
Title : Hypopseudouridylated Ribosome bound with TSV IRES, eEF2, GDP, and sordarin, Structure I
Authors : Zhao, Y.; Rai, J.; Li, H.
Deposited on : 2022-10-20
Resolution : 2.72 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:

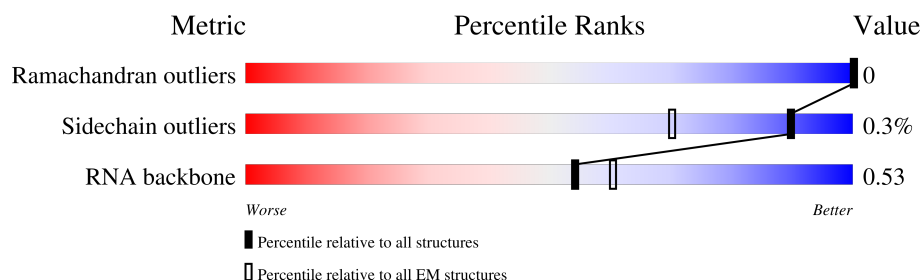
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 2.72 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.



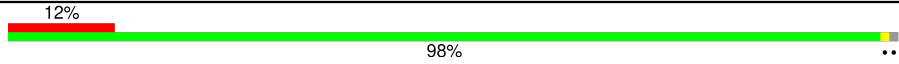
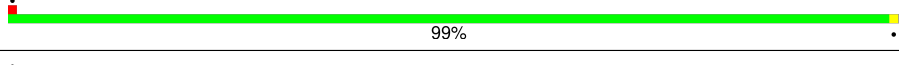
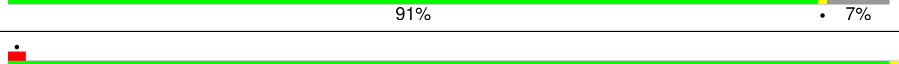
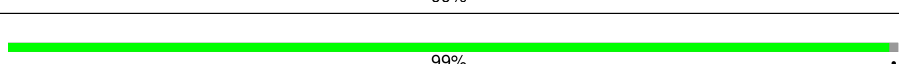
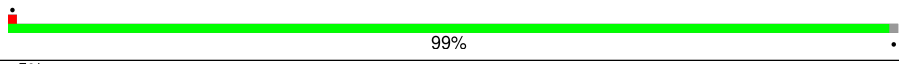
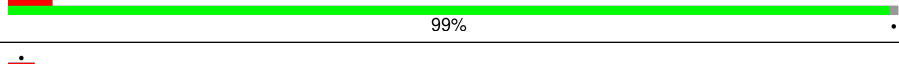
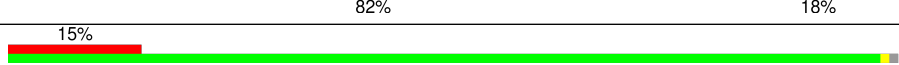
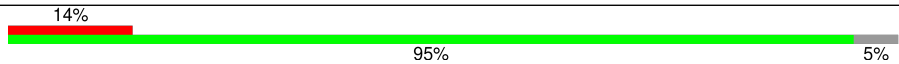
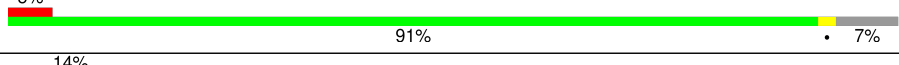
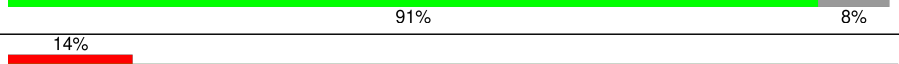
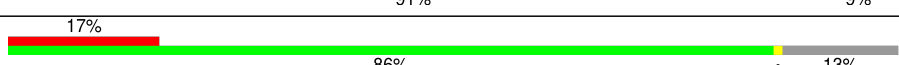
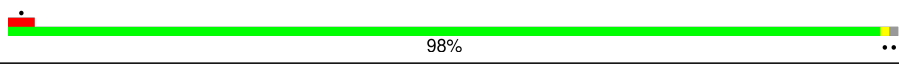

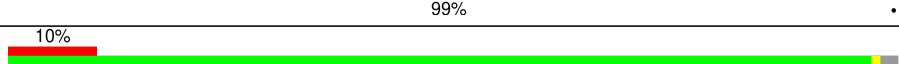

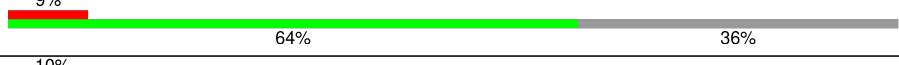
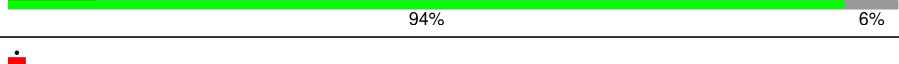
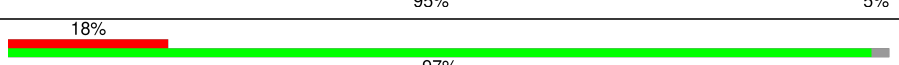





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	
2	BB	255	
3	BC	254	
4	BE	261	
5	BG	236	
6	BH	190	
7	BI	200	
8	BJ	197	

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Mol	Chain	Length	Quality of chain
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	BR	136	
25	BS	146	
26	BT	144	
27	BU	121	
28	BZ	108	
29	Bc	67	
30	Bd	56	
31	Bg	319	
32	Bf	152	
33	BM	143	

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Mol	Chain	Length	Quality of chain
34	B5	1798	
35	AA	254	
36	AB	387	
37	AC	362	
38	A1	3360	
39	A3	121	
40	A4	158	
41	AD	297	
42	AE	176	
43	AF	244	
44	AG	256	
45	AH	191	
46	AI	221	
47	AJ	174	
48	AL	199	
49	AM	138	
50	AN	204	
51	AO	199	
52	AP	184	
53	AQ	186	
54	AR	189	
55	AS	178	
56	AT	160	
57	AU	121	
58	AV	137	

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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	SO1	DC	903	X	-	-	-

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 214176 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
1	BA	206	Total	C	N	O	S	0	0
			1612	1034	285	291	2		

- Molecule 2 is a protein called RPS1A isoform 1.

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

- Molecule 3 is a protein called RPS2 isoform 1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called RPS22A isoform 1.

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

- 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	conflict	GB 1329886537
B5	1773	4AC	C	conflict	GB 1329886537

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	386	Total	C	N	O	S	0	0
			3080	1955	584	533	8		

- Molecule 37 is a protein called RPL4A isoform 1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A1	3198	Total	C	N	O	P	0	0
			68445	30596	12331	22320	3198		

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

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

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

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

- 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	S	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	S	0	0
			993	625	192	176			

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

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

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

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

- Molecule 64 is a protein called RPL29 isoform 1.

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

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

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

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

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

- Molecule 67 is a protein called RPL32 isoform 1.

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

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

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

- 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 Taura syndrome virus (TSV) internal ribosome entry site (IRES) RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	EC	200	Total	C	N	O	P	0	0
			4235	1891	751	1393	200		

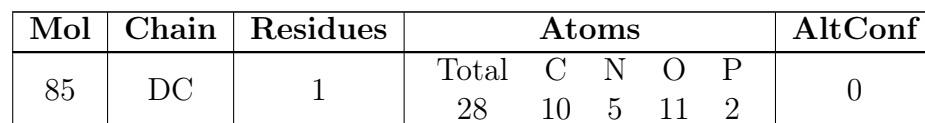
- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	BN	1	Total 1	Mg 1	0
83	Ba	1	Total 1	Mg 1	0
83	B5	53	Total 53	Mg 53	0
83	AB	1	Total 1	Mg 1	0
83	AC	1	Total 1	Mg 1	0
83	A1	172	Total 172	Mg 172	0
83	A3	2	Total 2	Mg 2	0
83	A4	3	Total 3	Mg 3	0
83	AI	1	Total 1	Mg 1	0
83	AL	1	Total 1	Mg 1	0
83	AP	1	Total 1	Mg 1	0
83	Ae	2	Total 2	Mg 2	0
83	Ah	1	Total 1	Mg 1	0
83	DC	1	Total 1	Mg 1	0

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

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

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



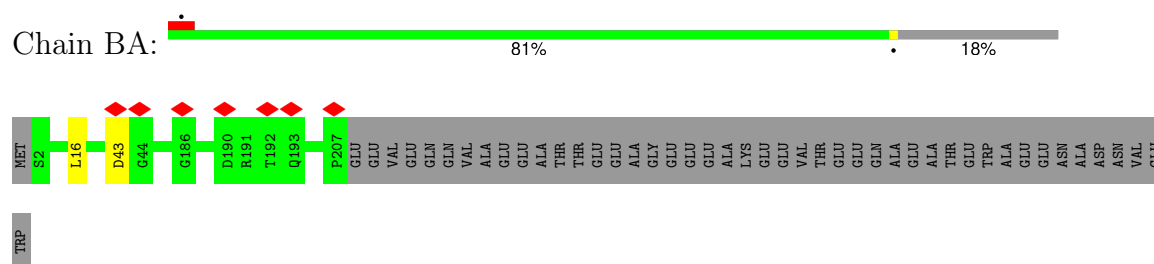
-
- ORTEP diagram of compound 501. The structure is a complex polycyclic molecule. The main ring system is shown in green, with atoms labeled C1 through C25 and O1 through O16. A side chain is attached to the main ring, with atoms labeled C26 through C35 and O17 through O20. The side chain includes a hydroxyl group (O20) and a methoxy group (O19). The structure is drawn with thermal ellipsoids at the 50% probability level. Bonds to the side chain are highlighted in red. Hydrogen atoms are shown as small spheres of arbitrary radii.

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

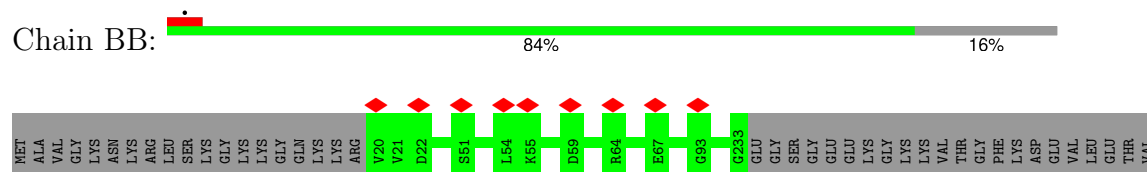
3 Residue-property plots [i](#)

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

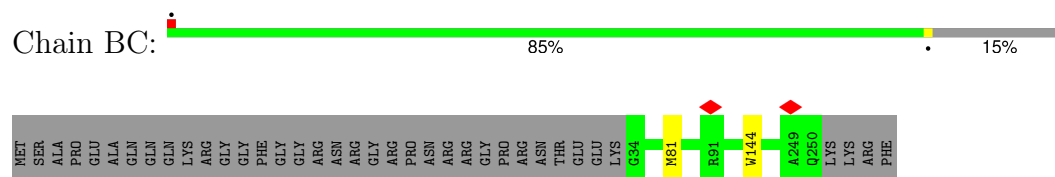
- Molecule 1: 40S ribosomal protein S0-A



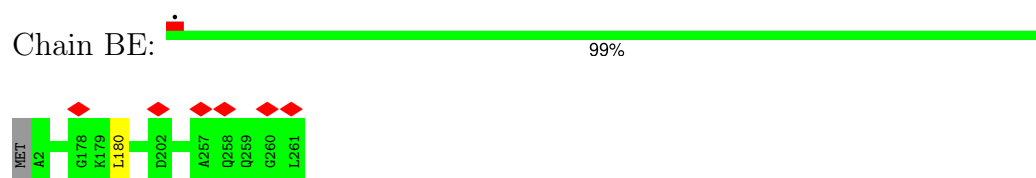
- Molecule 2: RPS1A isoform 1



- Molecule 3: RPS2 isoform 1

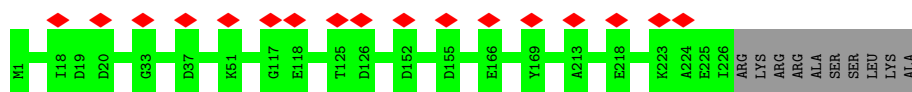


- Molecule 4: 40S ribosomal protein S4-A



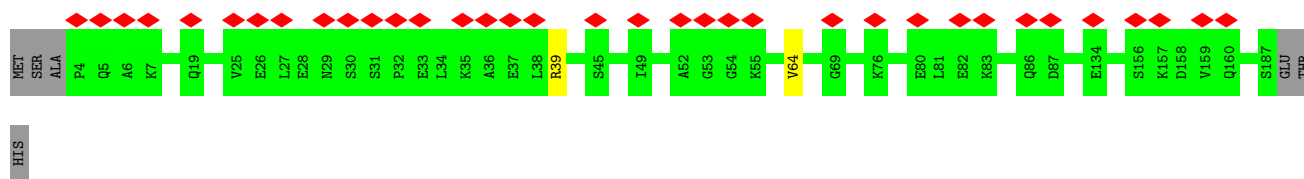
- Molecule 5: 40S ribosomal protein S6-A





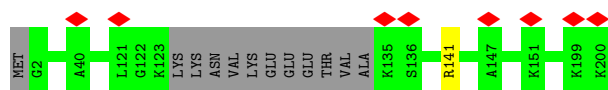
- Molecule 6: 40S ribosomal protein S7-A

Chain BH: 18% 96%



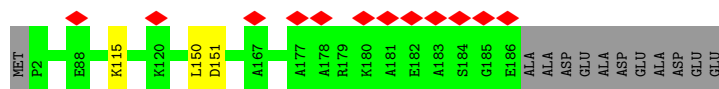
- Molecule 7: 40S ribosomal protein S8-A

Chain BI: 94% 6%



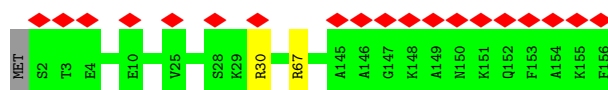
- Molecule 8: 40S ribosomal protein S9-A

Chain BJ: 6% 92% 6%



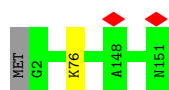
- Molecule 9: 40S ribosomal protein S11-A

Chain BL: 12% 98%



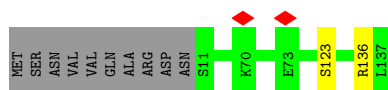
- Molecule 10: 40S ribosomal protein S13

Chain BN: 99%



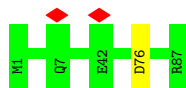
- Molecule 11: 40S ribosomal protein S14-A

Chain BO: 91% 7%



- Molecule 12: 40S ribosomal protein S21-A

Chain BV: 99%



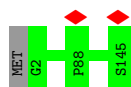
- Molecule 13: RPS22A isoform 1

Chain BW: 99%



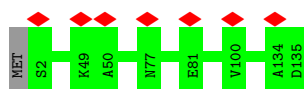
- Molecule 14: 40S ribosomal protein S23-A

Chain BX: 99%



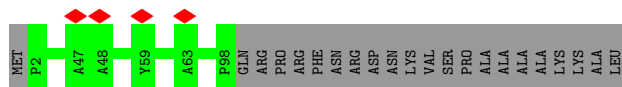
- Molecule 15: 40S ribosomal protein S24-A

Chain BY: 5% 99%



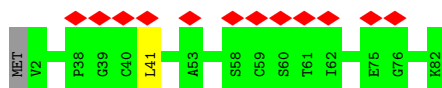
- Molecule 16: RPS26B isoform 1

Chain Ba: 82% 18%

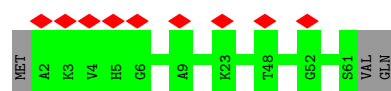


- Molecule 17: 40S ribosomal protein S27-A

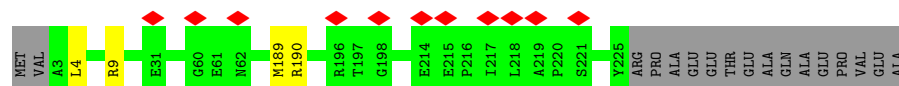
Chain Bb: 15% 98%



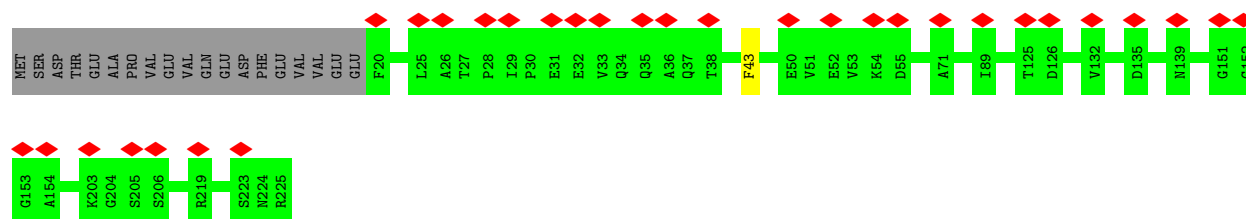
- Molecule 18: 40S ribosomal protein S30-A



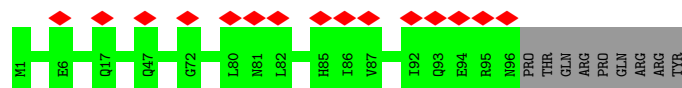
- Molecule 19: RPS3 isoform 1



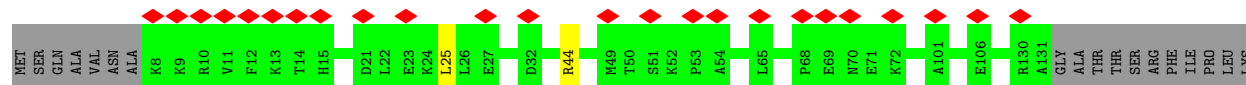
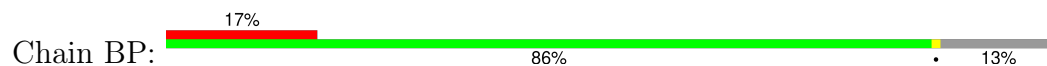
- Molecule 20: Rps5p



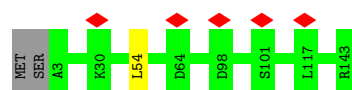
- Molecule 21: 40S ribosomal protein S10-A



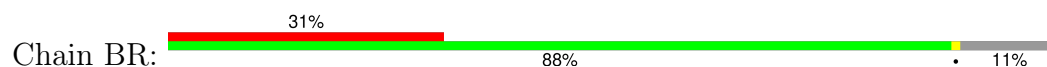
- Molecule 22: RPS15 isoform 1

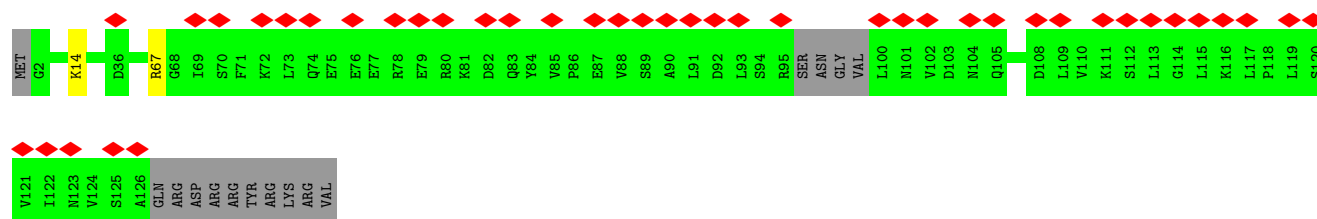


- Molecule 23: 40S ribosomal protein S16-A

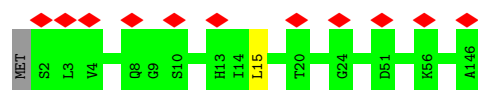


- Molecule 24: 40S ribosomal protein S17-A

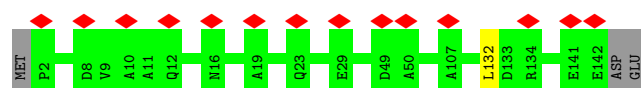




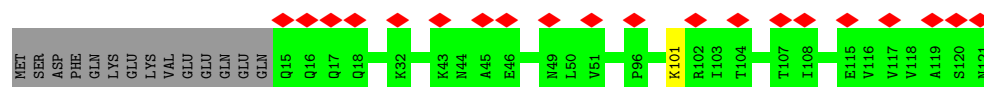
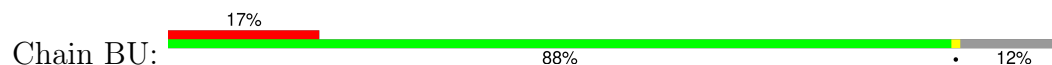
- Molecule 25: 40S ribosomal protein S18-A



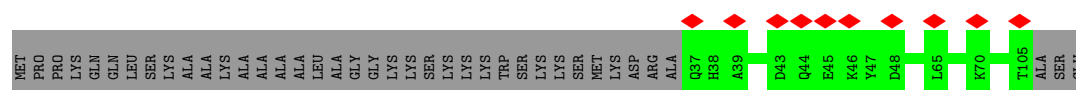
- Molecule 26: 40S ribosomal protein S19-A



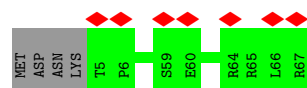
- Molecule 27: RPS20 isoform 1



- Molecule 28: RPS25A isoform 1

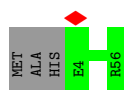


- Molecule 29: RPS28A isoform 1

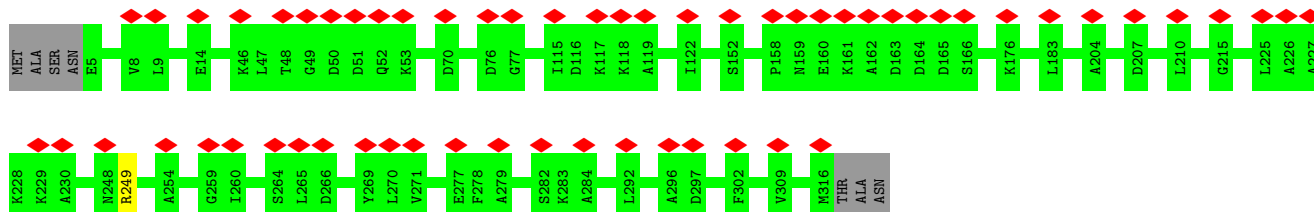


- Molecule 30: RPS29A isoform 1

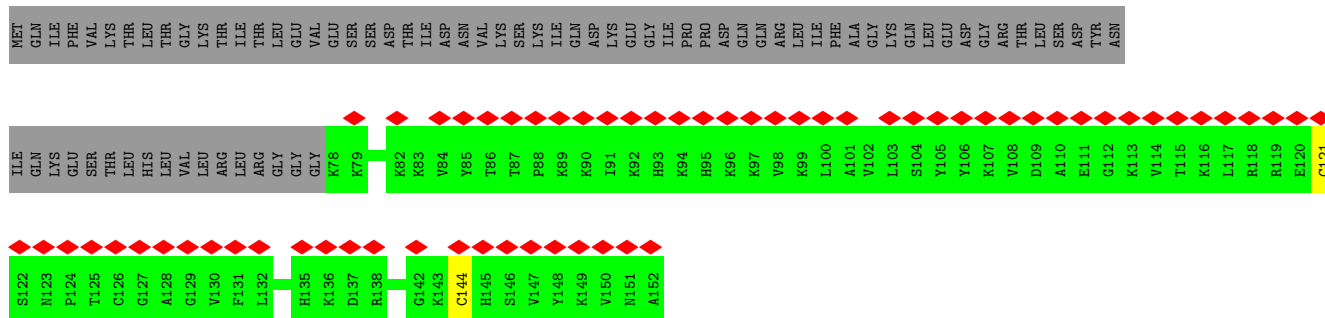
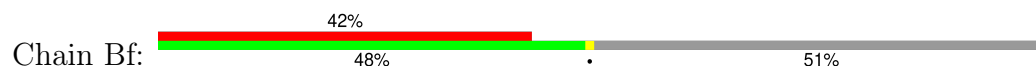




