



Full wwPDB EM Validation Report ⓘ

Dec 30, 2024 – 12:40 PM EST

PDB ID : 8CEH
EMDB ID : EMD-16609
Title : Translocation intermediate 4 (TI-4) of 80S *S. cerevisiae* ribosome with ligands and eEF2 in the presence of sordarin
Authors : Milicevic, N.; Jenner, L.; Myasnikov, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2023-02-01
Resolution : 2.05 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:

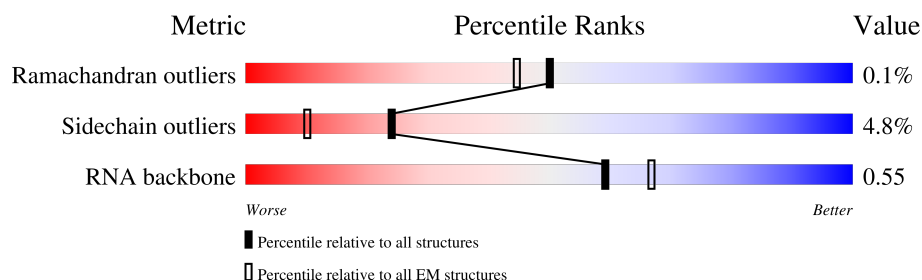
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, 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 2.05 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.




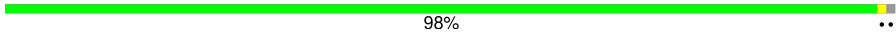

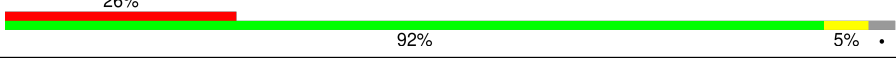

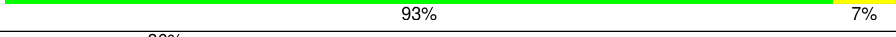

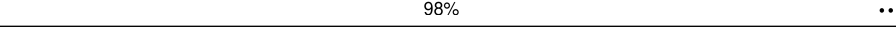
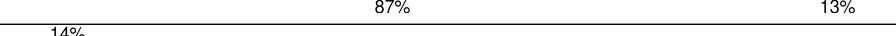

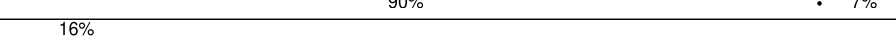
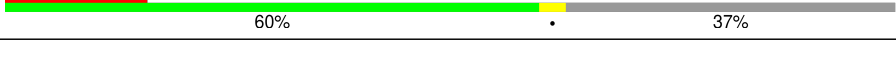

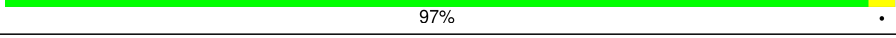
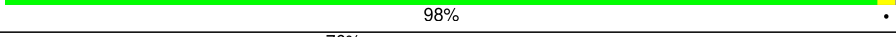
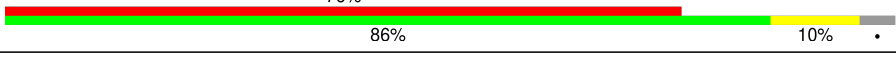
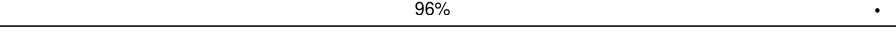
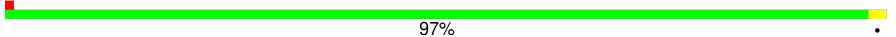

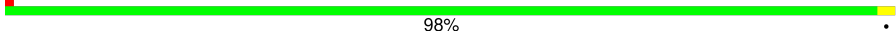

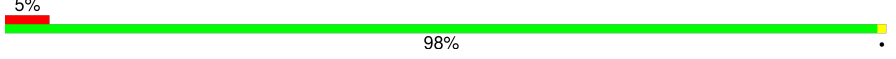



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	0	135	<div> <div>11%</div> <div>93%</div> <div>6%</div> </div>
2	1	108	<div> <div>63%</div> <div>57%</div> <div>7%</div> <div>35%</div> </div>
3	2	119	<div> <div>76%</div> <div>5%</div> <div>18%</div> </div>
4	3	82	<div> <div>10%</div> <div>98%</div> </div>
5	4	67	<div> <div>37%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
6	5	56	<div> <div>80%</div> <div>7%</div> <div>12%</div> </div>
7	6	63	<div> <div>10%</div> <div>73%</div> <div>11%</div> <div>16%</div> </div>
8	7	319	<div> <div>56%</div> <div>93%</div> <div>7%</div> </div>


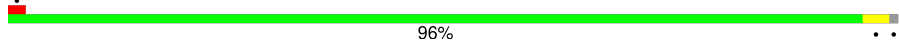
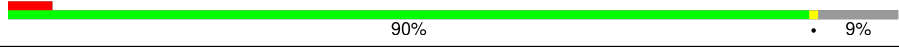
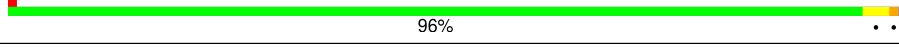
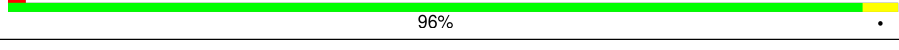
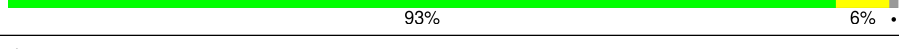
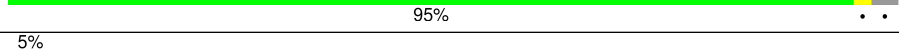
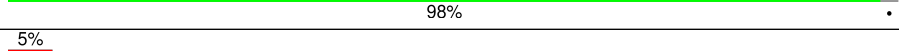
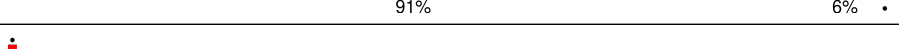
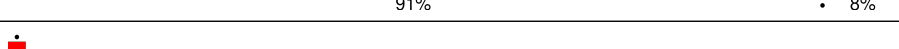
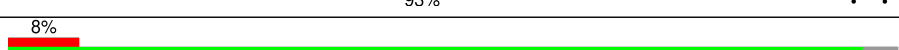
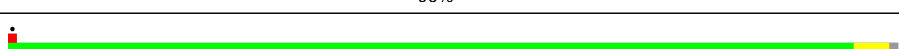
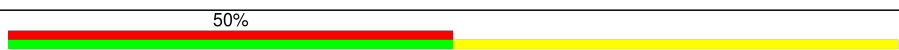
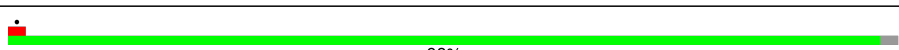
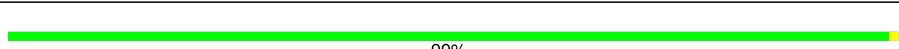
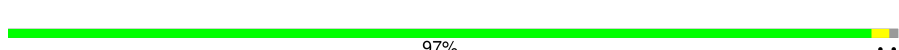

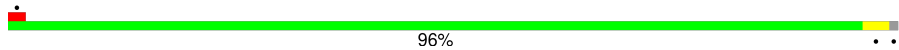
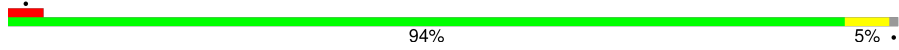
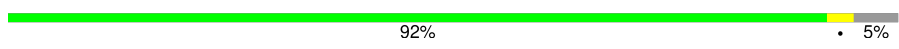
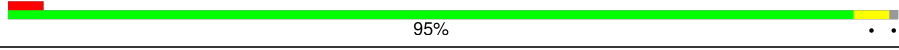
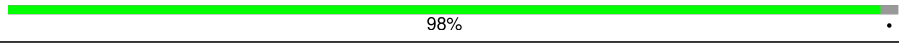