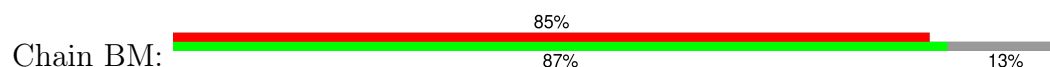
- Molecule 31: Guanine nucleotide-binding protein subunit beta-like protein



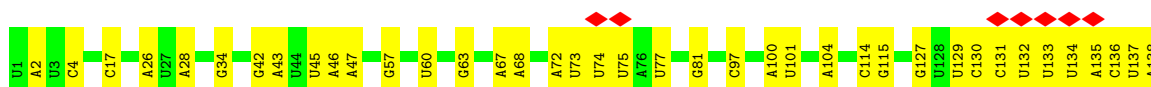
- Molecule 32: Ubiquitin-40S ribosomal protein S31



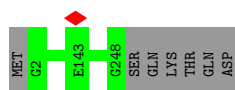
- Molecule 33: 40S ribosomal protein S12



- Molecule 34: 18S rRNA







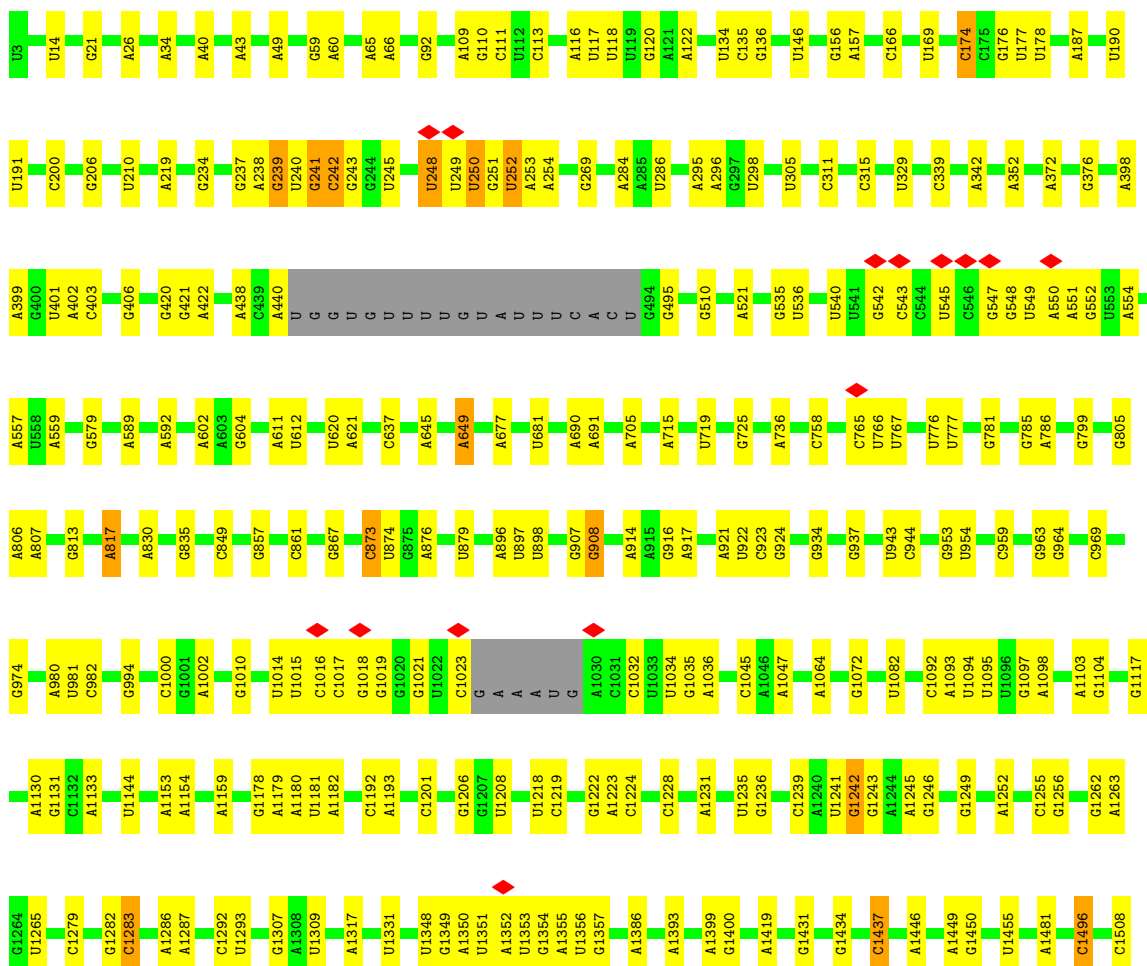
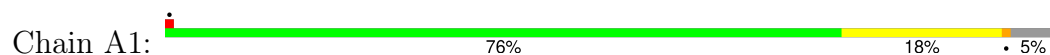
- Molecule 36: 60S ribosomal protein L3

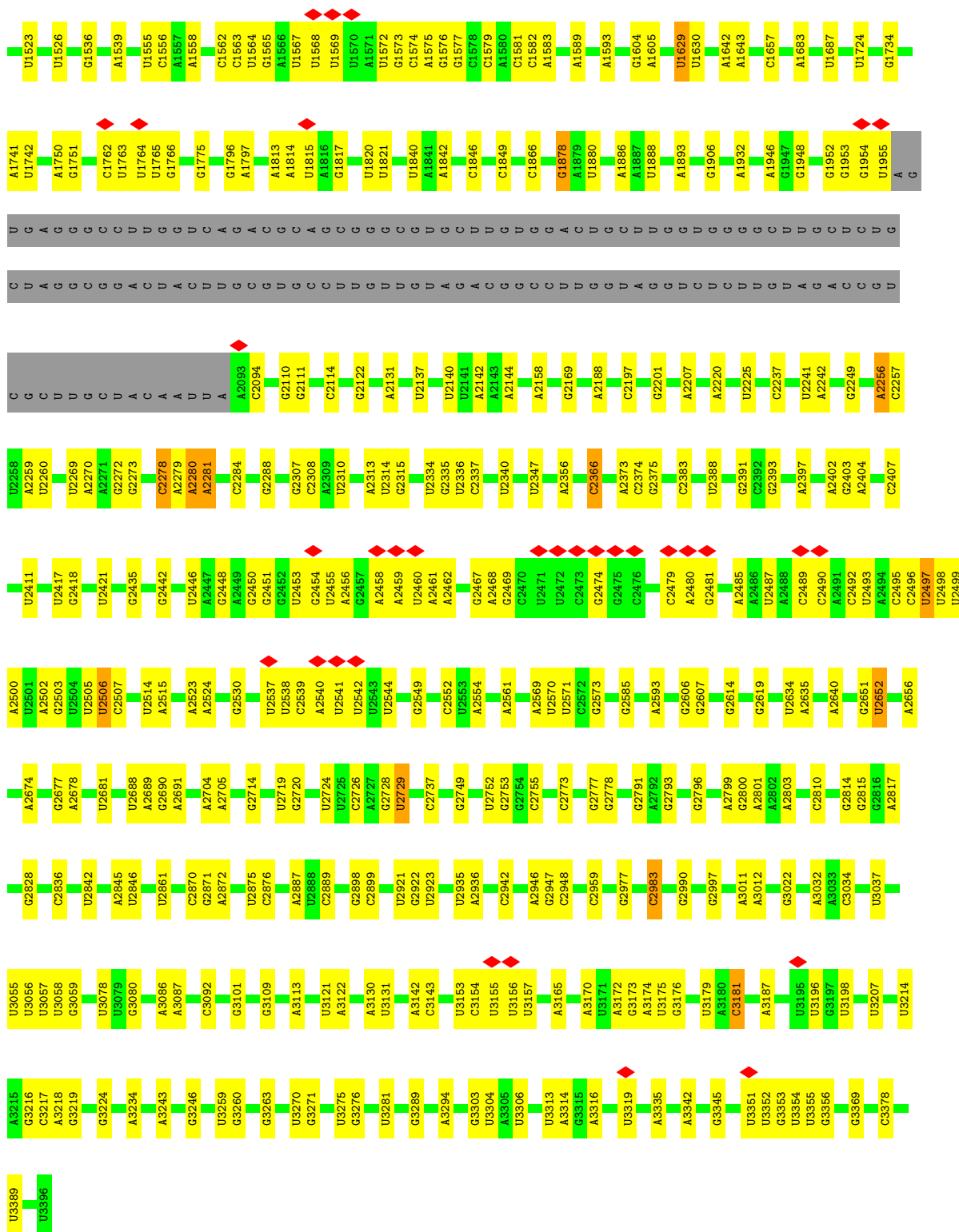


- Molecule 37: RPL4A isoform 1



- Molecule 38: 25S rRNA

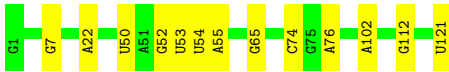




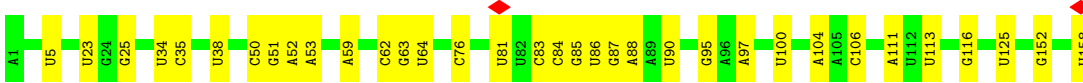
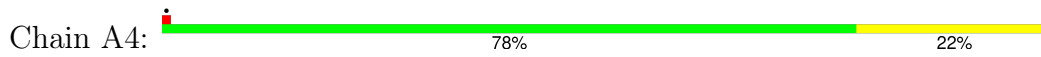
• Molecule 39: 5s rRNA

Chain A3:

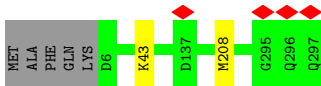




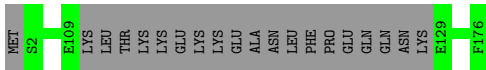
- Molecule 40: 5.8 S rRNA



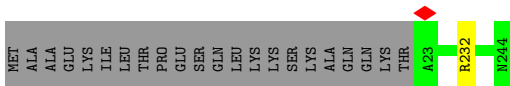
- Molecule 41: RPL5 isoform 1



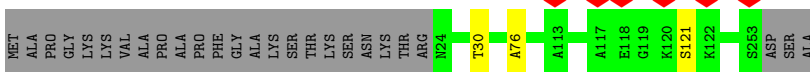
- Molecule 42: 60S ribosomal protein L6-A



- Molecule 43: 60S ribosomal protein L7-A



- Molecule 44: 60S ribosomal protein L8-A

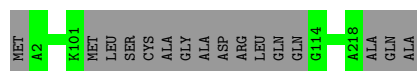


- Molecule 45: 60S ribosomal protein L9-A



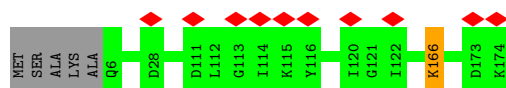
- Molecule 46: RPL10 isoform 1

Chain AI:  93% 7%



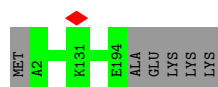
- Molecule 47: RPL11A isoform 1

Chain AJ:  6% 97%



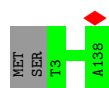
- Molecule 48: 60S ribosomal protein L13-A

Chain AL:  97%



- Molecule 49: 60S ribosomal protein L14-A

Chain AM:  99%



- Molecule 50: 60S ribosomal protein L15-A

Chain AN:  100%



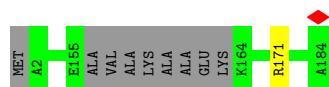
- Molecule 51: 60S ribosomal protein L16-A

Chain AO:  99%



- Molecule 52: 60S ribosomal protein L17-A

Chain AP:  95% 5%



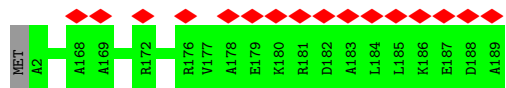
- Molecule 53: 60S ribosomal protein L18-A

Chain AQ:  99%



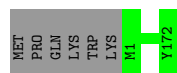
- Molecule 54: 60S ribosomal protein L19-A

Chain AR:  8% 99%



- Molecule 55: 60S ribosomal protein L20

Chain AS:  97%




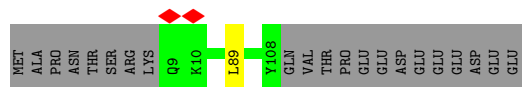
- Molecule 56: 60S ribosomal protein L21-A

Chain AT:  99%



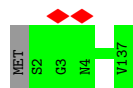
- Molecule 57: 60S ribosomal protein L22-A

Chain AU:  82% 17%



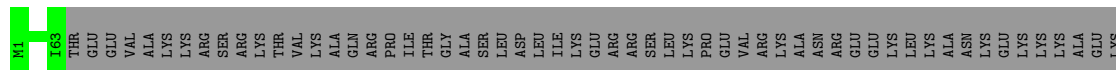
- Molecule 58: 60S ribosomal protein L23-A

Chain AV:  99%




- Molecule 59: RPL24A isoform 1

Chain AW:  41% 59%



ALA
ALA
ARG
LYS
LYS
GLU
LYS
LYS
ALA
SER
ALA
SER
ALA
GLY
THR
GLN
SER
SER
LYS
PHE
SER
LYS
GLN
ALA
LYS
GLY
ALA
PHE
GLN
LYS
VAL
ALA
ALA
THR
SER
ARG

- Molecule 60: 60S ribosomal protein L25

Chain AX:  85% 15%

MET
ALA
PRO
SER
ALA
LYS
ALA
THR
ALA
LYS
LYS
VAL
VAL
LYS
THR
GLY
ASN
GLY
LYS
K22
A23
T142

- Molecule 61: 60S ribosomal protein L26-A

Chain AY:  99% .

MET
A2
E127

- Molecule 62: 60S ribosomal protein L27-A

Chain AZ:  99% .

MET
A2
F136

- Molecule 63: 60S ribosomal protein L28

Chain Aa:  99% .

MET
P2
A149

- Molecule 64: RPL29 isoform 1

Chain Ab:  98% .

MET
A2
K58
K59

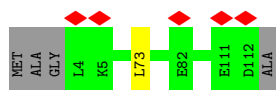
- Molecule 65: 60S ribosomal protein L30

Chain Ac:  92% 8%

MET
ALA
PRO
VAL
LYS
SER
GLN
GLU
S9
L104
A105

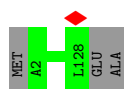
- Molecule 66: 60S ribosomal protein L31-A

Chain Ad:  96% . .



- Molecule 67: RPL32 isoform 1

Chain Ae: 98%



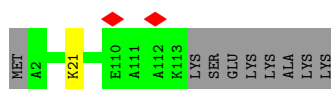
- Molecule 68: 60S ribosomal protein L33-A

Chain Af: 99%



- Molecule 69: 60S ribosomal protein L34-A

Chain Ag: 92% 7%



- Molecule 70: 60S ribosomal protein L35-A

Chain Ah: 99%



- Molecule 71: 60S ribosomal protein L36-A

Chain Ai: 99%

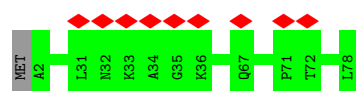


- Molecule 72: 60S ribosomal protein L37-A

Chain Aj: 99%



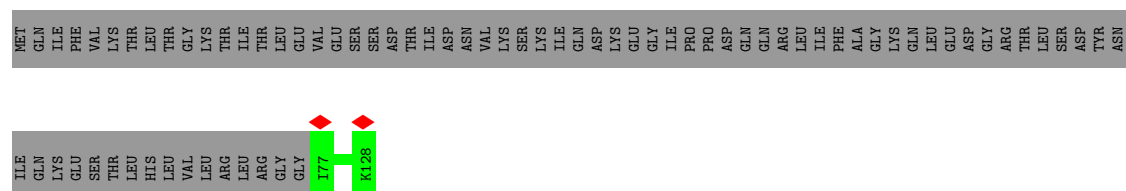
- Molecule 73: RPL38 isoform 1



- Molecule 74: 60S ribosomal protein L39



- Molecule 75: Ubiquitin-60S ribosomal protein L40



- Molecule 76: 60S ribosomal protein L41-A

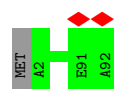


There are no outlier residues recorded for this chain.

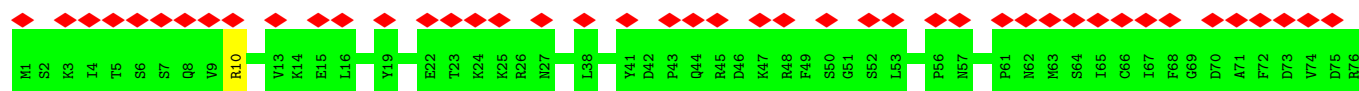
- Molecule 77: 60S ribosomal protein L42-A

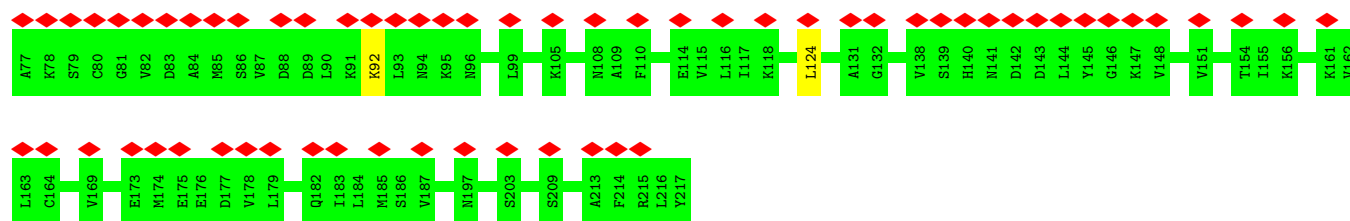


- Molecule 78: 60S ribosomal protein L43-A



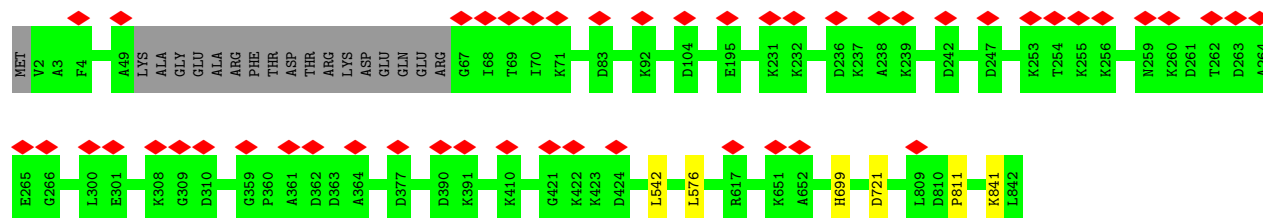
- Molecule 79: RPL1A isoform 1





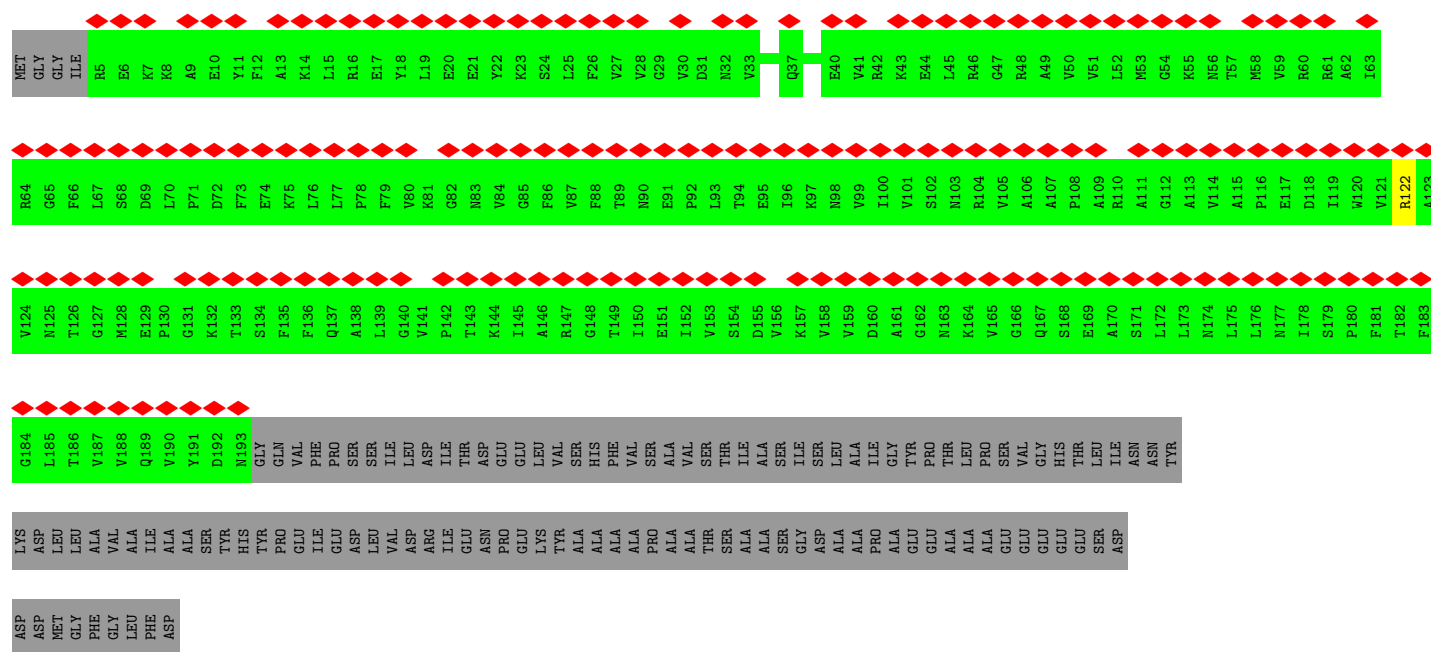
• Molecule 80: Elongation factor 2

Chain DC: 6% 97%



• Molecule 81: 60S acidic ribosomal protein P0

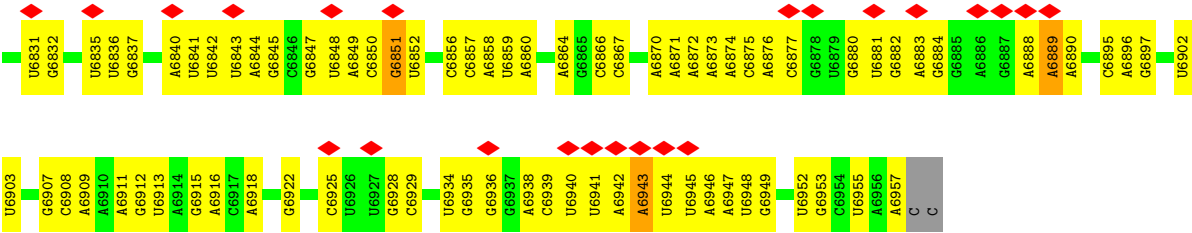
Chain V: 55% 60% 39%



• Molecule 82: Taura syndrome virus (TSV) internal ribosome entry site (IRES) RNA

Chain EC: 22% 40% 58%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82327	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.565	Depositor
Minimum map value	-2.598	Depositor
Average map value	0.049	Depositor
Map value standard deviation	0.250	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, OMG, XSX, A2M, UR3, OMU, HIC, 5MC, MG, G7M, MA6, SO1, 4AC, ZN, DDE, GDP, OMC

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	0.29	0/1653	0.65	2/2261 (0.1%)
2	BB	0.28	0/1735	0.63	0/2335
3	BC	0.28	0/1665	0.56	1/2263 (0.0%)
4	BE	0.27	0/2109	0.66	1/2839 (0.0%)
5	BG	0.25	0/1844	0.58	0/2464
6	BH	0.28	0/1506	0.64	0/2028
7	BI	0.26	0/1514	0.63	0/2021
8	BJ	0.26	0/1519	0.65	2/2035 (0.1%)
9	BL	0.28	0/1272	0.58	0/1712
10	BN	0.27	0/1215	0.57	0/1638
11	BO	0.30	0/952	0.72	0/1279
12	BV	0.30	0/693	0.72	1/935 (0.1%)
13	BW	0.27	0/1038	0.60	0/1395
14	BX	0.25	0/1139	0.61	0/1518
15	BY	0.28	0/1087	0.62	0/1449
16	Ba	0.26	0/782	0.69	0/1047
17	Bb	0.28	0/620	0.67	1/838 (0.1%)
18	Be	0.25	0/483	0.65	0/643
19	BD	0.27	0/1759	0.64	2/2368 (0.1%)
20	BF	0.27	0/1629	0.64	1/2202 (0.0%)
21	BK	0.28	0/837	0.63	0/1131
22	BP	0.27	0/1012	0.71	1/1356 (0.1%)
23	BQ	0.28	0/1125	0.63	1/1510 (0.1%)
24	BR	0.27	0/984	0.63	0/1318
25	BS	0.27	0/1211	0.68	1/1628 (0.1%)
26	BT	0.30	0/1113	0.68	2/1494 (0.1%)
27	BU	0.26	0/865	0.59	0/1169
28	BZ	0.25	0/566	0.56	0/761
29	Bc	0.26	0/499	0.74	0/670
30	Bd	0.28	0/452	0.63	0/600
31	Bg	0.26	0/2454	0.62	0/3340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Bf	0.27	0/616	0.70	2/817 (0.2%)
33	BM	0.26	0/943	0.61	0/1274
34	B5	0.27	0/41880	0.89	66/65248 (0.1%)
35	AA	0.28	0/1912	0.59	0/2569
36	AB	0.28	0/3138	0.59	1/4217 (0.0%)
37	AC	0.27	0/2800	0.56	1/3790 (0.0%)
38	A1	0.33	0/75561	0.88	81/117806 (0.1%)
39	A3	0.29	0/2883	0.84	1/4491 (0.0%)
40	A4	0.31	0/3746	0.85	4/5832 (0.1%)
41	AD	0.27	0/2390	0.56	1/3225 (0.0%)
42	AE	0.29	0/1260	0.58	0/1694
43	AF	0.27	0/1821	0.51	0/2451
44	AG	0.26	0/1830	0.54	0/2469
45	AH	0.29	0/1531	0.59	1/2062 (0.0%)
46	AI	0.27	0/1708	0.55	0/2290
47	AJ	0.28	0/1374	0.65	0/1842
48	AL	0.26	0/1568	0.58	0/2106
49	AM	0.25	0/1068	0.52	0/1438
50	AN	0.28	0/1757	0.60	0/2354
51	AO	0.29	0/1585	0.57	0/2128
52	AP	0.28	0/1410	0.57	0/1893
53	AQ	0.27	0/1465	0.59	0/1965
54	AR	0.25	0/1538	0.59	0/2050
55	AS	0.29	0/1481	0.56	0/1990
56	AT	0.28	0/1300	0.54	0/1743
57	AU	0.29	0/812	0.62	1/1099 (0.1%)
58	AV	0.29	0/1018	0.58	0/1369
59	AW	0.28	0/533	0.58	0/707
60	AX	0.28	0/983	0.54	0/1325
61	AY	0.27	0/1004	0.63	0/1341
62	AZ	0.27	0/1118	0.54	0/1497
63	Aa	0.28	0/1204	0.58	0/1612
64	Ab	0.25	0/473	0.51	0/629
65	Ac	0.27	0/751	0.48	0/1008
66	Ad	0.26	0/904	0.60	1/1213 (0.1%)
67	Ae	0.26	0/1041	0.56	0/1394
68	Af	0.30	0/868	0.59	0/1168
69	Ag	0.29	0/890	0.60	0/1189
70	Ah	0.26	0/978	0.53	0/1301
71	Ai	0.26	0/778	0.59	0/1034
72	Aj	0.28	0/696	0.63	0/923
73	Ak	0.28	0/618	0.60	0/826
74	Al	0.25	0/443	0.60	0/588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Am	0.27	0/423	0.59	0/562
76	An	0.29	0/234	0.89	0/300
77	Ao	0.28	0/860	0.59	0/1136
78	Ap	0.27	0/701	0.60	0/934
79	E	0.27	0/1745	0.56	1/2342 (0.0%)
80	DC	0.27	0/6521	0.62	5/8830 (0.1%)
81	V	0.30	0/1498	0.68	0/2025
82	EC	0.31	1/4733 (0.0%)	0.92	4/7369 (0.1%)
All	All	0.30	1/227724 (0.0%)	0.78	186/333712 (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	1
6	BH	0	1
11	BO	0	1
41	AD	0	1
43	AF	0	1
44	AG	0	3
47	AJ	0	1
77	Ao	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	EC	6758	A	OP3-P	-10.55	1.48	1.61

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	965	U	C2-N1-C1'	9.84	129.51	117.70
34	B5	1389	C	C2-N1-C1'	8.16	127.78	118.80
23	BQ	54	LEU	CA-CB-CG	8.08	133.88	115.30
38	A1	3181	C	N1-C2-O2	7.95	123.67	118.90
32	Bf	144	CYS	CA-CB-SG	7.82	128.07	114.00
34	B5	1473	U	C2-N1-C1'	7.74	126.98	117.70
38	A1	406	G	O4'-C1'-N9	7.72	114.37	108.20
38	A1	3034	C	C2-N1-C1'	7.66	127.22	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1217	A	OP2-P-O3'	7.64	122.02	105.20
38	A1	922	U	C2-N1-C1'	7.63	126.86	117.70
34	B5	965	U	N1-C2-O2	7.58	128.10	122.80
22	BP	25	LEU	CA-CB-CG	7.36	132.24	115.30
34	B5	1458	G	N3-C4-C5	-7.32	124.94	128.60
25	BS	15	LEU	CA-CB-CG	7.31	132.12	115.30
34	B5	1286	U	N1-C2-O2	7.14	127.80	122.80
34	B5	224	C	N1-C2-O2	7.13	123.18	118.90
38	A1	241	G	P-O3'-C3'	7.08	128.20	119.70
38	A1	922	U	N1-C2-O2	7.08	127.75	122.80
34	B5	1473	U	N1-C2-O2	7.03	127.72	122.80
80	DC	576	LEU	CA-CB-CG	7.03	131.46	115.30
38	A1	1255	C	N3-C2-O2	-6.95	117.03	121.90
34	B5	965	U	N3-C2-O2	-6.92	117.36	122.20
38	A1	3034	C	N3-C2-O2	-6.91	117.06	121.90
37	AC	182	LEU	CA-CB-CG	6.89	131.15	115.30
34	B5	1286	U	N3-C2-O2	-6.85	117.40	122.20
34	B5	1286	U	C2-N1-C1'	6.83	125.89	117.70
34	B5	965	U	C6-N1-C1'	-6.81	111.67	121.20
34	B5	1458	G	C2-N3-C4	6.78	115.29	111.90
38	A1	2506	U	C2-N1-C1'	6.74	125.79	117.70
38	A1	3181	C	N3-C2-O2	-6.72	117.19	121.90
38	A1	1496	C	C2-N1-C1'	6.62	126.08	118.80
38	A1	252	U	N1-C2-O2	6.58	127.41	122.80
34	B5	224	C	N3-C2-O2	-6.58	117.30	121.90
34	B5	1162	C	C2-N1-C1'	6.57	126.02	118.80
19	BD	4	LEU	CA-CB-CG	6.56	130.39	115.30
40	A4	5	U	C2-N1-C1'	6.55	125.57	117.70
34	B5	1706	C	N3-C2-O2	-6.54	117.32	121.90
66	Ad	73	LEU	CA-CB-CG	6.52	130.30	115.30
38	A1	3181	C	C2-N1-C1'	6.48	125.93	118.80
34	B5	1307	U	C2-N1-C1'	6.48	125.47	117.70
41	AD	208	MET	CA-CB-CG	6.44	124.25	113.30
38	A1	2225	U	N3-C2-O2	-6.41	117.71	122.20
38	A1	982	C	C2-N1-C1'	6.40	125.84	118.80
26	BT	132	LEU	CB-CG-CD2	-6.35	100.20	111.00
17	Bb	41	LEU	CA-CB-CG	6.35	129.91	115.30
38	A1	2237	C	N3-C2-O2	-6.35	117.46	121.90
38	A1	922	U	N3-C2-O2	-6.35	117.76	122.20
34	B5	1560	U	C2-N1-C1'	6.33	125.29	117.70
80	DC	721	ASP	CB-CG-OD1	6.30	123.97	118.30
38	A1	3034	C	N1-C2-O2	6.29	122.67	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	3034	C	C6-N1-C2	-6.27	117.79	120.30
38	A1	2497	U	P-O3'-C3'	6.27	127.23	119.70
38	A1	239	G	OP1-P-O3'	6.25	118.95	105.20
34	B5	959	U	N1-C2-O2	6.25	127.17	122.80
38	A1	2225	U	N1-C2-O2	6.24	127.17	122.80
32	Bf	121	CYS	CA-CB-SG	6.24	125.23	114.00
38	A1	2836	C	C2-N1-C1'	6.24	125.66	118.80
38	A1	252	U	N3-C2-O2	-6.22	117.84	122.20
34	B5	959	U	C2-N1-C1'	6.20	125.14	117.70
38	A1	3037	U	C2-N1-C1'	6.20	125.14	117.70
34	B5	1380	U	C2-N1-C1'	6.19	125.13	117.70
57	AU	89	LEU	CA-CB-CG	6.17	129.49	115.30
34	B5	1162	C	N1-C2-O2	6.15	122.59	118.90
38	A1	1283	C	C6-N1-C2	-6.13	117.85	120.30
34	B5	1380	U	N3-C2-O2	-6.12	117.92	122.20
38	A1	2225	U	C2-N1-C1'	6.11	125.03	117.70
82	EC	6943	A	P-O3'-C3'	6.11	127.03	119.70
38	A1	3058	U	C2-N1-C1'	6.09	125.01	117.70
38	A1	1283	C	C5-C6-N1	6.08	124.04	121.00
38	A1	1604	G	C4-N9-C1'	6.08	134.40	126.50
40	A4	100	U	C2-N1-C1'	6.04	124.95	117.70
20	BF	43	PHE	C-N-CA	6.03	136.77	121.70
40	A4	5	U	N3-C2-O2	-6.02	117.98	122.20
3	BC	81	MET	CA-CB-CG	6.02	123.53	113.30
34	B5	610	G	N3-C4-C5	-6.02	125.59	128.60
38	A1	3306	U	C2-N1-C1'	6.02	124.92	117.70
34	B5	1307	U	N1-C2-O2	6.01	127.01	122.80
80	DC	811	PRO	N-CD-CG	-5.99	94.21	103.20
82	EC	6889	A	P-O3'-C3'	5.96	126.85	119.70
34	B5	1473	U	N3-C2-O2	-5.95	118.03	122.20
38	A1	1577	G	N1-C6-O6	-5.95	116.33	119.90
38	A1	3037	U	N3-C2-O2	-5.92	118.06	122.20
34	B5	819	G	P-O3'-C3'	5.91	126.79	119.70
38	A1	2237	C	N1-C2-O2	5.90	122.44	118.90
38	A1	2836	C	N3-C2-O2	-5.87	117.79	121.90
4	BE	180	LEU	CA-CB-CG	5.87	128.80	115.30
34	B5	862	A	P-O3'-C3'	5.86	126.73	119.70
38	A1	174	C	C6-N1-C2	-5.86	117.96	120.30
38	A1	242	C	N1-C2-O2	5.83	122.40	118.90
38	A1	2726	C	C2-N1-C1'	5.82	125.20	118.80
38	A1	174	C	C5-C6-N1	5.81	123.91	121.00
34	B5	1706	C	N1-C2-O2	5.81	122.39	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1560	U	N3-C2-O2	-5.80	118.14	122.20
38	A1	1577	G	C5-C6-O6	5.80	132.08	128.60
34	B5	861	U	C2-N1-C1'	5.78	124.64	117.70
38	A1	2846	U	C2-N1-C1'	5.78	124.64	117.70
19	BD	189	MET	CA-CB-CG	5.77	123.11	113.30
34	B5	530	C	N1-C2-O2	5.76	122.36	118.90
34	B5	1000	C	C2-N1-C1'	5.74	125.11	118.80
34	B5	1716	C	C2-N1-C1'	5.73	125.10	118.80
38	A1	242	C	C2-N1-C1'	5.72	125.09	118.80
38	A1	2983	C	C2-N1-C1'	5.71	125.08	118.80
45	AH	138	THR	C-N-CA	5.70	135.94	121.70
34	B5	959	U	N3-C2-O2	-5.68	118.22	122.20
34	B5	1458	G	N3-C4-N9	5.67	129.40	126.00
34	B5	1389	C	C6-N1-C1'	-5.63	114.04	120.80
34	B5	1354	G	C4-N9-C1'	5.62	133.81	126.50
34	B5	1716	C	N1-C2-O2	5.62	122.28	118.90
38	A1	2836	C	C6-N1-C2	-5.62	118.05	120.30
38	A1	315	C	C2-N1-C1'	5.61	124.97	118.80
38	A1	2366	C	C2-N1-C1'	5.60	124.96	118.80
38	A1	239	G	P-O3'-C3'	5.60	126.42	119.70
36	AB	351	LEU	CA-CB-CG	5.59	128.16	115.30
38	A1	174	C	N1-C2-O2	5.58	122.25	118.90
38	A1	1255	C	N1-C2-O2	5.56	122.24	118.90
34	B5	1567	U	C2-N1-C1'	5.56	124.37	117.70
39	A3	50	U	C2-N1-C1'	5.56	124.37	117.70
1	BA	43	ASP	CB-CG-OD1	5.55	123.29	118.30
34	B5	238	U	C2-N1-C1'	5.54	124.35	117.70
40	A4	64	U	N3-C2-O2	-5.52	118.33	122.20
26	BT	132	LEU	CA-CB-CG	5.51	127.97	115.30
34	B5	1021	C	C2-N1-C1'	5.51	124.86	118.80
38	A1	954	U	C2-N1-C1'	5.50	124.31	117.70
80	DC	542	LEU	CA-CB-CG	5.49	127.94	115.30
38	A1	113	C	C2-N1-C1'	5.44	124.79	118.80
38	A1	2899	C	C2-N1-C1'	5.43	124.77	118.80
34	B5	1380	U	N1-C2-O2	5.43	126.60	122.80
34	B5	1514	U	N3-C2-O2	-5.43	118.40	122.20
38	A1	1878	G	C4-N9-C1'	5.43	133.56	126.50
34	B5	1217	A	P-O3'-C3'	5.43	126.21	119.70
38	A1	1222	G	O4'-C1'-N9	5.42	112.53	108.20
8	BJ	151	ASP	CB-CG-OD1	5.40	123.16	118.30
34	B5	1560	U	N1-C2-O2	5.39	126.57	122.80
38	A1	3214	U	C2-N1-C1'	5.38	124.16	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	BJ	150	LEU	CA-CB-CG	5.38	127.66	115.30
34	B5	575	C	C2-N1-C1'	5.37	124.71	118.80
38	A1	169	U	N3-C2-O2	-5.35	118.45	122.20
34	B5	1389	C	C6-N1-C2	-5.32	118.17	120.30
34	B5	1258	U	N1-C2-O2	5.32	126.52	122.80
38	A1	873	C	P-O3'-C3'	5.30	126.06	119.70
38	A1	3058	U	N1-C2-O2	5.28	126.49	122.80
34	B5	1473	U	C6-N1-C1'	-5.27	113.83	121.20
38	A1	2137	U	C2-N1-C1'	5.26	124.02	117.70
38	A1	1604	G	N3-C4-C5	-5.26	125.97	128.60
12	BV	76	ASP	CB-CG-OD1	5.25	123.03	118.30
38	A1	954	U	N3-C2-O2	-5.24	118.53	122.20
38	A1	2407	C	C5-C6-N1	5.23	123.61	121.00
38	A1	954	U	N1-C2-O2	5.23	126.46	122.80
34	B5	1688	U	N3-C2-O2	-5.22	118.54	122.20
34	B5	1307	U	N3-C2-O2	-5.22	118.55	122.20
38	A1	252	U	C2-N1-C1'	5.20	123.94	117.70
38	A1	1629	U	P-O3'-C3'	5.19	125.92	119.70
34	B5	1162	C	N3-C2-O2	-5.18	118.28	121.90
38	A1	969	C	N1-C2-O2	5.17	122.00	118.90
34	B5	575	C	N1-C2-O2	5.16	122.00	118.90
82	EC	6889	A	OP1-P-O3'	5.16	116.55	105.20
1	BA	16	LEU	CA-CB-CG	5.16	127.17	115.30
34	B5	1389	C	N1-C2-O2	5.16	122.00	118.90
34	B5	610	G	C2-N3-C4	5.16	114.48	111.90
34	B5	1258	U	C2-N1-C1'	5.15	123.88	117.70
34	B5	934	C	C2-N1-C1'	5.13	124.44	118.80
82	EC	6851	G	P-O3'-C3'	5.13	125.85	119.70
79	E	124	LEU	CA-CB-CG	5.13	127.09	115.30
34	B5	1344	A	OP1-P-O3'	5.10	116.43	105.20
34	B5	536	C	C2-N1-C1'	5.10	124.41	118.80
34	B5	1332	C	C2-N1-C1'	5.10	124.41	118.80
38	A1	2846	U	N3-C2-O2	-5.10	118.63	122.20
38	A1	1604	G	C8-N9-C1'	-5.10	120.37	127.00
38	A1	2836	C	N1-C2-O2	5.10	121.96	118.90
38	A1	2652	U	N3-C2-O2	-5.09	118.64	122.20
38	A1	1878	G	N3-C4-C5	-5.09	126.06	128.60
80	DC	811	PRO	CA-N-CD	-5.08	104.39	111.50
38	A1	3058	U	N3-C2-O2	-5.07	118.65	122.20
34	B5	850	A	N3-C4-N9	5.07	131.45	127.40
38	A1	250	U	N1-C2-O2	5.05	126.34	122.80
38	A1	835	G	O4'-C1'-N9	5.05	112.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1596	C	C2-N1-C1'	5.05	124.36	118.80
38	A1	248	U	N3-C2-O2	-5.04	118.68	122.20
38	A1	922	U	C6-N1-C1'	-5.03	114.17	121.20
38	A1	1242	G	P-O3'-C3'	5.03	125.73	119.70
38	A1	3057	U	N1-C2-O2	5.02	126.31	122.80
38	A1	1563	C	C5-C4-N4	5.02	123.71	120.20
38	A1	3057	U	N3-C2-O2	-5.02	118.69	122.20
34	B5	1567	U	N1-C2-O2	5.01	126.31	122.80
38	A1	2899	C	N1-C2-O2	5.01	121.91	118.90
34	B5	1162	C	C6-N1-C2	-5.01	118.30	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	AD	43	LYS	Peptide
43	AF	232	ARG	Peptide
44	AG	121	SER	Peptide
44	AG	30	THR	Peptide
44	AG	76	ALA	Peptide
47	AJ	166	LYS	Peptide
77	Ao	103	ALA	Peptide
3	BC	144	TRP	Peptide
6	BH	64	VAL	Peptide
11	BO	123	SER	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	204/252 (81%)	181 (89%)	23 (11%)	0	100	100
2	BB	212/255 (83%)	188 (89%)	24 (11%)	0	100	100
3	BC	215/254 (85%)	206 (96%)	9 (4%)	0	100	100
4	BE	258/261 (99%)	233 (90%)	25 (10%)	0	100	100
5	BG	224/236 (95%)	220 (98%)	4 (2%)	0	100	100
6	BH	182/190 (96%)	168 (92%)	14 (8%)	0	100	100
7	BI	184/200 (92%)	164 (89%)	20 (11%)	0	100	100
8	BJ	183/197 (93%)	171 (93%)	12 (7%)	0	100	100
9	BL	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
10	BN	148/151 (98%)	135 (91%)	13 (9%)	0	100	100
11	BO	125/137 (91%)	111 (89%)	14 (11%)	0	100	100
12	BV	85/87 (98%)	74 (87%)	11 (13%)	0	100	100
13	BW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
14	BX	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
15	BY	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
16	Ba	95/119 (80%)	82 (86%)	13 (14%)	0	100	100
17	Bb	79/82 (96%)	69 (87%)	10 (13%)	0	100	100
18	Be	58/63 (92%)	52 (90%)	6 (10%)	0	100	100
19	BD	221/240 (92%)	211 (96%)	10 (4%)	0	100	100
20	BF	204/225 (91%)	185 (91%)	19 (9%)	0	100	100
21	BK	94/105 (90%)	85 (90%)	9 (10%)	0	100	100
22	BP	122/142 (86%)	113 (93%)	9 (7%)	0	100	100
23	BQ	139/143 (97%)	134 (96%)	5 (4%)	0	100	100
24	BR	117/136 (86%)	108 (92%)	9 (8%)	0	100	100
25	BS	143/146 (98%)	130 (91%)	13 (9%)	0	100	100
26	BT	139/144 (96%)	128 (92%)	11 (8%)	0	100	100
27	BU	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
28	BZ	67/108 (62%)	64 (96%)	3 (4%)	0	100	100
29	Bc	61/67 (91%)	55 (90%)	6 (10%)	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%)	70 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	BM	122/143 (85%)	111 (91%)	11 (9%)	0	100	100
35	AA	245/254 (96%)	232 (95%)	13 (5%)	0	100	100
36	AB	383/387 (99%)	364 (95%)	19 (5%)	0	100	100
37	AC	359/362 (99%)	340 (95%)	19 (5%)	0	100	100
41	AD	290/297 (98%)	276 (95%)	14 (5%)	0	100	100
42	AE	152/176 (86%)	143 (94%)	9 (6%)	0	100	100
43	AF	220/244 (90%)	210 (96%)	10 (4%)	0	100	100
44	AG	228/256 (89%)	209 (92%)	19 (8%)	0	100	100
45	AH	188/191 (98%)	171 (91%)	17 (9%)	0	100	100
46	AI	201/221 (91%)	191 (95%)	10 (5%)	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%)	128 (96%)	6 (4%)	0	100	100
50	AN	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
51	AO	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
52	AP	171/184 (93%)	165 (96%)	6 (4%)	0	100	100
53	AQ	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
54	AR	186/189 (98%)	178 (96%)	8 (4%)	0	100	100
55	AS	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
56	AT	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
57	AU	98/121 (81%)	92 (94%)	6 (6%)	0	100	100
58	AV	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
59	AW	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
60	AX	119/142 (84%)	115 (97%)	4 (3%)	0	100	100
61	AY	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
62	AZ	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
63	Aa	146/149 (98%)	131 (90%)	15 (10%)	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%)	103 (96%)	4 (4%)	0	100	100
67	Ae	125/130 (96%)	123 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	Af	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
69	Ag	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
70	Ah	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
71	Ai	97/100 (97%)	90 (93%)	7 (7%)	0	100	100
72	Aj	85/88 (97%)	80 (94%)	5 (6%)	0	100	100
73	Ak	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
74	Al	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
75	Am	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	89 (86%)	14 (14%)	0	100	100
78	Ap	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
79	E	215/217 (99%)	198 (92%)	17 (8%)	0	100	100
80	DC	819/842 (97%)	768 (94%)	51 (6%)	0	100	100
81	V	187/312 (60%)	176 (94%)	11 (6%)	0	100	100
All	All	12115/13257 (91%)	11334 (94%)	781 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	173/210 (82%)	173 (100%)	0	100	100
2	BB	191/224 (85%)	191 (100%)	0	100	100
3	BC	176/205 (86%)	176 (100%)	0	100	100
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%)	164 (99%)	1 (1%)	84	93
7	BI	150/161 (93%)	149 (99%)	1 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BJ	158/166 (95%)	157 (99%)	1 (1%)	84	93
9	BL	136/137 (99%)	134 (98%)	2 (2%)	60	82
10	BN	127/128 (99%)	126 (99%)	1 (1%)	79	91
11	BO	96/105 (91%)	95 (99%)	1 (1%)	73	88
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%)	180 (99%)	2 (1%)	70	87
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%)	73	88
23	BQ	117/119 (98%)	117 (100%)	0	100	100
24	BR	110/124 (89%)	108 (98%)	2 (2%)	54	78
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	113 (100%)	0	100	100
27	BU	100/114 (88%)	99 (99%)	1 (1%)	73	88
28	BZ	61/89 (68%)	61 (100%)	0	100	100
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%)	255 (100%)	1 (0%)	89	96
32	Bf	66/135 (49%)	66 (100%)	0	100	100
33	BM	100/119 (84%)	100 (100%)	0	100	100
35	AA	189/196 (96%)	189 (100%)	0	100	100
36	AB	321/322 (100%)	320 (100%)	1 (0%)	91	97
37	AC	288/289 (100%)	287 (100%)	1 (0%)	91	97
41	AD	241/245 (98%)	241 (100%)	0	100	100
42	AE	134/153 (88%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	67	85
46	AI	176/187 (94%)	176 (100%)	0	100	100
47	AJ	147/150 (98%)	146 (99%)	1 (1%)	81	92
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%)	160 (100%)	0	100	100
52	AP	141/146 (97%)	140 (99%)	1 (1%)	81	92
53	AQ	150/151 (99%)	150 (100%)	0	100	100
54	AR	153/154 (99%)	153 (100%)	0	100	100
55	AS	156/162 (96%)	156 (100%)	0	100	100
56	AT	136/137 (99%)	135 (99%)	1 (1%)	81	92
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
68	Af	90/91 (99%)	90 (100%)	0	100	100
69	Ag	95/103 (92%)	94 (99%)	1 (1%)	70	87
70	Ah	104/105 (99%)	104 (100%)	0	100	100
71	Ai	81/82 (99%)	81 (100%)	0	100	100
72	Aj	70/71 (99%)	70 (100%)	0	100	100
73	Ak	68/69 (99%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	89 (99%)	1 (1%)	70	87
78	Ap	71/72 (99%)	71 (100%)	0	100	100
79	E	198/198 (100%)	196 (99%)	2 (1%)	73	88
80	DC	699/714 (98%)	698 (100%)	1 (0%)	92	98
81	V	160/254 (63%)	159 (99%)	1 (1%)	84	93
All	All	10346/11154 (93%)	10319 (100%)	27 (0%)	90	97