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Mol	Chain	Length	Quality of chain
9	8	152	
10	A	199	
11	AA	3396	
12	Aa	842	
13	B	184	
14	BB	121	
15	Bb	76	
16	C	186	
17	CC	158	
18	Cc	77	
19	D	189	
20	DD	312	
21	Dd	39	
22	E	172	
23	EE	254	
24	Ee	165	
25	F	160	
26	FF	387	
27	G	121	
28	GG	362	
29	H	137	
30	HH	297	
31	I	155	
32	II	176	
33	J	142	

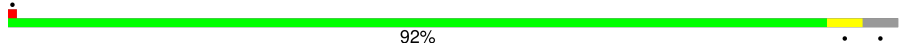
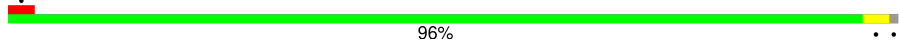




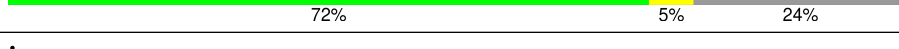
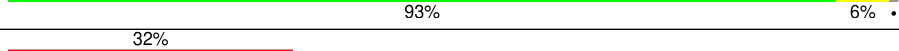
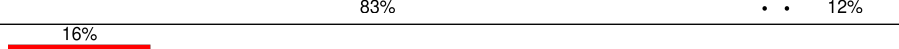
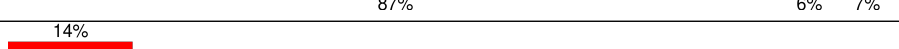
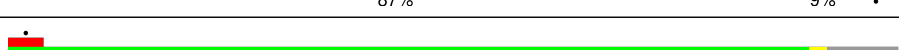



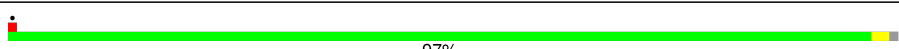




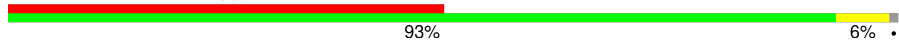
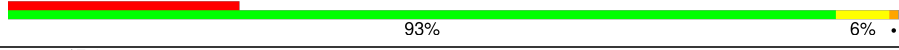
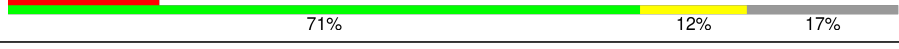
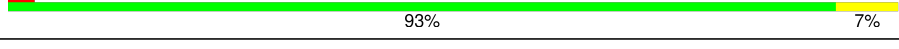
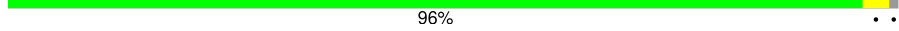

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Mol	Chain	Length	Quality of chain
34	JJ	244	
35	K	127	
36	KK	256	
37	L	136	
38	LL	191	
39	M	149	
40	MM	221	
41	N	59	
42	NN	174	
43	O	105	
44	OO	199	
45	P	113	
46	PP	138	
47	Pp	2	
48	Q	130	
49	QQ	204	
50	R	107	
51	S	121	
52	T	120	
53	U	100	
54	V	88	
55	W	78	
56	X	51	
57	Y	128	
58	Z	25	

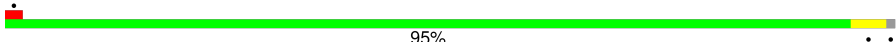
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Mol	Chain	Length	Quality of chain
59	a	106	
60	b	92	
61	c	1800	
62	d	252	
63	e	255	
64	f	254	
65	g	240	
66	h	261	
67	i	225	
68	j	236	
69	k	190	
70	l	200	
71	m	197	
72	n	105	
73	o	156	
74	p	151	
75	q	137	
76	r	142	
77	s	143	
78	t	136	
79	u	146	
80	v	144	
81	w	121	
82	x	87	
83	y	130	