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

Mol	Chain	Res	Type
6	BH	39	ARG
7	BI	141	ARG
8	BJ	115	LYS
9	BL	30	ARG
9	BL	67	ARG
10	BN	76	LYS
11	BO	136	ARG
19	BD	9	ARG
19	BD	190	ARG
22	BP	44	ARG
24	BR	14	LYS
24	BR	67	ARG
27	BU	101	LYS
31	Bg	249	ARG
36	AB	332	ARG
37	AC	300	ARG
45	AH	23	ARG
45	AH	166	ARG
47	AJ	166	LYS
52	AP	171	ARG
56	AT	83	ARG
69	Ag	21	LYS
77	Ao	80	ARG
79	E	10	ARG
79	E	92	LYS
80	DC	841	LYS

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Mol	Chain	Res	Type
81	V	122	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	33	GLN
2	BB	124	ASN
2	BB	194	ASN
2	BB	209	ASN
3	BC	201	ASN
3	BC	209	ASN
3	BC	220	ASN
4	BE	157	ASN
4	BE	201	HIS
5	BG	199	GLN
5	BG	201	GLN
6	BH	89	HIS
7	BI	32	GLN
7	BI	64	ASN
7	BI	87	ASN
7	BI	94	ASN
7	BI	159	GLN
8	BJ	48	GLN
8	BJ	123	HIS
10	BN	21	ASN
12	BV	70	ASN
12	BV	74	GLN
13	BW	39	GLN
14	BX	18	HIS
14	BX	22	ASN
14	BX	63	GLN
14	BX	75	GLN
14	BX	94	ASN
15	BY	77	ASN
16	Ba	25	ASN
19	BD	159	HIS
19	BD	165	ASN
19	BD	174	HIS
20	BF	34	GLN
20	BF	37	GLN
20	BF	63	GLN
20	BF	100	ASN

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Mol	Chain	Res	Type
20	BF	103	ASN
20	BF	104	ASN
21	BK	9	ASN
21	BK	81	ASN
23	BQ	93	HIS
24	BR	62	GLN
25	BS	8	GLN
26	BT	64	HIS
26	BT	77	ASN
28	BZ	38	HIS
29	Bc	27	GLN
31	Bg	69	GLN
31	Bg	159	ASN
33	BM	38	HIS
35	AA	79	ASN
35	AA	86	GLN
36	AB	212	ASN
36	AB	293	ASN
36	AB	313	HIS
36	AB	319	ASN
37	AC	48	GLN
41	AD	178	ASN
42	AE	172	HIS
43	AF	64	GLN
43	AF	104	GLN
43	AF	199	ASN
45	AH	9	GLN
45	AH	37	ASN
45	AH	51	GLN
45	AH	64	HIS
45	AH	100	ASN
45	AH	139	ASN
47	AJ	20	ASN
47	AJ	101	ASN
48	AL	103	ASN
49	AM	59	ASN
49	AM	119	GLN
53	AQ	45	ASN
54	AR	66	HIS
55	AS	62	ASN
55	AS	157	GLN
56	AT	103	GLN

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Mol	Chain	Res	Type
56	AT	112	ASN
58	AV	98	ASN
58	AV	132	ASN
60	AX	85	GLN
61	AY	42	GLN
61	AY	81	GLN
61	AY	98	ASN
62	AZ	78	ASN
64	Ab	42	ASN
66	Ad	57	GLN
67	Ae	13	HIS
67	Ae	20	HIS
67	Ae	71	HIS
68	Af	87	ASN
69	Ag	3	GLN
69	Ag	52	GLN
70	Ah	76	GLN
71	Ai	63	ASN
71	Ai	91	ASN
72	Aj	13	ASN
73	Ak	10	GLN
73	Ak	40	GLN
74	Al	43	ASN
78	Ap	25	GLN
78	Ap	33	GLN
79	E	8	GLN
79	E	21	ASN
79	E	119	GLN
79	E	197	ASN
79	E	200	ASN
80	DC	108	HIS
80	DC	145	GLN
80	DC	259	ASN
80	DC	461	GLN
80	DC	528	HIS
80	DC	603	ASN
80	DC	607	ASN
80	DC	649	GLN
81	V	103	ASN
81	V	125	ASN
81	V	193	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1775/1798 (98%)	418 (23%)	15 (0%)
38	A1	3194/3360 (95%)	570 (17%)	17 (0%)
39	A3	120/121 (99%)	11 (9%)	1 (0%)
40	A4	157/158 (99%)	31 (19%)	0
82	EC	197/202 (97%)	116 (58%)	10 (5%)
All	All	5443/5639 (96%)	1146 (21%)	43 (0%)

All (1146) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	2	A
34	B5	4	C
34	B5	17	C
34	B5	26	A
34	B5	34	G
34	B5	42	G
34	B5	43	A
34	B5	45	U
34	B5	46	A
34	B5	47	A
34	B5	57	G
34	B5	60	U
34	B5	63	G
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	97	C
34	B5	101	U
34	B5	104	A
34	B5	114	C
34	B5	115	G
34	B5	127	G
34	B5	129	U
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	158	U
34	B5	162	A
34	B5	163	G
34	B5	166	C
34	B5	176	C
34	B5	178	U
34	B5	179	A
34	B5	181	A
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	200	A
34	B5	204	G
34	B5	217	A
34	B5	218	A
34	B5	224	C
34	B5	225	A
34	B5	226	A
34	B5	227	U
34	B5	228	G
34	B5	229	U
34	B5	230	C
34	B5	233	C
34	B5	234	G
34	B5	240	U
34	B5	241	U
34	B5	246	G
34	B5	250	C

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Mol	Chain	Res	Type
34	B5	260	U
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	287	G
34	B5	299	A
34	B5	305	C
34	B5	314	C
34	B5	316	A
34	B5	319	U
34	B5	320	U
34	B5	321	C
34	B5	322	G
34	B5	333	A
34	B5	337	G
34	B5	338	C
34	B5	346	G
34	B5	352	A
34	B5	353	A
34	B5	359	A
34	B5	360	A
34	B5	361	C
34	B5	390	G
34	B5	396	G
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	427	C
34	B5	434	G
34	B5	439	U
34	B5	444	C
34	B5	452	A
34	B5	459	G
34	B5	460	A

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Mol	Chain	Res	Type
34	B5	470	A
34	B5	473	A
34	B5	475	A
34	B5	477	A
34	B5	480	G
34	B5	484	C
34	B5	485	A
34	B5	486	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	501	U
34	B5	503	G
34	B5	506	A
34	B5	507	U
34	B5	514	G
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	544	A
34	B5	549	G
34	B5	555	A
34	B5	557	G
34	B5	558	U
34	B5	559	C
34	B5	562	OMG
34	B5	563	U
34	B5	564	G
34	B5	565	C
34	B5	568	G

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Mol	Chain	Res	Type
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	610	G
34	B5	611	U
34	B5	619	A2M
34	B5	620	A
34	B5	621	A
34	B5	622	A
34	B5	623	A
34	B5	624	G
34	B5	634	G
34	B5	635	A
34	B5	638	U
34	B5	639	U
34	B5	650	U
34	B5	652	G
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	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

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Mol	Chain	Res	Type
34	B5	718	U
34	B5	719	U
34	B5	721	U
34	B5	722	G
34	B5	725	U
34	B5	726	C
34	B5	727	U
34	B5	728	U
34	B5	730	G
34	B5	731	C
34	B5	732	G
34	B5	733	A
34	B5	735	C
34	B5	740	A
34	B5	741	C
34	B5	753	A
34	B5	755	A
34	B5	765	G
34	B5	766	U
34	B5	774	A
34	B5	775	G
34	B5	778	G
34	B5	781	U
34	B5	782	U
34	B5	783	G
34	B5	784	C
34	B5	789	A
34	B5	794	U
34	B5	807	A
34	B5	814	A
34	B5	815	G
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	839	U
34	B5	840	U
34	B5	846	G
34	B5	851	U

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Mol	Chain	Res	Type
34	B5	859	A
34	B5	863	A
34	B5	877	G
34	B5	886	U
34	B5	895	G
34	B5	898	A
34	B5	899	G
34	B5	906	A
34	B5	907	A
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	988	A
34	B5	992	A
34	B5	993	A
34	B5	1004	U
34	B5	1005	A
34	B5	1020	A
34	B5	1021	C
34	B5	1026	A
34	B5	1028	C
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	1098	U
34	B5	1100	G

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Mol	Chain	Res	Type
34	B5	1138	A
34	B5	1150	G
34	B5	1158	C
34	B5	1159	C
34	B5	1166	A
34	B5	1171	A
34	B5	1173	C
34	B5	1183	A
34	B5	1185	U
34	B5	1186	U
34	B5	1194	A
34	B5	1195	C
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	1230	A
34	B5	1243	G
34	B5	1244	A
34	B5	1245	G
34	B5	1246	C
34	B5	1251	U
34	B5	1253	U
34	B5	1256	A
34	B5	1257	U
34	B5	1267	G
34	B5	1268	G
34	B5	1269	OMU
34	B5	1286	U
34	B5	1301	U
34	B5	1314	U
34	B5	1315	U
34	B5	1321	A
34	B5	1338	C
34	B5	1340	U

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Mol	Chain	Res	Type
34	B5	1344	A
34	B5	1345	A
34	B5	1346	A
34	B5	1349	G
34	B5	1352	G
34	B5	1353	U
34	B5	1355	C
34	B5	1362	U
34	B5	1363	U
34	B5	1364	G
34	B5	1366	U
34	B5	1367	G
34	B5	1368	G
34	B5	1370	U
34	B5	1371	A
34	B5	1372	U
34	B5	1373	C
34	B5	1378	U
34	B5	1390	U
34	B5	1398	U
34	B5	1399	C
34	B5	1400	A
34	B5	1402	G
34	B5	1413	U
34	B5	1415	U
34	B5	1426	C
34	B5	1427	A
34	B5	1428	OMG
34	B5	1436	A
34	B5	1447	C
34	B5	1459	C
34	B5	1460	A
34	B5	1461	C
34	B5	1469	A
34	B5	1471	A
34	B5	1481	C
34	B5	1486	G
34	B5	1491	U
34	B5	1492	A
34	B5	1493	A
34	B5	1496	U
34	B5	1506	G

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Mol	Chain	Res	Type
34	B5	1515	A
34	B5	1516	A
34	B5	1520	U
34	B5	1521	G
34	B5	1522	U
34	B5	1523	G
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	1565	C
34	B5	1575	G7M
34	B5	1584	G
34	B5	1601	G
34	B5	1607	G
34	B5	1616	G
34	B5	1619	C
34	B5	1634	C
34	B5	1635	A
34	B5	1636	C
34	B5	1646	C
34	B5	1651	A
34	B5	1657	U
34	B5	1658	G
34	B5	1680	G
34	B5	1682	U
34	B5	1683	C
34	B5	1684	U
34	B5	1688	U
34	B5	1693	A
34	B5	1698	G
34	B5	1700	C
34	B5	1701	A
34	B5	1703	C
34	B5	1711	C
34	B5	1715	G
34	B5	1716	C
34	B5	1717	G
34	B5	1760	G
34	B5	1762	A

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Mol	Chain	Res	Type
34	B5	1766	A
34	B5	1767	G
34	B5	1769	U
34	B5	1780	G
34	B5	1792	G
34	B5	1793	G
34	B5	1794	A
34	B5	1796	C
34	B5	1799	U
38	A1	14	U
38	A1	21	G
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	92	G
38	A1	109	A
38	A1	110	G
38	A1	111	C
38	A1	116	A
38	A1	117	U
38	A1	118	U
38	A1	120	G
38	A1	122	A
38	A1	134	U
38	A1	135	C
38	A1	136	G
38	A1	146	U
38	A1	156	G
38	A1	157	A
38	A1	166	C
38	A1	174	C
38	A1	176	G
38	A1	177	U
38	A1	178	U
38	A1	187	A
38	A1	190	U

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Mol	Chain	Res	Type
38	A1	191	U
38	A1	200	C
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	245	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	269	G
38	A1	284	A
38	A1	286	U
38	A1	295	A
38	A1	296	A
38	A1	298	U
38	A1	305	U
38	A1	311	C
38	A1	329	U
38	A1	339	C
38	A1	342	A
38	A1	352	A
38	A1	372	A
38	A1	376	G
38	A1	398	A
38	A1	399	A
38	A1	401	U
38	A1	402	A
38	A1	403	C
38	A1	420	G
38	A1	421	G

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Mol	Chain	Res	Type
38	A1	422	A
38	A1	438	A
38	A1	440	A
38	A1	495	G
38	A1	510	G
38	A1	521	A
38	A1	535	G
38	A1	536	U
38	A1	540	U
38	A1	542	G
38	A1	543	C
38	A1	545	U
38	A1	547	G
38	A1	548	G
38	A1	549	U
38	A1	550	A
38	A1	551	A
38	A1	552	G
38	A1	554	A
38	A1	557	A
38	A1	559	A
38	A1	579	G
38	A1	589	A
38	A1	592	A
38	A1	602	A
38	A1	604	G
38	A1	611	A
38	A1	612	U
38	A1	620	U
38	A1	621	A
38	A1	637	C
38	A1	649	A2M
38	A1	677	A
38	A1	681	U
38	A1	690	A
38	A1	691	A
38	A1	705	A
38	A1	715	A
38	A1	719	U
38	A1	725	G
38	A1	736	A
38	A1	758	C

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Mol	Chain	Res	Type
38	A1	765	C
38	A1	766	U
38	A1	767	U
38	A1	776	U
38	A1	777	U
38	A1	781	G
38	A1	785	G
38	A1	786	A
38	A1	799	G
38	A1	806	A
38	A1	813	G
38	A1	817	A2M
38	A1	830	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	924	G
38	A1	934	G
38	A1	937	G
38	A1	943	U
38	A1	944	C
38	A1	953	G
38	A1	959	C
38	A1	963	G
38	A1	964	G
38	A1	974	G
38	A1	980	A
38	A1	981	U
38	A1	994	G
38	A1	1000	C
38	A1	1002	A

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Mol	Chain	Res	Type
38	A1	1010	G
38	A1	1014	U
38	A1	1015	U
38	A1	1016	C
38	A1	1017	C
38	A1	1018	G
38	A1	1019	G
38	A1	1021	G
38	A1	1023	C
38	A1	1032	C
38	A1	1034	U
38	A1	1035	G
38	A1	1036	A
38	A1	1045	C
38	A1	1047	A
38	A1	1064	A
38	A1	1072	G
38	A1	1082	U
38	A1	1092	C
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	1144	U
38	A1	1153	A
38	A1	1154	A
38	A1	1159	A
38	A1	1178	G
38	A1	1179	A
38	A1	1180	A
38	A1	1181	U
38	A1	1182	A
38	A1	1192	C
38	A1	1193	A
38	A1	1201	C
38	A1	1206	G

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Mol	Chain	Res	Type
38	A1	1208	U
38	A1	1219	C
38	A1	1223	A
38	A1	1224	C
38	A1	1228	C
38	A1	1231	A
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	1249	G
38	A1	1252	A
38	A1	1256	G
38	A1	1262	G
38	A1	1263	A
38	A1	1265	U
38	A1	1279	C
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	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
38	A1	1355	A
38	A1	1356	U
38	A1	1357	G
38	A1	1386	A
38	A1	1393	A

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Mol	Chain	Res	Type
38	A1	1399	A
38	A1	1400	G
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	1481	A
38	A1	1496	C
38	A1	1508	C
38	A1	1523	U
38	A1	1526	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	1564	U
38	A1	1565	G
38	A1	1567	U
38	A1	1568	U
38	A1	1569	U
38	A1	1572	U
38	A1	1573	G
38	A1	1574	C
38	A1	1575	A
38	A1	1576	G
38	A1	1579	C
38	A1	1581	C
38	A1	1582	C
38	A1	1583	A
38	A1	1589	A
38	A1	1593	A
38	A1	1605	A
38	A1	1629	U
38	A1	1630	U
38	A1	1642	A
38	A1	1643	A
38	A1	1657	C
38	A1	1683	A

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Mol	Chain	Res	Type
38	A1	1687	U
38	A1	1724	U
38	A1	1734	G
38	A1	1741	A
38	A1	1742	U
38	A1	1750	A
38	A1	1751	G
38	A1	1762	C
38	A1	1763	U
38	A1	1764	U
38	A1	1765	U
38	A1	1766	G
38	A1	1775	G
38	A1	1796	G
38	A1	1797	A
38	A1	1813	A
38	A1	1814	A
38	A1	1815	U
38	A1	1817	G
38	A1	1820	U
38	A1	1821	U
38	A1	1840	U
38	A1	1842	A
38	A1	1846	C
38	A1	1849	C
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	1946	A
38	A1	1948	G
38	A1	1952	G
38	A1	1953	G
38	A1	1954	G
38	A1	1955	U
38	A1	2094	C
38	A1	2110	G
38	A1	2111	G
38	A1	2114	C

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Mol	Chain	Res	Type
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	2188	A
38	A1	2197	OMC
38	A1	2201	G
38	A1	2207	A
38	A1	2242	A
38	A1	2249	G
38	A1	2256	A2M
38	A1	2257	C
38	A1	2259	A
38	A1	2260	U
38	A1	2269	U
38	A1	2270	A
38	A1	2272	G
38	A1	2273	G
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	2308	C
38	A1	2310	U
38	A1	2313	A
38	A1	2314	U
38	A1	2315	G
38	A1	2334	U
38	A1	2335	G
38	A1	2336	U
38	A1	2340	U
38	A1	2356	A
38	A1	2366	C
38	A1	2373	A
38	A1	2374	C
38	A1	2375	G
38	A1	2383	C
38	A1	2388	U

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Mol	Chain	Res	Type
38	A1	2391	G
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	2442	G
38	A1	2446	U
38	A1	2448	G
38	A1	2450	G
38	A1	2451	G
38	A1	2453	U
38	A1	2454	G
38	A1	2455	U
38	A1	2456	A
38	A1	2458	A
38	A1	2459	A
38	A1	2460	U
38	A1	2461	A
38	A1	2462	A
38	A1	2467	G
38	A1	2468	A
38	A1	2469	G
38	A1	2474	G
38	A1	2479	C
38	A1	2480	A
38	A1	2481	G
38	A1	2485	A
38	A1	2487	U
38	A1	2489	C
38	A1	2490	C
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

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Mol	Chain	Res	Type
38	A1	2502	A
38	A1	2503	G
38	A1	2505	U
38	A1	2506	U
38	A1	2507	C
38	A1	2514	U
38	A1	2515	A
38	A1	2523	A
38	A1	2524	A
38	A1	2530	G
38	A1	2537	U
38	A1	2538	U
38	A1	2539	C
38	A1	2540	A
38	A1	2541	U
38	A1	2542	U
38	A1	2544	U
38	A1	2549	G
38	A1	2552	C
38	A1	2554	A
38	A1	2561	A
38	A1	2569	A
38	A1	2570	U
38	A1	2571	U
38	A1	2573	G
38	A1	2585	G
38	A1	2593	A
38	A1	2606	G
38	A1	2607	G
38	A1	2614	G
38	A1	2635	A
38	A1	2651	G
38	A1	2652	U
38	A1	2656	A
38	A1	2674	A
38	A1	2677	G
38	A1	2678	A
38	A1	2681	U
38	A1	2688	U
38	A1	2689	A
38	A1	2690	G
38	A1	2691	A

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Mol	Chain	Res	Type
38	A1	2704	A
38	A1	2705	A
38	A1	2714	G
38	A1	2719	U
38	A1	2720	G
38	A1	2728	G
38	A1	2729	OMU
38	A1	2737	C
38	A1	2749	G
38	A1	2752	U
38	A1	2753	G
38	A1	2755	C
38	A1	2773	C
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	2817	A
38	A1	2828	G
38	A1	2842	U
38	A1	2845	A
38	A1	2861	U
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	2935	U
38	A1	2936	A
38	A1	2942	C
38	A1	2947	G
38	A1	2977	G
38	A1	2983	C
38	A1	2990	G

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Mol	Chain	Res	Type
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	3080	G
38	A1	3086	A
38	A1	3087	A
38	A1	3092	C
38	A1	3101	G
38	A1	3109	G
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
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	3207	U
38	A1	3216	G
38	A1	3217	C
38	A1	3218	A

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Mol	Chain	Res	Type
38	A1	3219	G
38	A1	3224	G
38	A1	3234	A
38	A1	3243	A
38	A1	3246	G
38	A1	3259	U
38	A1	3260	G
38	A1	3263	G
38	A1	3270	U
38	A1	3271	G
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	3314	A
38	A1	3316	A
38	A1	3319	U
38	A1	3335	A
38	A1	3342	A
38	A1	3345	G
38	A1	3351	U
38	A1	3352	U
38	A1	3353	G
38	A1	3354	U
38	A1	3355	U
38	A1	3356	G
38	A1	3369	G
38	A1	3378	C
38	A1	3389	U
39	A3	7	G
39	A3	22	A
39	A3	53	U
39	A3	54	U
39	A3	55	A
39	A3	65	G
39	A3	74	C
39	A3	76	A
39	A3	102	A

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Mol	Chain	Res	Type
39	A3	112	G
39	A3	121	U
40	A4	23	U
40	A4	25	G
40	A4	34	U
40	A4	35	C
40	A4	38	U
40	A4	50	C
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	83	C
40	A4	84	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
40	A4	97	A
40	A4	104	A
40	A4	106	C
40	A4	111	A
40	A4	113	U
40	A4	116	G
40	A4	125	U
40	A4	152	G
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

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Mol	Chain	Res	Type
82	EC	6776	A
82	EC	6777	C
82	EC	6778	C
82	EC	6779	C
82	EC	6780	A
82	EC	6781	U
82	EC	6782	C
82	EC	6786	A
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	6805	C
82	EC	6811	G
82	EC	6816	A
82	EC	6817	A
82	EC	6818	G
82	EC	6819	G
82	EC	6820	C
82	EC	6821	U
82	EC	6822	U
82	EC	6823	U
82	EC	6824	C
82	EC	6825	A
82	EC	6831	U
82	EC	6832	G
82	EC	6835	U
82	EC	6836	U
82	EC	6837	G
82	EC	6840	A
82	EC	6841	U
82	EC	6842	U
82	EC	6843	U
82	EC	6844	A

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Mol	Chain	Res	Type
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	6856	C
82	EC	6857	C
82	EC	6858	A
82	EC	6859	U
82	EC	6860	A
82	EC	6864	A
82	EC	6866	C
82	EC	6867	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	6883	A
82	EC	6884	G
82	EC	6888	A
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	6907	G
82	EC	6908	C
82	EC	6909	A
82	EC	6911	A
82	EC	6912	G
82	EC	6913	U
82	EC	6915	G
82	EC	6916	A

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Mol	Chain	Res	Type
82	EC	6918	A
82	EC	6922	G
82	EC	6925	C
82	EC	6928	G
82	EC	6929	C
82	EC	6934	U
82	EC	6935	G
82	EC	6936	G
82	EC	6938	A
82	EC	6939	C
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	6947	A
82	EC	6948	U
82	EC	6949	G
82	EC	6953	G
82	EC	6955	U
82	EC	6957	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	B5	224	C
34	B5	345	U
34	B5	752	A
34	B5	819	G
34	B5	862	A
34	B5	950	C
34	B5	1217	A
34	B5	1285	U
34	B5	1344	A
34	B5	1369	U
34	B5	1427	A
34	B5	1458	G
34	B5	1521	G
34	B5	1600	A
34	B5	1645	G

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Mol	Chain	Res	Type
38	A1	122	A
38	A1	239	G
38	A1	241	G
38	A1	873	C
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	1572	U
38	A1	1629	U
38	A1	2241	U
38	A1	2497	U
38	A1	2506	U
38	A1	2875	U
38	A1	3121	U
39	A3	52	G
82	EC	6789	G
82	EC	6817	A
82	EC	6831	U
82	EC	6844	A
82	EC	6851	G
82	EC	6876	A
82	EC	6889	A
82	EC	6939	C
82	EC	6943	A
82	EC	6952	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	A2M	B5	796	34	18,25,26	0.90	1 (5%)	20,36,39	1.51	4 (20%)
38	A2M	A1	876	38	18,25,26	0.88	1 (5%)	20,36,39	1.25	2 (10%)
38	OMG	A1	805	38	19,26,27	0.88	1 (5%)	21,38,41	1.09	2 (9%)
38	OMU	A1	2729	38	19,22,23	1.28	4 (21%)	25,31,34	1.80	5 (20%)
38	A2M	A1	649	38	18,25,26	0.81	0	20,36,39	1.18	2 (10%)
34	A2M	B5	100	34,83	18,25,26	0.89	1 (5%)	20,36,39	1.25	2 (10%)
38	OMU	A1	1888	38	19,22,23	1.27	4 (21%)	25,31,34	1.85	4 (16%)
38	A2M	A1	1133	38	18,25,26	0.86	0	20,36,39	1.26	2 (10%)
38	OMG	A1	2922	38	19,26,27	0.88	1 (5%)	21,38,41	1.04	2 (9%)
38	OMU	A1	2421	38	19,22,23	1.28	3 (15%)	25,31,34	1.79	5 (20%)
38	OMG	A1	908	38	19,26,27	0.94	1 (5%)	21,38,41	1.16	2 (9%)
38	OMC	A1	2337	38	19,22,23	0.79	0	25,31,34	0.89	1 (4%)
38	1MA	A1	2142	38,83	17,25,26	1.48	2 (11%)	17,37,40	1.20	2 (11%)
34	A2M	B5	436	34	18,25,26	0.89	1 (5%)	20,36,39	1.35	3 (15%)
36	HIC	AB	243	36	8,11,12	1.64	2 (25%)	5,14,16	0.98	0
38	A2M	A1	807	38	18,25,26	0.86	0	20,36,39	1.37	3 (15%)
34	OMC	B5	414	34	19,22,23	0.83	0	25,31,34	0.97	1 (4%)
34	A2M	B5	541	34	18,25,26	0.87	0	20,36,39	1.25	2 (10%)
38	OMC	A1	2959	38	19,22,23	0.81	0	25,31,34	0.86	1 (4%)
38	A2M	A1	1449	38,83	18,25,26	0.91	1 (5%)	20,36,39	1.12	2 (10%)
34	A2M	B5	974	34	18,25,26	0.86	0	20,36,39	1.22	2 (10%)
34	OMU	B5	578	34	19,22,23	1.21	2 (10%)	25,31,34	1.79	5 (20%)
38	OMC	A1	2197	38	19,22,23	0.79	0	25,31,34	0.79	0
34	OMG	B5	1572	34	19,26,27	0.87	1 (5%)	21,38,41	1.12	2 (9%)
38	OMG	A1	2619	38	19,26,27	0.89	1 (5%)	21,38,41	1.01	2 (9%)
38	OMC	A1	1437	38	19,22,23	0.81	0	25,31,34	1.10	2 (8%)
38	OMU	A1	2347	38	19,22,23	1.31	4 (21%)	25,31,34	1.86	6 (24%)
34	OMC	B5	1007	34	19,22,23	0.79	0	25,31,34	0.82	1 (4%)
34	G7M	B5	1575	34	20,26,27	2.72	5 (25%)	16,39,42	1.53	3 (18%)
38	OMG	A1	2288	38	19,26,27	0.89	1 (5%)	21,38,41	1.05	2 (9%)
34	OMG	B5	1271	34	19,26,27	0.88	1 (5%)	21,38,41	0.99	1 (4%)
38	OMC	A1	650	38	19,22,23	0.79	0	25,31,34	0.81	0
38	5MC	A1	2278	38,83	19,22,23	1.60	3 (15%)	26,32,35	1.19	3 (11%)
38	A2M	A1	817	38,83	18,25,26	0.89	1 (5%)	20,36,39	1.30	2 (10%)
38	OMG	A1	1450	38	19,26,27	0.86	1 (5%)	21,38,41	1.02	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	A2M	B5	28	34,83	18,25,26	0.90	1 (5%)	20,36,39	1.34	3 (15%)
38	A2M	A1	2280	38	18,25,26	0.84	0	20,36,39	1.23	2 (10%)
38	UR3	A1	2634	38	19,22,23	0.97	0	26,32,35	1.73	3 (11%)
34	XSX	B5	1191	34	24,28,29	1.01	1 (4%)	30,40,43	3.76	5 (16%)
34	MA6	B5	1782	34	19,26,27	1.04	2 (10%)	18,38,41	1.93	3 (16%)
38	OMU	A1	2417	38	19,22,23	1.22	3 (15%)	25,31,34	1.80	5 (20%)
38	OMC	A1	2948	38	19,22,23	0.80	0	25,31,34	0.95	1 (4%)
38	OMC	A1	663	38	19,22,23	0.80	0	25,31,34	0.76	0
38	A2M	A1	2256	38	18,25,26	0.91	0	20,36,39	1.67	5 (25%)
80	DDE	DC	699	80	15,20,21	0.94	1 (6%)	11,28,30	1.21	1 (9%)
34	4AC	B5	1773	34	21,24,25	1.06	1 (4%)	28,34,37	1.46	5 (17%)
38	OMG	A1	2791	38	19,26,27	0.90	1 (5%)	21,38,41	0.99	1 (4%)
34	A2M	B5	619	34,83	18,25,26	0.81	0	20,36,39	1.33	2 (10%)
38	5MC	A1	2870	38,83	19,22,23	1.52	3 (15%)	26,32,35	1.28	2 (7%)
38	A2M	A1	2220	38	18,25,26	0.85	1 (5%)	20,36,39	1.30	2 (10%)
34	OMU	B5	1269	34	19,22,23	1.21	2 (10%)	25,31,34	1.82	5 (20%)
34	A2M	B5	420	34	18,25,26	0.91	1 (5%)	20,36,39	1.26	3 (15%)
38	OMG	A1	2815	38	19,26,27	0.90	1 (5%)	21,38,41	1.03	2 (9%)
34	OMG	B5	1428	34,83	19,26,27	0.90	1 (5%)	21,38,41	1.05	2 (9%)
38	1MA	A1	645	38,83	17,25,26	1.50	2 (11%)	17,37,40	1.16	2 (11%)
34	OMG	B5	562	34	19,26,27	0.88	1 (5%)	21,38,41	1.16	2 (9%)
34	4AC	B5	1280	34	21,24,25	1.04	1 (4%)	28,34,37	1.13	2 (7%)
38	A2M	A1	2281	38	18,25,26	0.77	0	20,36,39	1.91	5 (25%)
38	OMU	A1	898	38	19,22,23	1.26	3 (15%)	25,31,34	1.79	4 (16%)
34	MA6	B5	1781	34	19,26,27	1.07	2 (10%)	18,38,41	2.00	3 (16%)
38	OMU	A1	2724	38	19,22,23	1.22	3 (15%)	25,31,34	1.81	6 (24%)
38	OMU	A1	2921	38	19,22,23	1.22	3 (15%)	25,31,34	1.81	5 (20%)
38	OMG	A1	867	38,83	19,26,27	0.85	1 (5%)	21,38,41	1.04	2 (9%)
34	OMG	B5	1126	34	19,26,27	0.90	1 (5%)	21,38,41	1.13	2 (9%)
38	A2M	A1	2946	38,83	18,25,26	0.88	1 (5%)	20,36,39	1.60	3 (15%)
38	OMG	A1	2793	38	19,26,27	0.88	1 (5%)	21,38,41	1.05	2 (9%)
38	A2M	A1	2640	38	18,25,26	0.86	0	20,36,39	1.16	2 (10%)
34	OMC	B5	1639	34	19,22,23	0.76	0	25,31,34	0.81	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	A2M	B5	796	34	-	1/5/27/28	0/3/3/3
38	A2M	A1	876	38	-	0/5/27/28	0/3/3/3
38	OMG	A1	805	38	-	0/5/27/28	0/3/3/3
38	OMU	A1	2729	38	-	3/9/27/28	0/2/2/2
38	A2M	A1	649	38	-	2/5/27/28	0/3/3/3
34	A2M	B5	100	34,83	-	0/5/27/28	0/3/3/3
38	OMU	A1	1888	38	-	0/9/27/28	0/2/2/2
38	A2M	A1	1133	38	-	0/5/27/28	0/3/3/3
38	OMG	A1	2922	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	908	38	-	0/5/27/28	0/3/3/3
38	OMC	A1	2337	38	-	0/9/27/28	0/2/2/2
38	1MA	A1	2142	38,83	-	0/3/25/26	0/3/3/3
34	A2M	B5	436	34	-	0/5/27/28	0/3/3/3
36	HIC	AB	243	36	-	2/5/6/8	0/1/1/1
38	A2M	A1	807	38	-	0/5/27/28	0/3/3/3
34	OMC	B5	414	34	-	1/9/27/28	0/2/2/2
34	A2M	B5	541	34	-	3/5/27/28	0/3/3/3
38	OMC	A1	2959	38	-	0/9/27/28	0/2/2/2
38	A2M	A1	1449	38,83	-	0/5/27/28	0/3/3/3
34	A2M	B5	974	34	-	1/5/27/28	0/3/3/3
34	OMU	B5	578	34	-	4/9/27/28	0/2/2/2
38	OMC	A1	2197	38	-	6/9/27/28	0/2/2/2
34	OMG	B5	1572	34	-	0/5/27/28	0/3/3/3
38	OMG	A1	2619	38	-	1/5/27/28	0/3/3/3
38	OMC	A1	1437	38	-	3/9/27/28	0/2/2/2
38	OMU	A1	2347	38	-	0/9/27/28	0/2/2/2
34	OMC	B5	1007	34	-	0/9/27/28	0/2/2/2
34	G7M	B5	1575	34	-	0/3/25/26	0/3/3/3
38	OMG	A1	2288	38	-	0/5/27/28	0/3/3/3
34	OMG	B5	1271	34	-	1/5/27/28	0/3/3/3
38	OMC	A1	650	38	-	0/9/27/28	0/2/2/2
38	5MC	A1	2278	38,83	-	0/7/25/26	0/2/2/2
38	A2M	A1	817	38,83	-	1/5/27/28	0/3/3/3
38	OMG	A1	1450	38	-	1/5/27/28	0/3/3/3
34	A2M	B5	28	34,83	-	1/5/27/28	0/3/3/3
38	A2M	A1	2280	38	-	2/5/27/28	0/3/3/3
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	XSX	B5	1191	34	-	5/16/34/35	0/2/2/2
34	MA6	B5	1782	34	-	3/7/29/30	0/3/3/3
38	OMU	A1	2417	38	-	1/9/27/28	0/2/2/2
38	OMC	A1	2948	38	-	1/9/27/28	0/2/2/2
38	OMC	A1	663	38	-	1/9/27/28	0/2/2/2
38	A2M	A1	2256	38	-	2/5/27/28	0/3/3/3
80	DDE	DC	699	80	-	8/20/21/23	0/1/1/1
34	4AC	B5	1773	34	-	6/11/29/30	0/2/2/2
38	OMG	A1	2791	38	-	1/5/27/28	0/3/3/3
34	A2M	B5	619	34,83	-	2/5/27/28	0/3/3/3
38	5MC	A1	2870	38,83	-	4/7/25/26	0/2/2/2
38	A2M	A1	2220	38	-	1/5/27/28	0/3/3/3
34	OMU	B5	1269	34	-	1/9/27/28	0/2/2/2
34	A2M	B5	420	34	-	1/5/27/28	0/3/3/3
38	OMG	A1	2815	38	-	0/5/27/28	0/3/3/3
34	OMG	B5	1428	34,83	-	3/5/27/28	0/3/3/3
38	1MA	A1	645	38,83	-	0/3/25/26	0/3/3/3
34	OMG	B5	562	34	-	2/5/27/28	0/3/3/3
34	4AC	B5	1280	34	-	4/11/29/30	0/2/2/2
38	A2M	A1	2281	38	-	2/5/27/28	0/3/3/3
38	OMU	A1	898	38	-	0/9/27/28	0/2/2/2
34	MA6	B5	1781	34	-	1/7/29/30	0/3/3/3
38	OMU	A1	2724	38	-	1/9/27/28	0/2/2/2
38	OMU	A1	2921	38	-	0/9/27/28	0/2/2/2
38	OMG	A1	867	38,83	-	1/5/27/28	0/3/3/3
34	OMG	B5	1126	34	-	0/5/27/28	0/3/3/3
38	A2M	A1	2946	38,83	-	1/5/27/28	0/3/3/3
38	OMG	A1	2793	38	-	0/5/27/28	0/3/3/3
38	A2M	A1	2640	38	-	1/5/27/28	0/3/3/3
34	OMC	B5	1639	34	-	1/9/27/28	0/2/2/2

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	C8-N7	6.95	1.45	1.33
34	B5	1575	G7M	C8-N9	6.88	1.45	1.33
38	A1	2278	5MC	C5-C4	5.70	1.48	1.44
38	A1	2870	5MC	C5-C4	5.13	1.48	1.44
38	A1	645	1MA	C2-N3	4.78	1.34	1.28
38	A1	2142	1MA	C2-N3	4.73	1.34	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	C5-C4	3.99	1.47	1.39
34	B5	1575	G7M	C2'-C3'	-3.83	1.43	1.53
36	AB	243	HIC	CD2-CG	3.50	1.41	1.36
38	A1	645	1MA	C6-N6	2.98	1.35	1.27
38	A1	2421	OMU	C4-N3	-2.93	1.33	1.38
38	A1	2142	1MA	C6-N6	2.93	1.35	1.27
34	B5	1781	MA6	C6-C5	2.91	1.49	1.44
38	A1	2870	5MC	C6-C5	2.90	1.39	1.34
34	B5	1773	4AC	C4-N4	-2.84	1.35	1.39
38	A1	898	OMU	C4-N3	-2.84	1.33	1.38
34	B5	1280	4AC	C4-N4	-2.81	1.35	1.39
38	A1	2729	OMU	C4-N3	-2.80	1.33	1.38
38	A1	2347	OMU	C4-N3	-2.79	1.33	1.38
38	A1	2278	5MC	C6-C5	2.75	1.39	1.34
38	A1	1888	OMU	C4-N3	-2.74	1.33	1.38
38	A1	2417	OMU	C4-N3	-2.73	1.33	1.38
34	B5	1782	MA6	C6-C5	2.71	1.49	1.44
38	A1	2921	OMU	C4-N3	-2.70	1.34	1.38
38	A1	2724	OMU	C4-N3	-2.64	1.34	1.38
34	B5	1269	OMU	C4-N3	-2.61	1.34	1.38
34	B5	578	OMU	C4-N3	-2.60	1.34	1.38
38	A1	2815	OMG	C6-N1	-2.59	1.33	1.37
38	A1	2791	OMG	C6-N1	-2.54	1.33	1.37
38	A1	2619	OMG	C6-N1	-2.53	1.33	1.37
38	A1	2288	OMG	C6-N1	-2.48	1.34	1.37
34	B5	1575	G7M	O3'-C3'	-2.48	1.36	1.43
38	A1	2347	OMU	C2-N1	2.46	1.42	1.38
34	B5	1428	OMG	C6-N1	-2.45	1.34	1.37
38	A1	2793	OMG	C6-N1	-2.45	1.34	1.37
38	A1	908	OMG	C6-N1	-2.44	1.34	1.37
34	B5	1126	OMG	C6-N1	-2.42	1.34	1.37
34	B5	562	OMG	C6-N1	-2.40	1.34	1.37
38	A1	2922	OMG	C6-N1	-2.39	1.34	1.37
38	A1	805	OMG	C6-N1	-2.38	1.34	1.37
38	A1	1450	OMG	C6-N1	-2.37	1.34	1.37
38	A1	2921	OMU	C2-N3	-2.35	1.33	1.38
38	A1	2421	OMU	C2-N3	-2.35	1.33	1.38
34	B5	1271	OMG	C6-N1	-2.34	1.34	1.37
38	A1	898	OMU	C2-N3	-2.33	1.33	1.38
38	A1	2729	OMU	C2-N3	-2.31	1.33	1.38
38	A1	2278	5MC	C6-N1	-2.30	1.34	1.38
38	A1	2417	OMU	C2-N3	-2.30	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	867	OMG	C6-N1	-2.30	1.34	1.37
38	A1	2347	OMU	C2-N3	-2.28	1.34	1.38
38	A1	1888	OMU	C2-N3	-2.28	1.34	1.38
34	B5	1572	OMG	C6-N1	-2.26	1.34	1.37
38	A1	898	OMU	C5-C4	-2.26	1.38	1.43
38	A1	2724	OMU	C5-C4	-2.25	1.38	1.43
38	A1	2870	5MC	C6-N1	-2.22	1.34	1.38
38	A1	2946	A2M	O4'-C1'	2.21	1.43	1.40
34	B5	1269	OMU	C2-N3	-2.21	1.34	1.38
34	B5	578	OMU	C2-N3	-2.19	1.34	1.38
38	A1	2729	OMU	C5-C4	-2.19	1.39	1.43
38	A1	2724	OMU	C2-N3	-2.19	1.34	1.38
38	A1	2347	OMU	C5-C4	-2.18	1.39	1.43
34	B5	28	A2M	O4'-C1'	2.18	1.43	1.40
34	B5	436	A2M	O4'-C1'	2.18	1.43	1.40
38	A1	2220	A2M	O4'-C1'	2.17	1.43	1.40
38	A1	2729	OMU	C2-N1	2.17	1.41	1.38
34	B5	420	A2M	O4'-C1'	2.14	1.43	1.40
38	A1	2417	OMU	C5-C4	-2.13	1.39	1.43
34	B5	796	A2M	O4'-C1'	2.13	1.43	1.40
34	B5	1191	XSX	C2-N1	2.13	1.41	1.38
38	A1	1449	A2M	O4'-C1'	2.12	1.43	1.40
38	A1	876	A2M	O4'-C1'	2.12	1.43	1.40
34	B5	1782	MA6	C6-N1	2.10	1.35	1.32
38	A1	1888	OMU	C5-C4	-2.10	1.39	1.43
36	AB	243	HIC	CZ-NE2	-2.09	1.42	1.48
80	DC	699	DDE	CD2-NE2	2.09	1.39	1.36
34	B5	100	A2M	O4'-C1'	2.09	1.43	1.40
38	A1	817	A2M	O4'-C1'	2.09	1.43	1.40
38	A1	1888	OMU	C2-N1	2.07	1.41	1.38
38	A1	2421	OMU	C5-C4	-2.07	1.39	1.43
38	A1	2921	OMU	C5-C4	-2.07	1.39	1.43
34	B5	1781	MA6	C6-N1	2.01	1.35	1.32