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Mol	Chain	Length	Quality of chain
84	z	145	 95%

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 207126 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 S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 2 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 3 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 4 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 5 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 6 is a protein called HLJ1_G0030400.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	49	Total	C	N	O	S	0	0
			404	249	86	65	4		

- Molecule 7 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	53	Total	C	N	O	S	0	0
			427	269	88	69	1		

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	318	Total	C	N	O	S	0	0
			2436	1541	418	469	8		

- Molecule 9 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	36	Total	C	N	O	S	0	0
			276	173	54	45	4		

- Molecule 10 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 11 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	3197	Total	C	N	O	P	0	0
			68429	30589	12334	22309	3197		

- Molecule 12 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Aa	816	Total	C	N	O	S	0	0
			6368	4051	1088	1198	31		

- Molecule 13 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	B	154	Total	C	N	O	0	0
			1222	761	237	224		

- Molecule 14 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 15 is a RNA chain called Transfer RNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Bb	76	Total	C	N	O	P	0	0
			1638	736	294	533	75		

- Molecule 16 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 17 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 18 is a RNA chain called Transfer RNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Cc	77	Total	C	N	O	P	0	0
			1644	732	298	537	77		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cc	18	C	U	conflict	GB 170517292

- Molecule 19 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	D	176	Total	C	N	O	0	0
			1423	875	308	240		

- Molecule 20 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DD	197	Total	C	N	O	S	0	0
			1531	980	266	281	4		

- Molecule 21 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Dd	6	Total	C	N	O	P	0	0
			125	56	18	45	6		

- Molecule 22 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	EE	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 24 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ee	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 25 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	FF	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 27 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	G	97	Total	C	N	O		
			770	499	126	145	0	0

- Molecule 28 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H	129	Total	C	N	O	S		
			963	607	180	169	7	0	0

- Molecule 30 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	HH	296	Total	C	N	O	S		
			2375	1501	414	458	2	0	0

- Molecule 31 is a protein called 60S ribosomal protein L24-A.

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

- Molecule 32 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	II	155	Total	C	N	O	S		
			1230	795	221	213	1	0	0

- Molecule 33 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	120	Total	C	N	O	S		
			959	617	168	172	2	0	0

- Molecule 34 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	126	Total	C	N	O	S	0	0
			993	625	192	176			

- Molecule 36 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	KK	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 37 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L	135	Total	C	N	O	S	0	0
			1092	710	202	180			

- Molecule 38 is a protein called RPL9A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LL	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 39 is a protein called 60S ribosomal protein L28.

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

- Molecule 40 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	MM	215	Total	C	N	O	S	0	0
			1743	1102	331	303	7		

- Molecule 41 is a protein called 60S ribosomal protein L29.

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

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

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

- Molecule 43 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	O	97	Total	C	N	O	S	0	0
			742	479	124	138	1		

- Molecule 44 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 45 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	P	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 46 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 47 is a protein called Polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Pp	2	Total	C	N	O	S	0	0
			19	14	2	2	1		

- Molecule 48 is a protein called 60S ribosomal protein L32.

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

- Molecule 49 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 50 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 51 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 52 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 53 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 54 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	V	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 55 is a protein called 60S ribosomal protein L38.

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

- Molecule 56 is a protein called 60S ribosomal protein L39.

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

- Molecule 57 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 58 is a protein called 60S ribosomal protein L41.

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

- Molecule 59 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	a	102	Total	C	N	O	S	0	0
			819	514	166	134	5		

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

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

- Molecule 61 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	c	1608	Total	C	N	O	P	0	0
			34321	15360	6093	11260	1608		

- Molecule 62 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	d	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 63 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	e	212	Total	C	N	O	S	0	0
			1689	1073	303	309	4		

- Molecule 64 is a protein called 40S ribosomal protein S2.