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1191	XSX	C3-C1-N3	19.14	145.62	112.16
38	A1	2634	UR3	C4-N3-C2	-6.89	119.03	124.58
34	B5	1781	MA6	C2-N1-C6	5.92	122.64	116.84
34	B5	1782	MA6	C2-N1-C6	5.64	122.37	116.84
34	B5	1773	4AC	N4-C4-N3	5.08	122.11	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2921	OMU	C4-N3-C2	-4.85	120.59	126.61
34	B5	578	OMU	C4-N3-C2	-4.81	120.64	126.61
34	B5	1191	XSX	C4-N3-C2	-4.81	119.01	124.66
38	A1	2421	OMU	C4-N3-C2	-4.78	120.68	126.61
34	B5	1269	OMU	C4-N3-C2	-4.75	120.72	126.61
38	A1	1888	OMU	C4-N3-C2	-4.72	120.75	126.61
38	A1	2417	OMU	C4-N3-C2	-4.71	120.77	126.61
38	A1	898	OMU	C4-N3-C2	-4.69	120.79	126.61
38	A1	2724	OMU	C4-N3-C2	-4.63	120.87	126.61
38	A1	2729	OMU	C4-N3-C2	-4.53	120.99	126.61
38	A1	2281	A2M	O4'-C1'-N9	4.49	114.70	108.75
38	A1	2421	OMU	N3-C2-N1	4.48	120.72	114.89
38	A1	1888	OMU	N3-C2-N1	4.47	120.71	114.89
38	A1	2347	OMU	C4-N3-C2	-4.42	121.12	126.61
38	A1	2417	OMU	N3-C2-N1	4.34	120.54	114.89
38	A1	2724	OMU	N3-C2-N1	4.30	120.49	114.89
38	A1	2921	OMU	N3-C2-N1	4.28	120.47	114.89
38	A1	898	OMU	N3-C2-N1	4.25	120.43	114.89
38	A1	2870	5MC	C5-C6-N1	-4.23	118.71	123.31
38	A1	2729	OMU	N3-C2-N1	4.22	120.39	114.89
34	B5	578	OMU	N3-C2-N1	4.12	120.26	114.89
34	B5	1269	OMU	N3-C2-N1	4.11	120.24	114.89
38	A1	2347	OMU	N3-C2-N1	4.04	120.15	114.89
38	A1	2220	A2M	N3-C2-N1	-4.03	123.20	128.67
38	A1	2921	OMU	C5-C4-N3	3.99	120.40	114.80
38	A1	2281	A2M	C4'-O4'-C1'	-3.96	106.30	109.92
34	B5	1782	MA6	N3-C2-N1	-3.94	123.32	128.67
34	B5	578	OMU	C5-C4-N3	3.91	120.28	114.80
38	A1	898	OMU	C5-C4-N3	3.90	120.27	114.80
38	A1	2256	A2M	O2'-C2'-C1'	3.89	116.52	109.00
34	B5	1269	OMU	C5-C4-N3	3.85	120.19	114.80
38	A1	2417	OMU	C5-C4-N3	3.83	120.17	114.80
34	B5	796	A2M	N3-C2-N1	-3.82	123.49	128.67
38	A1	2946	A2M	O4'-C1'-N9	3.82	113.81	108.75
34	B5	1280	4AC	N4-C4-N3	3.82	120.07	113.87
38	A1	649	A2M	N3-C2-N1	-3.81	123.50	128.67
38	A1	2347	OMU	C5-C4-N3	3.81	120.14	114.80
38	A1	817	A2M	N3-C2-N1	-3.81	123.50	128.67
38	A1	2729	OMU	C5-C4-N3	3.80	120.12	114.80
38	A1	2946	A2M	N3-C2-N1	-3.77	123.56	128.67
34	B5	436	A2M	N3-C2-N1	-3.76	123.56	128.67
34	B5	28	A2M	N3-C2-N1	-3.75	123.59	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	1888	OMU	C5-C4-N3	3.74	120.04	114.80
38	A1	2421	OMU	C5-C4-N3	3.74	120.03	114.80
34	B5	974	A2M	N3-C2-N1	-3.73	123.62	128.67
34	B5	1781	MA6	N3-C2-N1	-3.70	123.65	128.67
38	A1	2724	OMU	C5-C4-N3	3.69	119.97	114.80
38	A1	2281	A2M	N3-C2-N1	-3.68	123.67	128.67
38	A1	1133	A2M	N3-C2-N1	-3.65	123.72	128.67
38	A1	2256	A2M	N3-C2-N1	-3.63	123.74	128.67
38	A1	2280	A2M	N3-C2-N1	-3.63	123.75	128.67
34	B5	420	A2M	N3-C2-N1	-3.59	123.80	128.67
38	A1	2640	A2M	N3-C2-N1	-3.58	123.82	128.67
34	B5	619	A2M	N3-C2-N1	-3.57	123.82	128.67
34	B5	100	A2M	N3-C2-N1	-3.57	123.83	128.67
38	A1	1449	A2M	N3-C2-N1	-3.56	123.84	128.67
34	B5	541	A2M	N3-C2-N1	-3.55	123.86	128.67
38	A1	2347	OMU	C1'-N1-C2	3.52	123.91	117.59
38	A1	876	A2M	N3-C2-N1	-3.45	123.99	128.67
38	A1	2634	UR3	C5-C4-N3	3.42	119.55	115.04
34	B5	1781	MA6	C4-C5-N7	-3.36	105.78	109.34
34	B5	1575	G7M	O3'-C3'-C4'	3.28	120.51	111.08
34	B5	1782	MA6	C4-C5-N7	-3.26	105.89	109.34
34	B5	1575	G7M	O2'-C2'-C3'	3.21	122.11	111.82
38	A1	2724	OMU	O4-C4-C5	-3.19	119.65	125.16
38	A1	807	A2M	N3-C2-N1	-3.10	124.46	128.67
38	A1	2417	OMU	O4-C4-C5	-3.10	119.81	125.16
38	A1	2921	OMU	O4-C4-C5	-3.10	119.82	125.16
38	A1	1437	OMC	O2-C2-N3	-3.04	117.54	122.33
38	A1	2347	OMU	O4-C4-C5	-3.04	119.92	125.16
34	B5	1126	OMG	C8-N7-C5	3.04	107.72	102.55
34	B5	1269	OMU	O4-C4-C5	-3.03	119.93	125.16
38	A1	898	OMU	O4-C4-C5	-3.02	119.95	125.16
38	A1	2729	OMU	O4-C4-C5	-3.01	119.97	125.16
38	A1	2278	5MC	C5-C6-N1	-2.98	120.07	123.31
38	A1	1888	OMU	O4-C4-C5	-2.97	120.05	125.16
34	B5	578	OMU	O4-C4-C5	-2.95	120.07	125.16
80	DC	699	DDE	CAU-CBW-CBI	-2.95	105.45	111.22
38	A1	867	OMG	C8-N7-C5	2.92	107.53	102.55
34	B5	1572	OMG	C8-N7-C5	2.92	107.53	102.55
38	A1	2619	OMG	C8-N7-C5	2.91	107.51	102.55
38	A1	805	OMG	C8-N7-C5	2.87	107.43	102.55
38	A1	2815	OMG	C8-N7-C5	2.86	107.42	102.55
38	A1	2922	OMG	C8-N7-C5	2.86	107.42	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2791	OMG	C8-N7-C5	2.85	107.40	102.55
34	B5	1191	XSX	C5-C4-N3	2.85	119.58	115.64
34	B5	1773	4AC	C5-C4-N4	-2.84	118.15	122.94
34	B5	619	A2M	C4-C5-N7	-2.83	106.35	109.34
38	A1	2278	5MC	C5-C4-N3	-2.81	118.88	121.75
38	A1	2421	OMU	O4-C4-C5	-2.81	120.32	125.16
34	B5	796	A2M	C4-C5-N7	-2.80	106.38	109.34
34	B5	1271	OMG	C8-N7-C5	2.78	107.28	102.55
34	B5	562	OMG	C8-N7-C5	2.77	107.27	102.55
38	A1	2948	OMC	O2-C2-N3	-2.76	117.98	122.33
38	A1	645	1MA	C8-N7-C5	2.76	107.25	102.55
38	A1	2640	A2M	C4-C5-N7	-2.76	106.42	109.34
38	A1	2288	OMG	C8-N7-C5	2.75	107.24	102.55
38	A1	2793	OMG	C8-N7-C5	2.75	107.23	102.55
38	A1	817	A2M	C4-C5-N7	-2.75	106.43	109.34
34	B5	420	A2M	C4-C5-N7	-2.73	106.45	109.34
38	A1	2280	A2M	C4-C5-N7	-2.73	106.46	109.34
38	A1	2278	5MC	O2-C2-N3	-2.72	118.04	122.33
34	B5	1428	OMG	C8-N7-C5	2.72	107.18	102.55
34	B5	796	A2M	C2'-C1'-N9	-2.71	106.53	112.56
38	A1	908	OMG	C8-N7-C5	2.71	107.16	102.55
38	A1	1450	OMG	C8-N7-C5	2.70	107.14	102.55
38	A1	876	A2M	C4-C5-N7	-2.68	106.51	109.34
34	B5	28	A2M	C4-C5-N7	-2.67	106.51	109.34
34	B5	414	OMC	O2-C2-N3	-2.66	118.13	122.33
38	A1	807	A2M	C4-C5-N7	-2.63	106.56	109.34
38	A1	2142	1MA	C8-N7-C5	2.62	107.01	102.55
38	A1	2870	5MC	C5-C4-N3	-2.62	119.07	121.75
38	A1	807	A2M	O4'-C1'-N9	2.60	112.19	108.75
38	A1	2256	A2M	O3'-C3'-C2'	-2.59	103.92	111.19
38	A1	1133	A2M	C4-C5-N7	-2.59	106.60	109.34
34	B5	100	A2M	C4-C5-N7	-2.54	106.65	109.34
38	A1	2256	A2M	C4-C5-N7	-2.53	106.66	109.34
34	B5	974	A2M	C4-C5-N7	-2.49	106.70	109.34
38	A1	2142	1MA	C5-C6-N1	2.49	117.53	113.95
38	A1	2417	OMU	O2-C2-N1	-2.49	119.56	122.80
38	A1	649	A2M	C4-C5-N7	-2.47	106.73	109.34
38	A1	2946	A2M	C4-C5-N7	-2.46	106.74	109.34
38	A1	645	1MA	C5-C6-N1	2.45	117.46	113.95
34	B5	436	A2M	C4-C5-N7	-2.41	106.79	109.34
34	B5	1575	G7M	CN7-N7-C8	-2.41	113.83	125.43
34	B5	1269	OMU	O2-C2-N1	-2.40	119.67	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	28	A2M	O4'-C1'-N9	2.40	111.92	108.75
38	A1	1437	OMC	C1'-N1-C2	2.39	123.71	118.44
34	B5	541	A2M	C4-C5-N7	-2.38	106.83	109.34
38	A1	2220	A2M	C4-C5-N7	-2.36	106.84	109.34
38	A1	2337	OMC	O2-C2-N3	-2.35	118.63	122.33
38	A1	2724	OMU	C1'-N1-C2	2.30	121.72	117.59
34	B5	1773	4AC	C6-C5-C4	2.28	119.75	117.00
34	B5	562	OMG	C5-C6-N1	2.26	118.39	114.07
38	A1	1449	A2M	C4-C5-N7	-2.26	106.95	109.34
34	B5	420	A2M	O4'-C1'-N9	2.19	111.66	108.75
34	B5	1280	4AC	C6-C5-C4	2.18	119.63	117.00
38	A1	2281	A2M	C4-C5-N7	-2.18	107.03	109.34
34	B5	1773	4AC	C1'-N1-C2	2.18	123.25	118.44
34	B5	796	A2M	O4'-C1'-N9	2.17	111.63	108.75
38	A1	2921	OMU	O2-C2-N1	-2.17	119.97	122.80
34	B5	1191	XSX	C1'-N1-C2	2.17	120.59	117.04
34	B5	578	OMU	O2-C2-N1	-2.15	120.00	122.80
34	B5	1773	4AC	O2-C2-N3	-2.15	118.95	122.33
38	A1	2281	A2M	C2'-C1'-N9	-2.14	107.80	112.56
34	B5	436	A2M	O4'-C1'-N9	2.14	111.58	108.75
38	A1	2421	OMU	O2-C2-N1	-2.14	120.02	122.80
38	A1	2815	OMG	C5-C6-N1	2.13	118.14	114.07
34	B5	1572	OMG	C5-C6-N1	2.11	118.09	114.07
38	A1	2729	OMU	C1'-N1-C2	2.10	121.37	117.59
34	B5	1126	OMG	C5-C6-N1	2.10	118.07	114.07
38	A1	2256	A2M	O4'-C1'-N9	-2.10	105.96	108.75
38	A1	2959	OMC	O2-C2-N3	-2.09	119.03	122.33
38	A1	805	OMG	C5-C6-N1	2.09	118.05	114.07
38	A1	2724	OMU	O2-C2-N1	-2.07	120.10	122.80
38	A1	2347	OMU	O2-C2-N3	-2.07	117.68	121.49
34	B5	1639	OMC	O2-C2-N3	-2.06	119.09	122.33
34	B5	1191	XSX	C6-N1-C2	-2.06	120.12	121.80
34	B5	1007	OMC	O2-C2-N3	-2.05	119.10	122.33
34	B5	1428	OMG	C5-C6-N1	2.05	117.98	114.07
38	A1	2619	OMG	C5-C6-N1	2.05	117.97	114.07
38	A1	2793	OMG	C5-C6-N1	2.05	117.97	114.07
38	A1	867	OMG	C5-C6-N1	2.05	117.97	114.07
38	A1	1450	OMG	C5-C6-N1	2.03	117.94	114.07
38	A1	2922	OMG	C5-C6-N1	2.02	117.92	114.07
38	A1	2288	OMG	C5-C6-N1	2.02	117.92	114.07
38	A1	2634	UR3	C3U-N3-C2	2.01	120.83	117.33
38	A1	908	OMG	C5-C6-N1	2.01	117.89	114.07

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B5	414	OMC	C1'-C2'-O2'-CM2
34	B5	420	A2M	C1'-C2'-O2'-CM'
34	B5	562	OMG	O4'-C4'-C5'-O5'
34	B5	796	A2M	C1'-C2'-O2'-CM'
34	B5	974	A2M	C1'-C2'-O2'-CM'
34	B5	1191	XSX	C3-C1-N3-C2
34	B5	1191	XSX	C3-C1-N3-C4
34	B5	1191	XSX	N3-C1-C3-C7
34	B5	1271	OMG	C1'-C2'-O2'-CM2
34	B5	1428	OMG	C1'-C2'-O2'-CM2
34	B5	1782	MA6	O4'-C4'-C5'-O5'
34	B5	1782	MA6	C3'-C4'-C5'-O5'
36	AB	243	HIC	CA-CB-CG-ND1
36	AB	243	HIC	CA-CB-CG-CD2
80	DC	699	DDE	CBI-CBW-NCB-CAB
80	DC	699	DDE	CBI-CBW-NCB-CAC
80	DC	699	DDE	CBI-CBW-NCB-CAA
80	DC	699	DDE	CAU-CBW-NCB-CAB
80	DC	699	DDE	CAU-CBW-NCB-CAC
80	DC	699	DDE	CAU-CBW-NCB-CAA
80	DC	699	DDE	CE1-CAT-CAU-CBW
34	B5	1280	4AC	N3-C4-N4-C7
34	B5	1280	4AC	C5-C4-N4-C7
34	B5	1280	4AC	O7-C7-N4-C4
34	B5	1280	4AC	CM7-C7-N4-C4
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	649	A2M	C1'-C2'-O2'-CM'
38	A1	663	OMC	C1'-C2'-O2'-CM2
38	A1	867	OMG	C1'-C2'-O2'-CM2
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	2220	A2M	C1'-C2'-O2'-CM'
38	A1	2256	A2M	C1'-C2'-O2'-CM'
38	A1	2417	OMU	C1'-C2'-O2'-CM2
38	A1	2421	OMU	C1'-C2'-O2'-CM2
38	A1	2619	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
38	A1	2724	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	562	OMG	C3'-C4'-C5'-O5'
34	B5	1773	4AC	O4'-C4'-C5'-O5'
38	A1	2729	OMU	C3'-C4'-C5'-O5'
34	B5	541	A2M	O4'-C4'-C5'-O5'
38	A1	1437	OMC	O4'-C4'-C5'-O5'
38	A1	2197	OMC	O4'-C4'-C5'-O5'
38	A1	2280	A2M	O4'-C4'-C5'-O5'
38	A1	2280	A2M	C3'-C4'-C5'-O5'
38	A1	2729	OMU	O4'-C4'-C5'-O5'
34	B5	541	A2M	C3'-C4'-C5'-O5'
34	B5	578	OMU	O4'-C4'-C5'-O5'
34	B5	619	A2M	O4'-C4'-C5'-O5'
34	B5	1773	4AC	C3'-C4'-C5'-O5'
38	A1	1437	OMC	C3'-C4'-C5'-O5'
38	A1	2197	OMC	C3'-C4'-C5'-O5'
34	B5	1782	MA6	N1-C6-N6-C9
34	B5	1191	XSX	N4-C7-C9-O10
34	B5	619	A2M	C3'-C4'-C5'-O5'
38	A1	817	A2M	C4'-C5'-O5'-P
38	A1	2256	A2M	C4'-C5'-O5'-P
38	A1	2870	5MC	C2'-C1'-N1-C6
38	A1	2281	A2M	O4'-C4'-C5'-O5'
34	B5	1191	XSX	N4-C7-C9-O11
34	B5	1639	OMC	O4'-C4'-C5'-O5'
38	A1	2870	5MC	O4'-C1'-N1-C6
34	B5	1781	MA6	C5-C6-N6-C10
34	B5	541	A2M	C4'-C5'-O5'-P
38	A1	2197	OMC	O4'-C1'-N1-C6
38	A1	2281	A2M	C3'-C4'-C5'-O5'
34	B5	1269	OMU	C3'-C2'-O2'-CM2
80	DC	699	DDE	CAT-CAU-CBW-CBI
38	A1	2870	5MC	O4'-C1'-N1-C2
34	B5	28	A2M	C1'-C2'-O2'-CM'
38	A1	2640	A2M	C1'-C2'-O2'-CM'
38	A1	1450	OMG	C4'-C5'-O5'-P
34	B5	578	OMU	C3'-C4'-C5'-O5'
34	B5	1428	OMG	O4'-C4'-C5'-O5'
34	B5	1428	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
34	B5	578	OMU	C2'-C1'-N1-C6
38	A1	2870	5MC	C2'-C1'-N1-C2
38	A1	649	A2M	C4'-C5'-O5'-P
38	A1	2729	OMU	C4'-C5'-O5'-P
34	B5	578	OMU	O4'-C1'-N1-C6
38	A1	2197	OMC	O4'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 244 ligands modelled in this entry, 242 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	25,30,30	0.96	1 (4%)	30,47,47	1.16	3 (10%)
86	SO1	DC	903	-	34,39,39	0.68	1 (2%)	38,64,64	1.11	5 (13%)

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	-	0/12/32/32	0/3/3/3
86	SO1	DC	903	-	1/1/15/16	7/21/104/104	0/7/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	DC	903	SO1	O14-C5	-2.93	1.19	1.30
85	DC	901	GDP	C6-N1	-2.08	1.34	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	DC	903	SO1	C12-C6-C2	-3.70	99.36	105.09
85	DC	901	GDP	C8-N7-C5	2.91	107.51	102.55
86	DC	903	SO1	C1-C4-C13	-2.88	115.28	118.36
86	DC	903	SO1	C7-C2-C6	2.35	116.55	112.05
85	DC	901	GDP	C5-C6-N1	2.24	118.34	114.07
86	DC	903	SO1	C18-C9-C16	-2.08	100.87	103.72
86	DC	903	SO1	C24-C18-C9	-2.06	101.11	105.14
85	DC	901	GDP	O6-C6-C5	-2.06	120.23	124.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
86	DC	903	SO1	C4

All (7) torsion outliers are listed below:

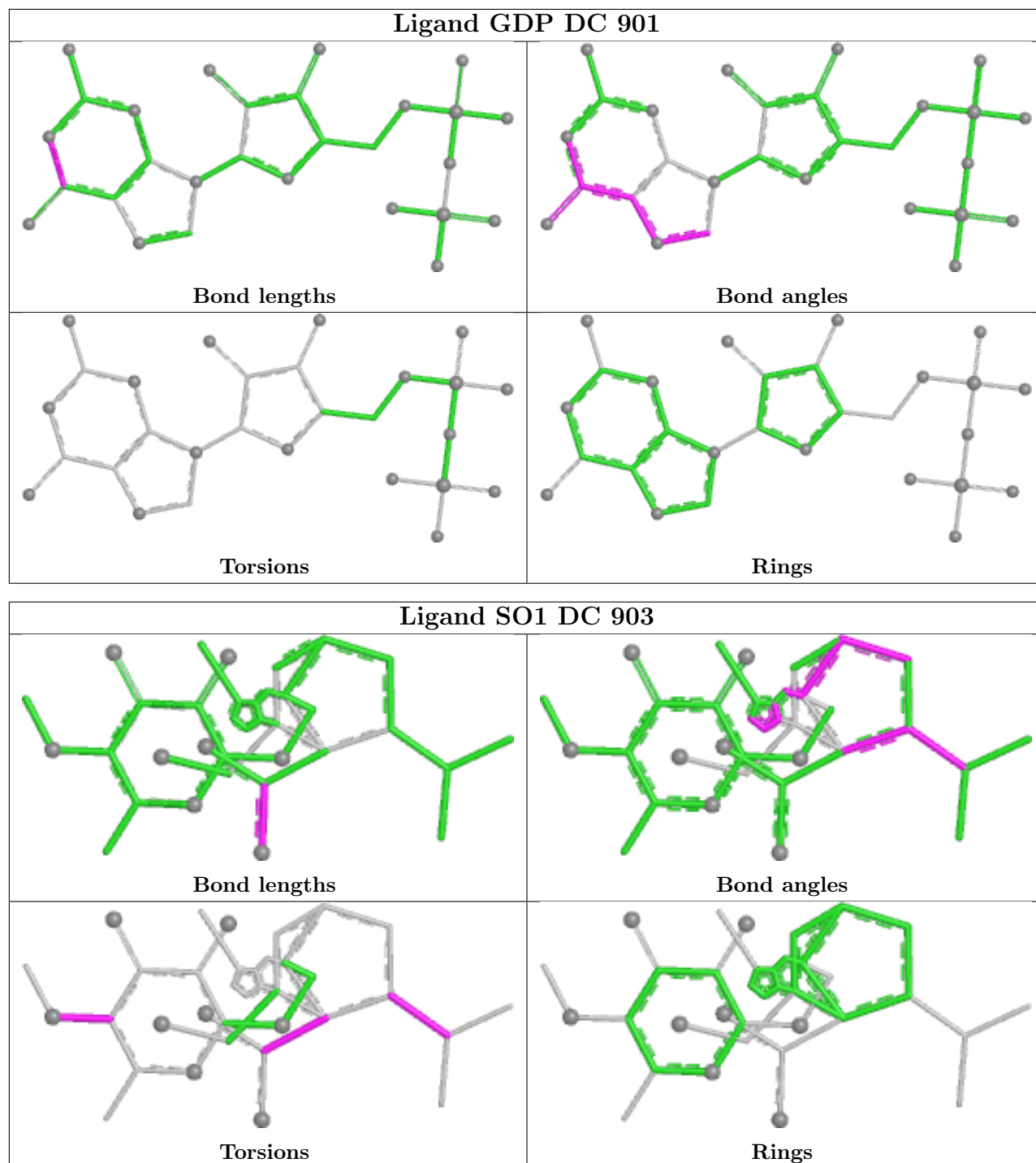
Mol	Chain	Res	Type	Atoms
86	DC	903	SO1	C2-C1-C5-O14
86	DC	903	SO1	C2-C1-C5-O15
86	DC	903	SO1	C21-C13-C4-C12
86	DC	903	SO1	C20-C13-C4-C12
86	DC	903	SO1	C54-C55-O64-C65
86	DC	903	SO1	C21-C13-C4-C1
86	DC	903	SO1	C20-C13-C4-C1

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 [i](#)

There are no chain breaks in this entry.