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

- Molecule 65 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	g	183	Total	C	N	O	S	0	0
			1412	893	260	253	6		

- Molecule 66 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	h	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 67 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	i	199	Total	C	N	O	S	0	0
			1572	987	290	292	3		

- Molecule 68 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	j	219	Total	C	N	O	S	0	0
			1766	1108	341	314	3		

- Molecule 69 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	k	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 70 is a protein called 40S ribosomal protein S8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	l	184	Total	C	N	O	S	0	0
			1457	906	291	258	2		

- Molecule 71 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	n	33	Total	C	N	O	0	0
			300	199	46	55		

- Molecule 73 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	o	142	Total	C	N	O	S	0	0
			1146	735	217	191	3		

- Molecule 74 is a protein called 40S ribosomal protein S13.

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

- Molecule 75 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	q	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 76 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	r	91	Total	C	N	O	S	0	0
			732	469	138	120	5		

- Molecule 77 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	s	137	Total	C	N	O	S	0	0
			1080	692	199	189			

- Molecule 78 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	t	121	Total	C	N	O	S	0	0
			961	599	182	178	2		

- Molecule 79 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 80 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	v	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 81 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	w	100	Total	C	N	O	S	0	0
			800	509	144	146	1		

- Molecule 82 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 83 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 84 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	2	1	Total	Zn	0
			1	1	
85	5	1	Total	Zn	0
			1	1	
85	8	1	Total	Zn	0
			1	1	
85	S	1	Total	Zn	0
			1	1	
85	V	1	Total	Zn	0
			1	1	
85	Y	1	Total	Zn	0
			1	1	
85	a	1	Total	Zn	0
			1	1	
85	b	1	Total	Zn	0
			1	1	

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	AA	198	Total	Mg	0
			198	198	
86	Aa	1	Total	Mg	0
			1	1	
86	B	1	Total	Mg	0
			1	1	
86	BB	5	Total	Mg	0
			5	5	
86	Bb	1	Total	Mg	0
			1	1	

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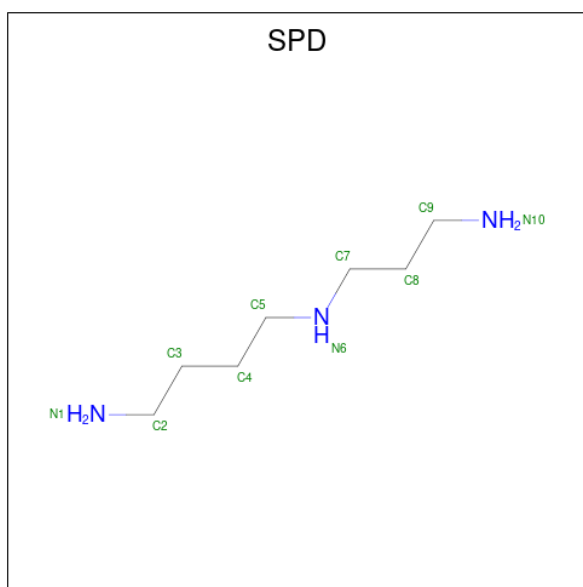
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Mol	Chain	Residues	Atoms		AltConf
86	CC	3	Total 3	Mg 3	0
86	Dd	1	Total 1	Mg 1	0
86	FF	1	Total 1	Mg 1	0
86	H	1	Total 1	Mg 1	0
86	QQ	1	Total 1	Mg 1	0
86	c	49	Total 49	Mg 49	0

- Molecule 87 is POTASSIUM ION (three-letter code: K) (formula: K).