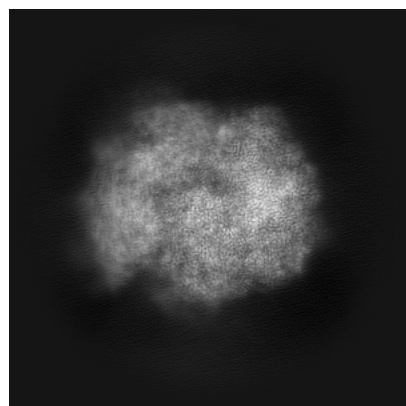
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28633. These allow visual inspection of the internal detail of the map and identification of artifacts.

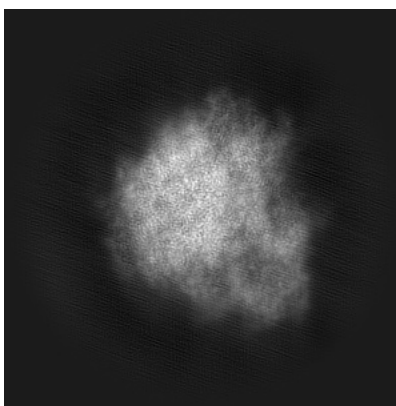
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

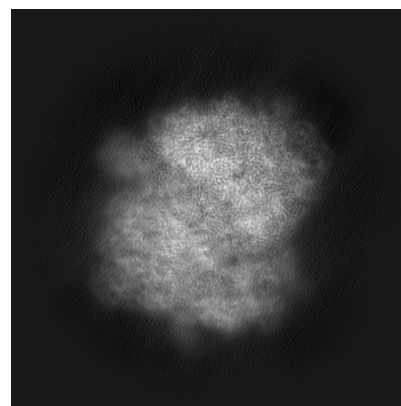
6.1.1 Primary map



X

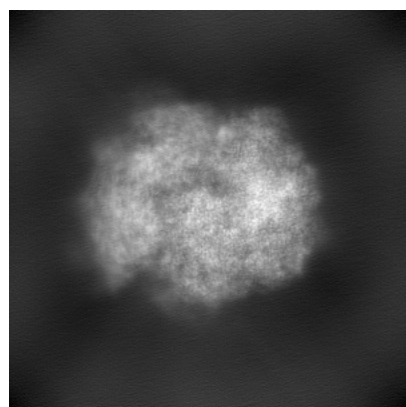


Y

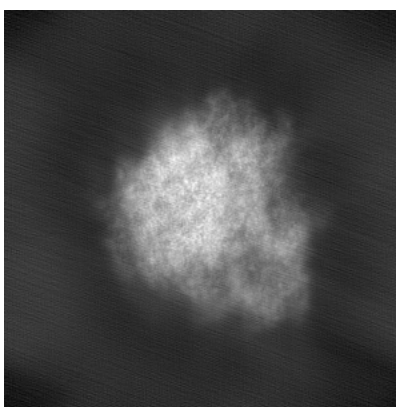


Z

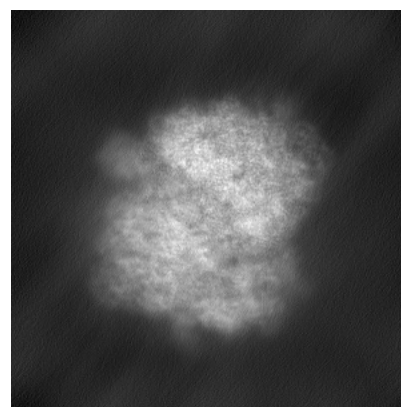
6.1.2 Raw map



X



Y

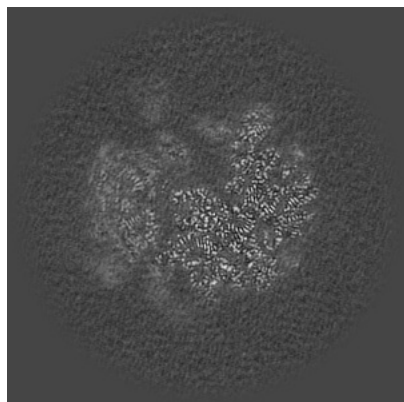


Z

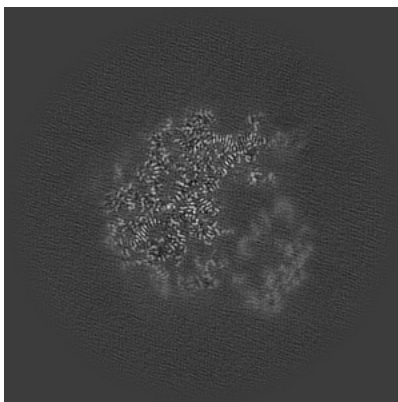
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

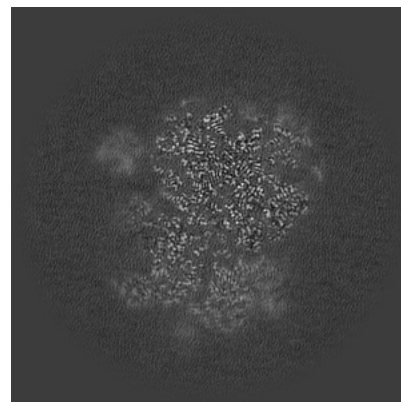
6.2.1 Primary map



X Index: 200

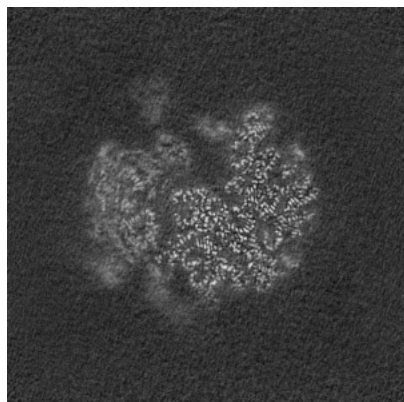


Y Index: 200

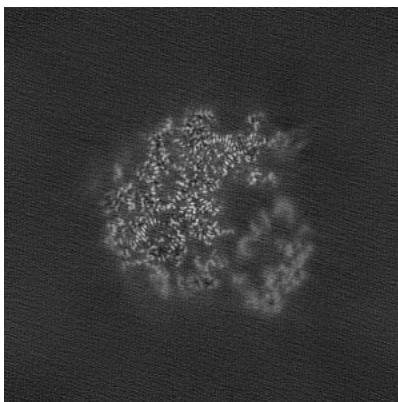


Z Index: 200

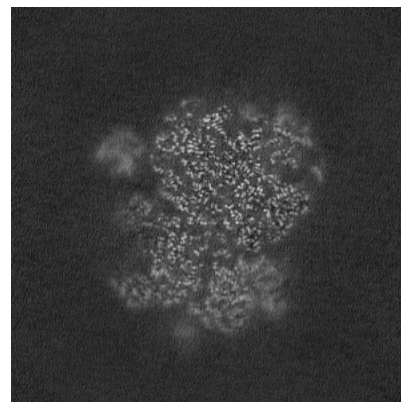
6.2.2 Raw map



X Index: 200



Y Index: 200

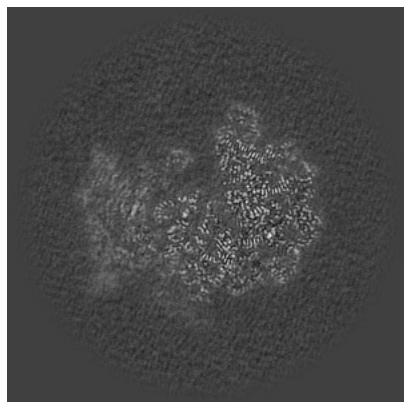


Z Index: 200

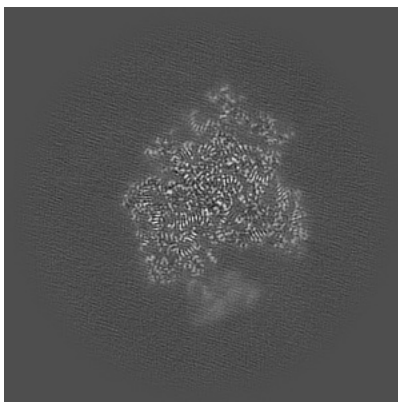
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

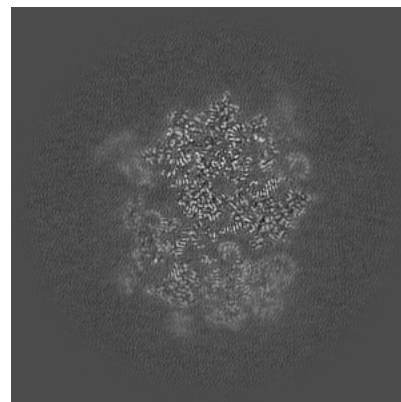
6.3.1 Primary map



X Index: 214

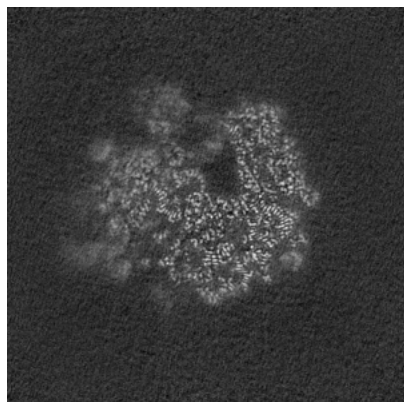


Y Index: 247

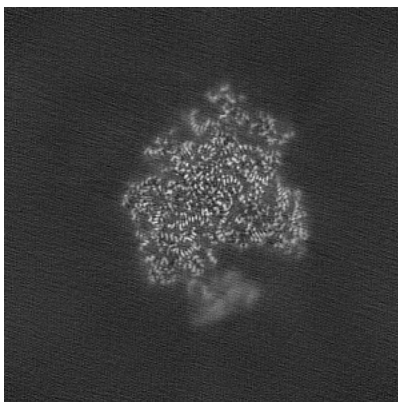


Z Index: 189

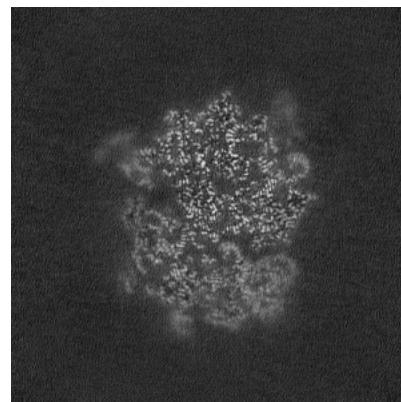
6.3.2 Raw map



X Index: 184



Y Index: 247

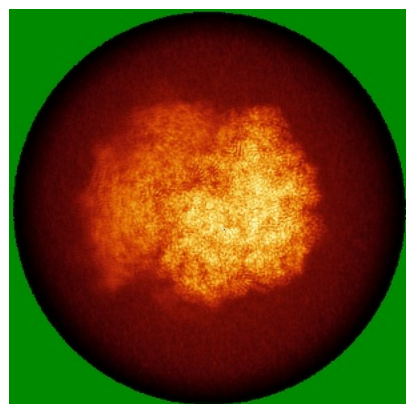


Z Index: 188

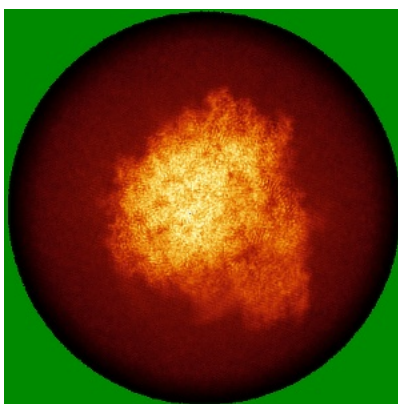
The images above show the largest variance slices of the map in three orthogonal directions.

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

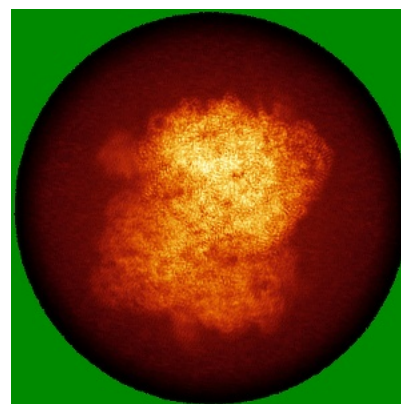
6.4.1 Primary map



X

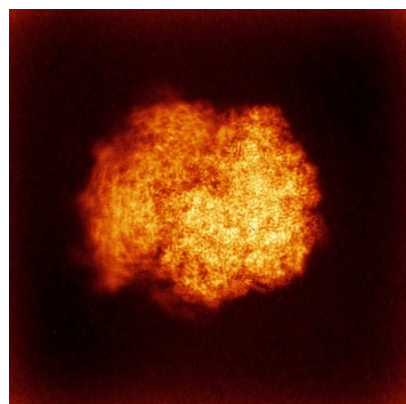


Y

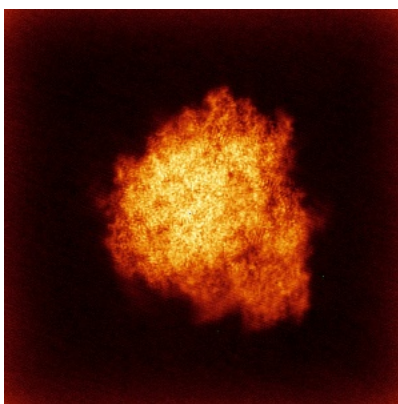


Z

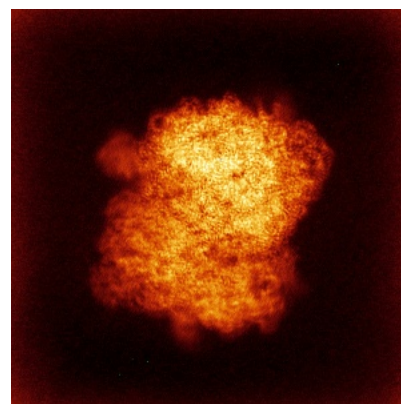
6.4.2 Raw map



X



Y

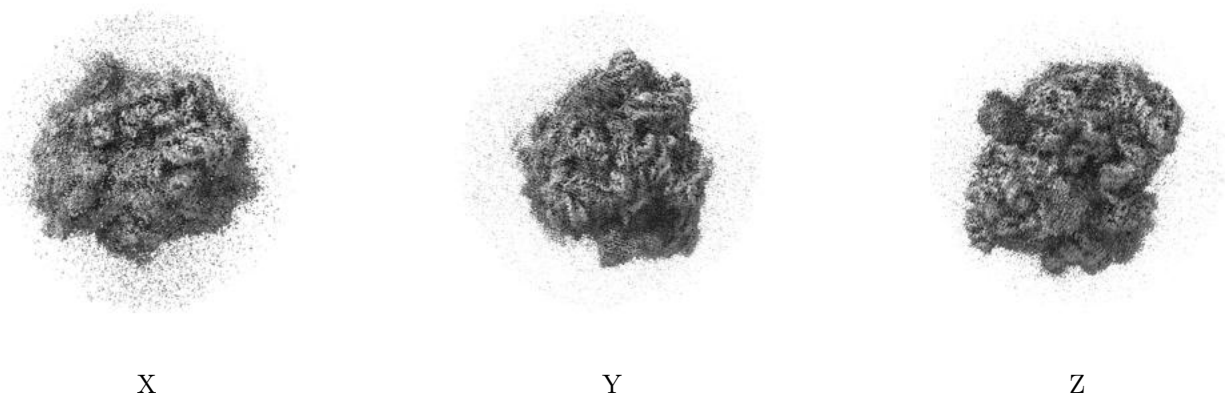


Z

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

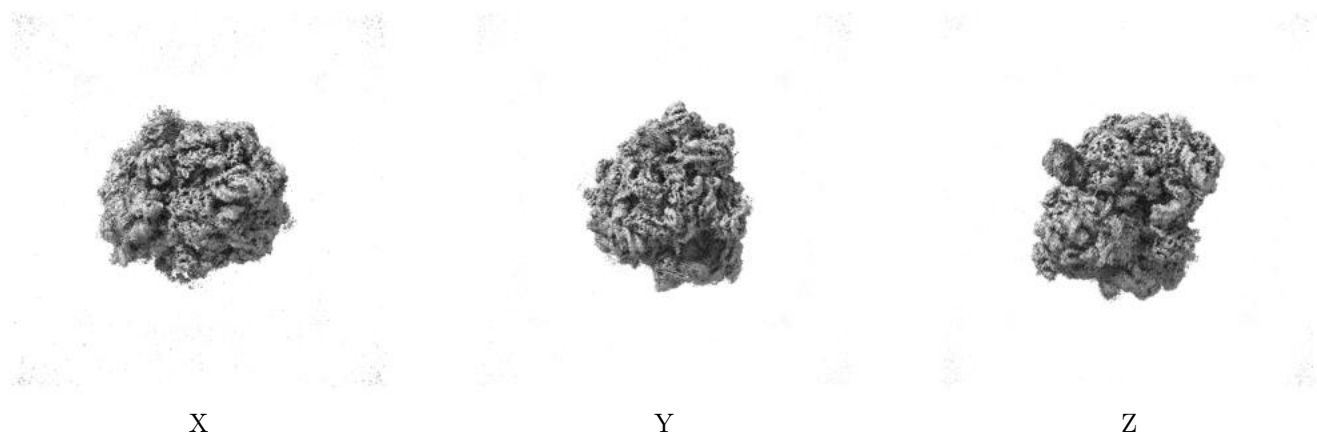
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

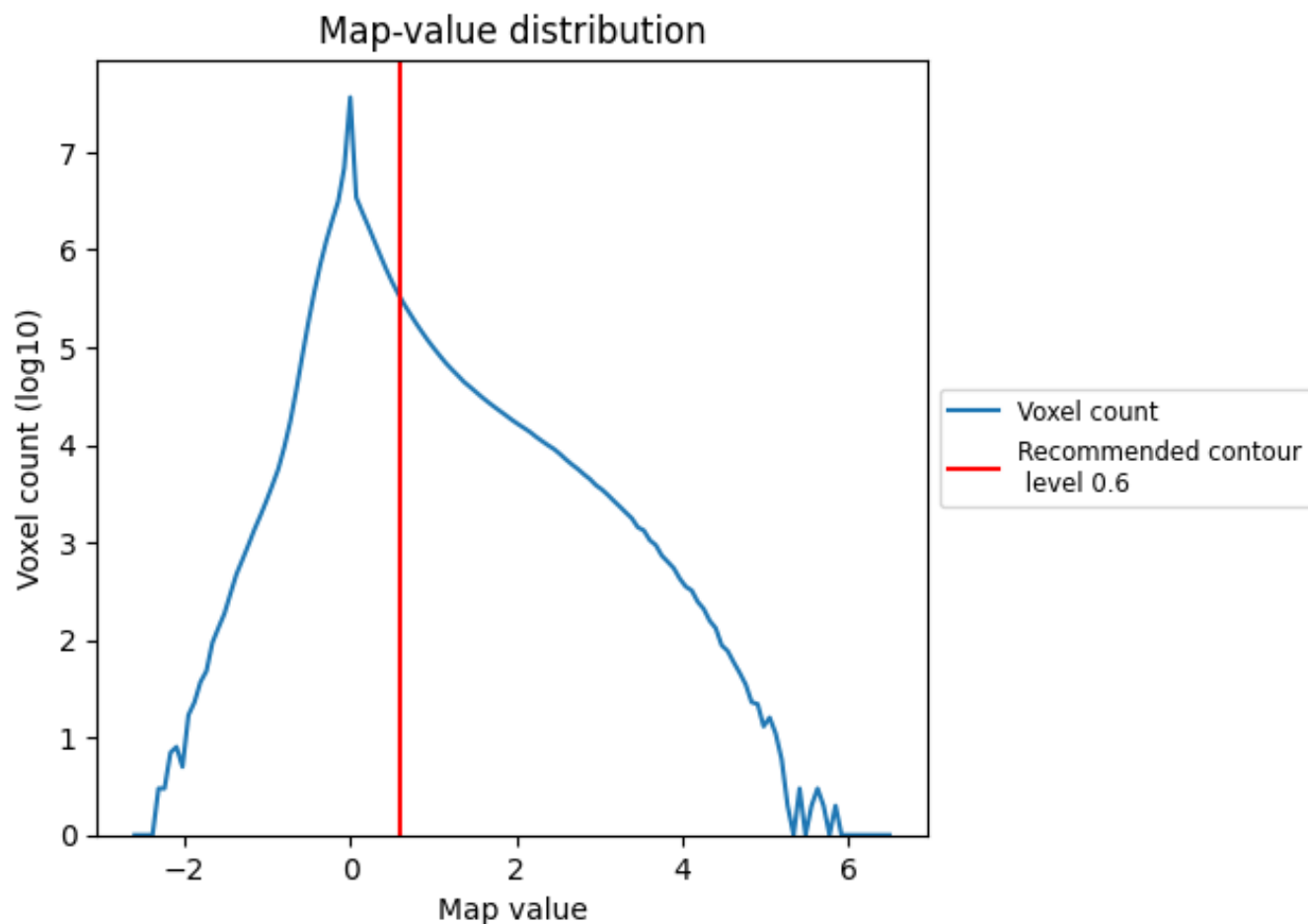
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

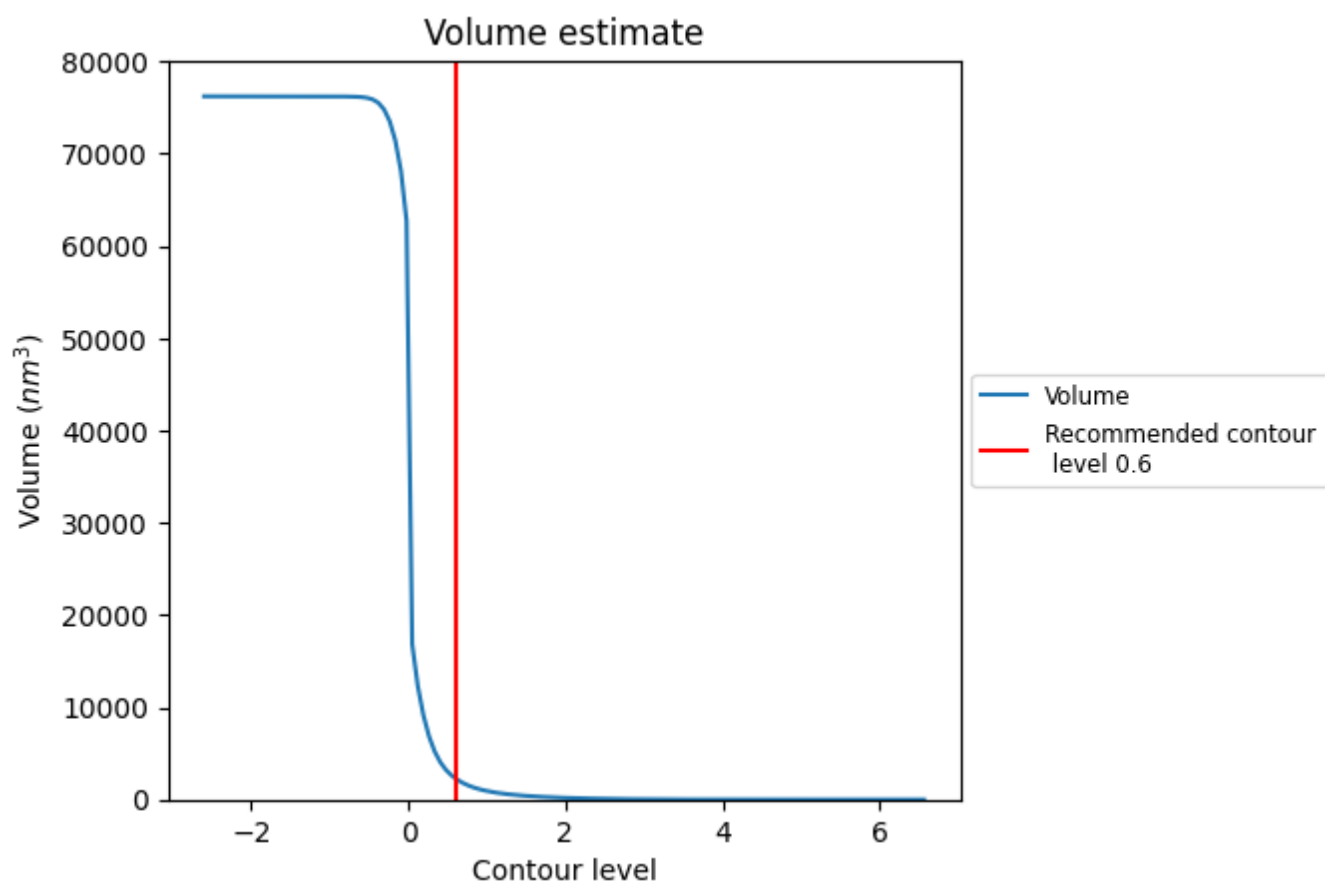
This section contains the results of statistical analysis of the map.

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.

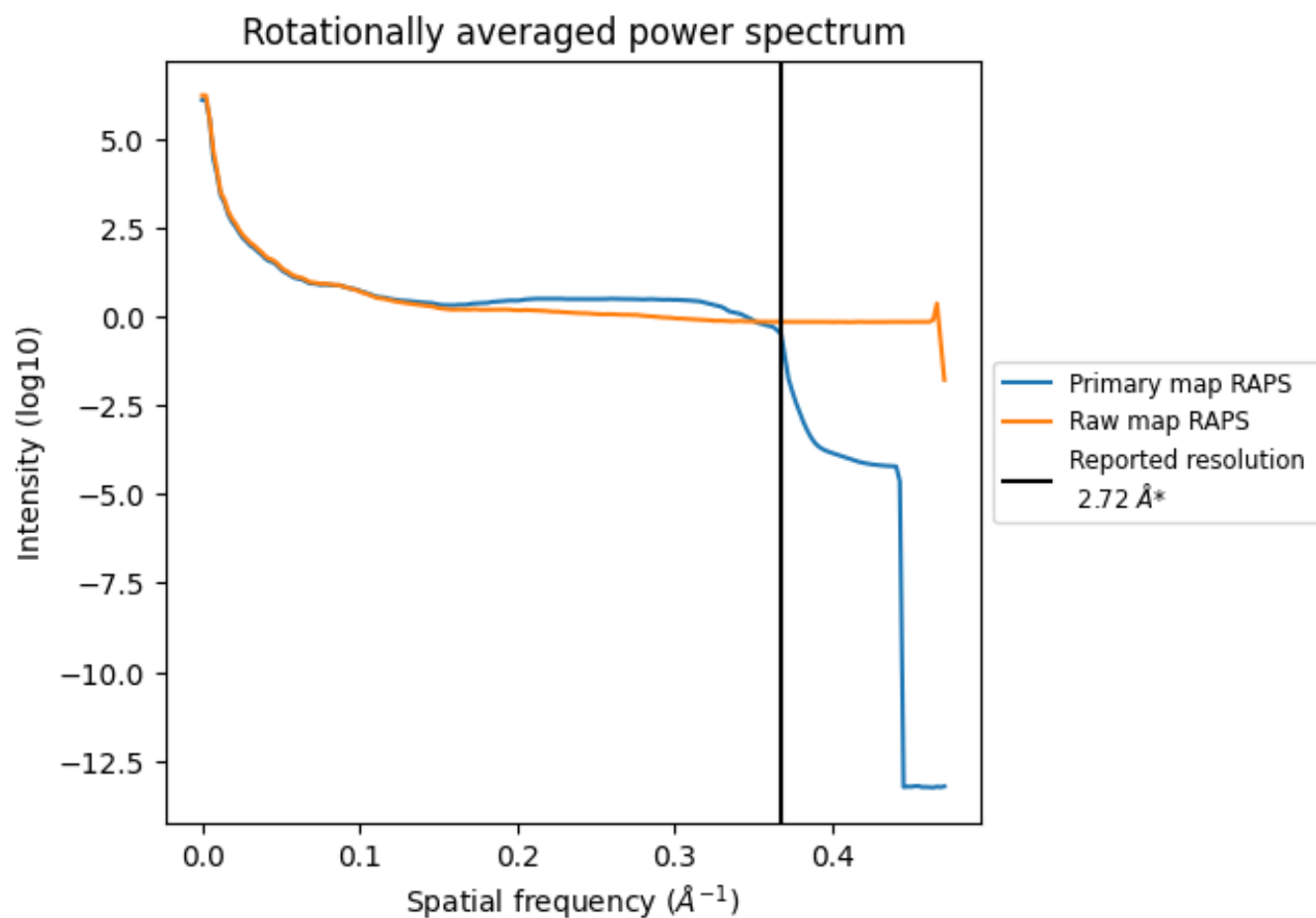
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2308 nm³; this corresponds to an approximate mass of 2085 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

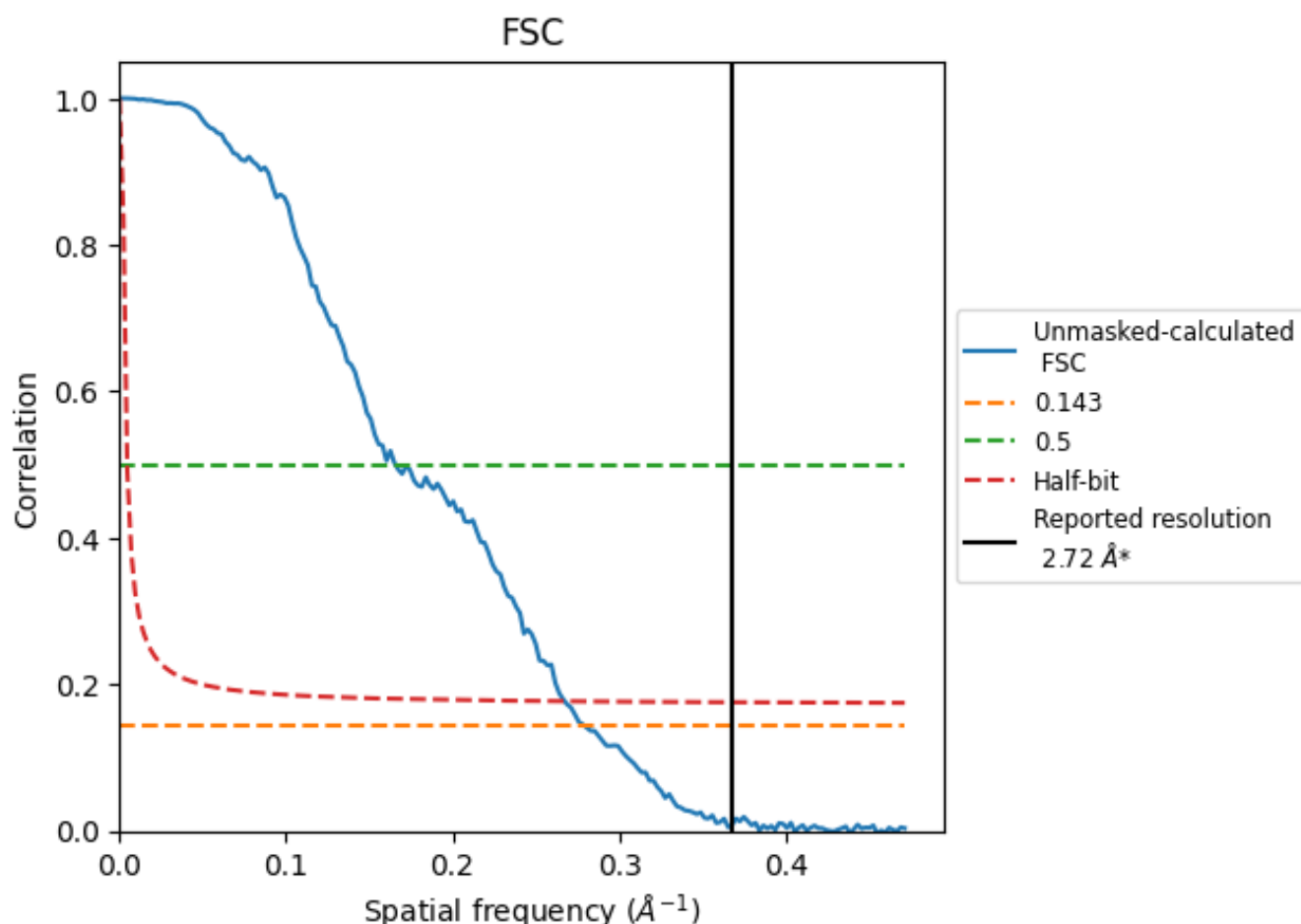


*Reported resolution corresponds to spatial frequency of 0.368 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8.2 Resolution estimates [i](#)

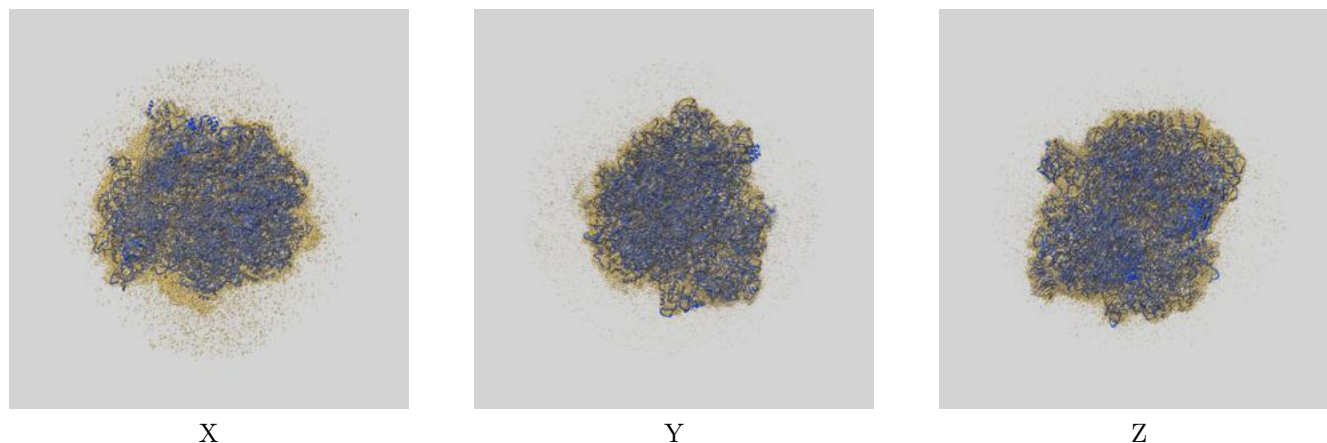
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	6.04	3.74

*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 3.58 differs from the reported value 2.72 by more than 10 %

9 Map-model fit [i](#)

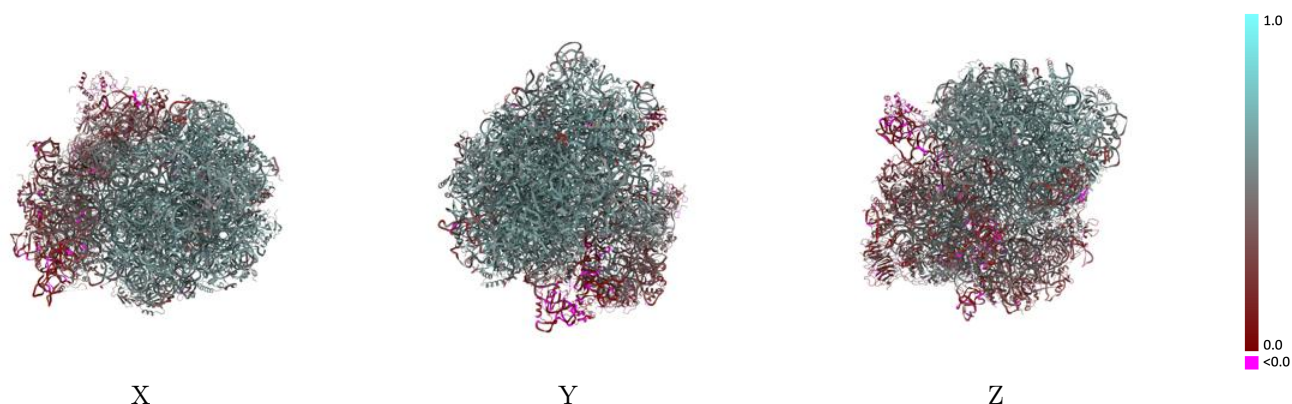
This section contains information regarding the fit between EMDB map EMD-28633 and PDB model 8EVQ. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



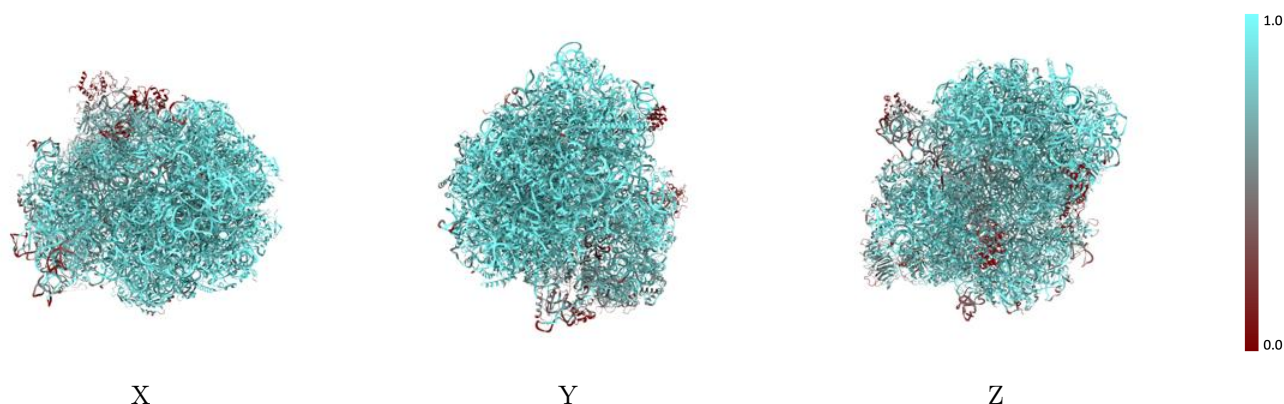
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



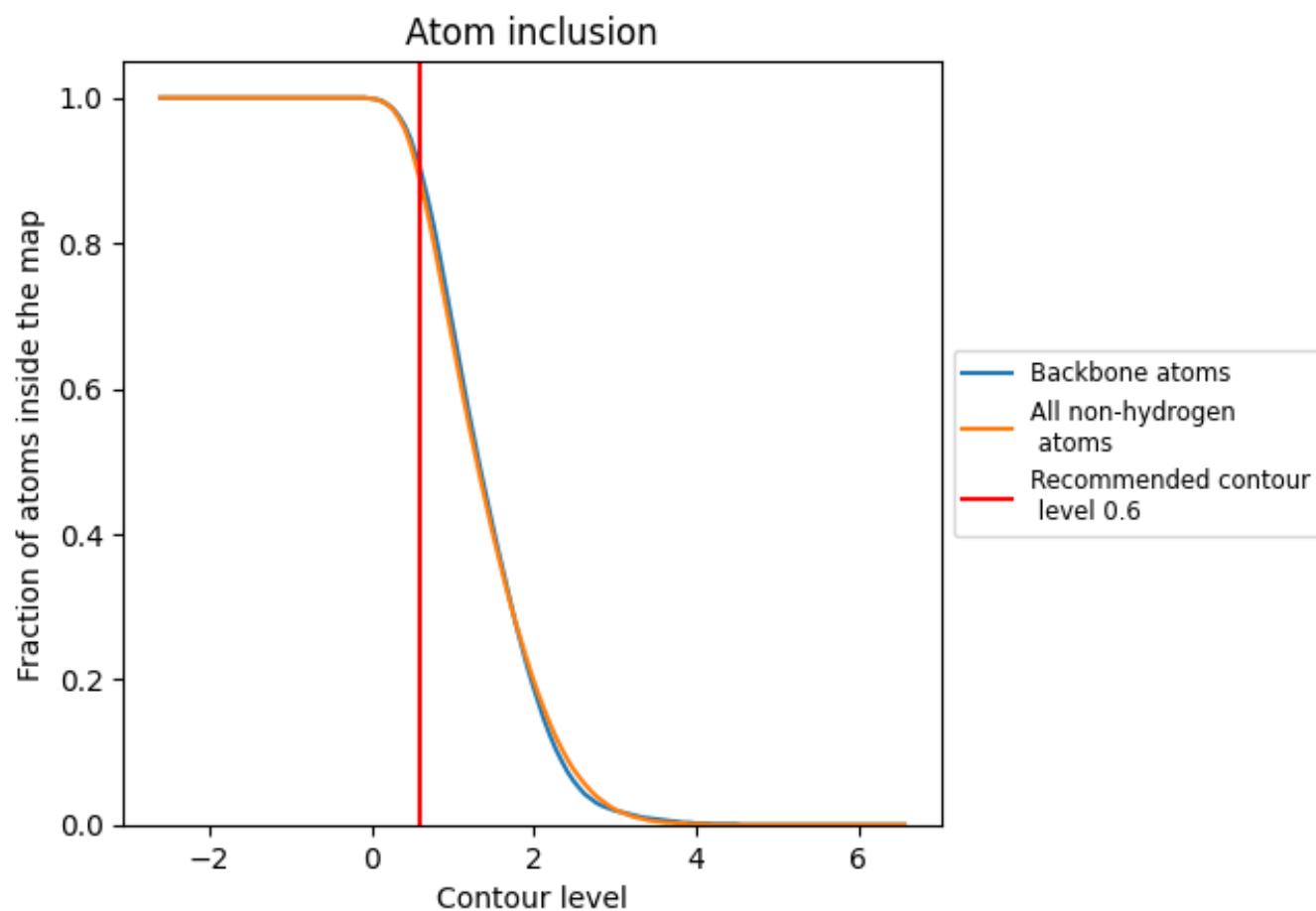
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



At the recommended contour level, 90% of all backbone atoms, 89% 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	 0.8860	 0.4870
A1	 0.9680	 0.5710
A3	 0.9920	 0.5790
A4	 0.9820	 0.5940
AA	 0.9740	 0.6210
AB	 0.9630	 0.5830
AC	 0.9640	 0.5870
AD	 0.9080	 0.5130
AE	 0.9380	 0.5380
AF	 0.9710	 0.5980
AG	 0.9170	 0.5510
AH	 0.9420	 0.5730
AI	 0.9640	 0.5820
AJ	 0.8110	 0.4340
AL	 0.9510	 0.5900
AM	 0.9490	 0.5750
AN	 0.9870	 0.6270
AO	 0.9670	 0.5930
AP	 0.9620	 0.5760
AQ	 0.9800	 0.6170
AR	 0.8500	 0.5090
AS	 0.9670	 0.5940
AT	 0.9570	 0.5780
AU	 0.8810	 0.4590
AV	 0.9510	 0.5870
AW	 0.9600	 0.5770
AX	 0.9410	 0.5650
AY	 0.9480	 0.5580
AZ	 0.9220	 0.5440
Aa	 0.9710	 0.6070
Ab	 0.9290	 0.5620
Ac	 0.8880	 0.5490
Ad	 0.9110	 0.5380
Ae	 0.9730	 0.6010
Af	 0.9840	 0.6100















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Chain	Atom inclusion	Q-score
Ag	 0.9250	 0.5740
Ah	 0.9500	 0.5620
Ai	 0.9520	 0.5550
Aj	 0.9860	 0.6150
Ak	 0.7400	 0.4660
Al	 0.9830	 0.5870
Am	 0.9280	 0.5810
An	 0.9530	 0.5560
Ao	 0.9060	 0.5770
Ap	 0.9360	 0.5900
B5	 0.8860	 0.4100
BA	 0.8120	 0.4410
BB	 0.7830	 0.4340
BC	 0.9050	 0.4790
BD	 0.7890	 0.3580
BE	 0.8460	 0.3580
BF	 0.7130	 0.3390
BG	 0.7650	 0.2800
BH	 0.6710	 0.3800
BI	 0.8450	 0.4230
BJ	 0.8310	 0.3500
BK	 0.6600	 0.2670
BL	 0.8150	 0.4430
BM	 0.0840	 0.1490
BN	 0.8610	 0.4860
BO	 0.8430	 0.4800
BP	 0.6570	 0.3210
BQ	 0.8180	 0.3840
BR	 0.5970	 0.2900
BS	 0.7450	 0.3280
BT	 0.7530	 0.3120
BU	 0.6860	 0.3050
BV	 0.8780	 0.4620
BW	 0.9420	 0.5280
BX	 0.8880	 0.4500
BY	 0.7920	 0.3020
BZ	 0.6880	 0.2880
Ba	 0.8740	 0.5090
Bb	 0.7440	 0.4510
Bc	 0.7210	 0.3900
Bd	 0.9170	 0.4040
Be	 0.7360	 0.3000

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Chain	Atom inclusion	Q-score
Bf	 0.1570	 0.1440
Bg	 0.6200	 0.2510
DC	 0.7890	 0.3990
E	 0.3980	 0.1190
EC	 0.5930	 0.1910
V	 0.1270	 0.2200