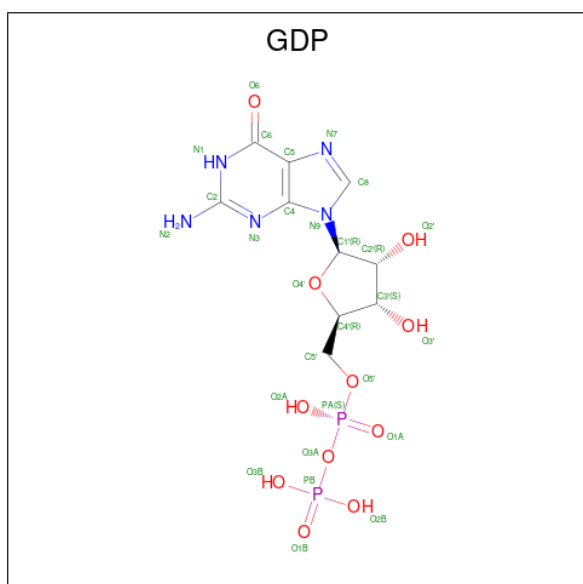
Mol	Chain	Residues	Atoms		AltConf
87	AA	14	Total 14	K 14	0
87	EE	1	Total 1	K 1	0
87	MM	1	Total 1	K 1	0
87	Q	1	Total 1	K 1	0
87	a	1	Total 1	K 1	0
87	c	2	Total 2	K 2	0
87	q	1	Total 1	K 1	0

- Molecule 88 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



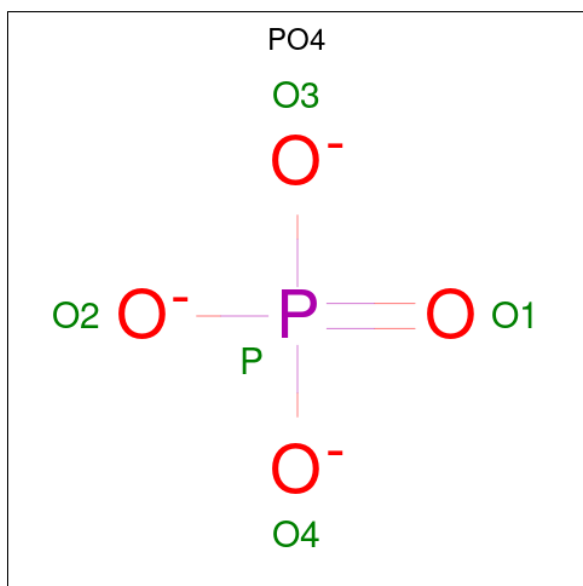
Mol	Chain	Residues	Atoms			AltConf
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	

- Molecule 89 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



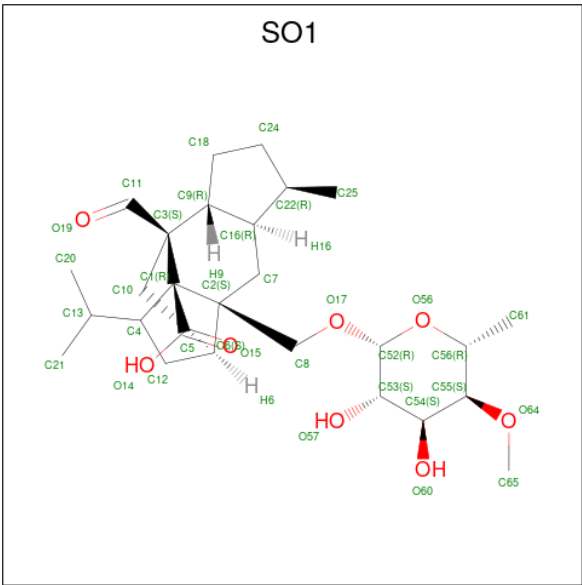
Mol	Chain	Residues	Atoms					AltConf
89	Aa	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 90 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
90	Aa	1	Total	O	P	0
			5	4	1	

- Molecule 91 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.B.ETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula: C₂₇H₄₂O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
91	Aa	1	Total	C	O	0
			35	27	8	

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	2	1	Total	O	0
			1	1	
92	A	2	Total	O	0
			2	2	
92	AA	778	Total	O	0
			778	778	
92	B	3	Total	O	0
			3	3	
92	BB	13	Total	O	0
			13	13	
92	CC	13	Total	O	0
			13	13	
92	Cc	1	Total	O	0
			1	1	
92	D	1	Total	O	0
			1	1	
92	EE	6	Total	O	0
			6	6	
92	F	4	Total	O	0
			4	4	
92	FF	3	Total	O	0
			3	3	

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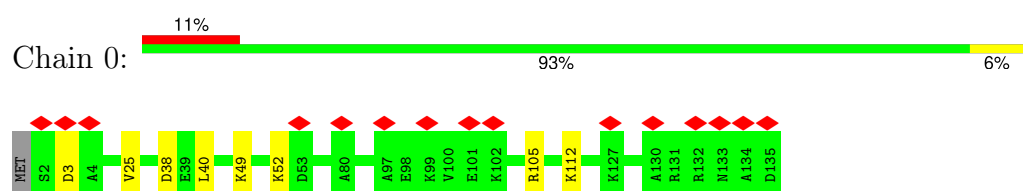
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Mol	Chain	Residues	Atoms		AltConf
92	GG	3	Total 3	O 3	0
92	H	3	Total 3	O 3	0
92	HH	1	Total 1	O 1	0
92	J	1	Total 1	O 1	0
92	JJ	1	Total 1	O 1	0
92	M	2	Total 2	O 2	0
92	MM	2	Total 2	O 2	0
92	N	1	Total 1	O 1	0
92	Q	4	Total 4	O 4	0
92	QQ	6	Total 6	O 6	0
92	V	2	Total 2	O 2	0
92	c	118	Total 118	O 118	0
92	h	2	Total 2	O 2	0
92	o	2	Total 2	O 2	0
92	p	2	Total 2	O 2	0

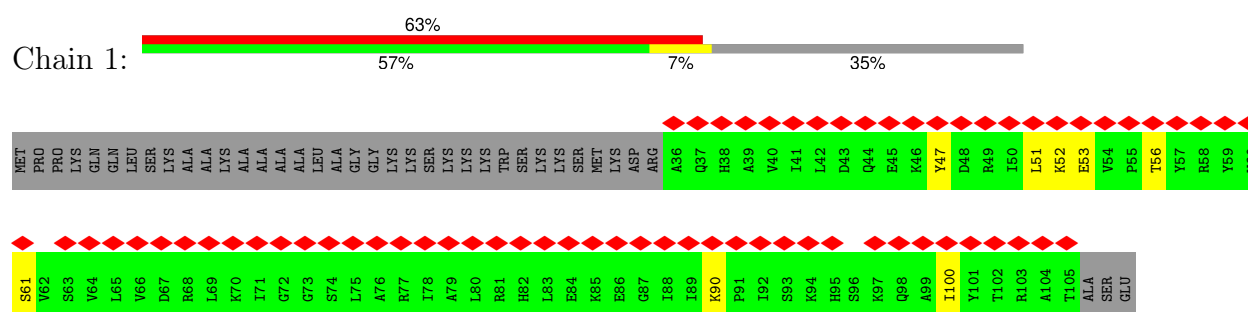
3 Residue-property plots [i](#)

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

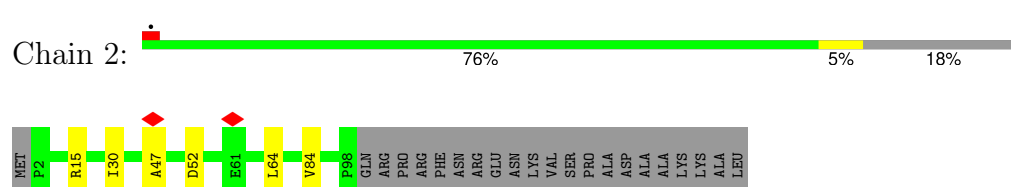
- Molecule 1: 40S ribosomal protein S24-A



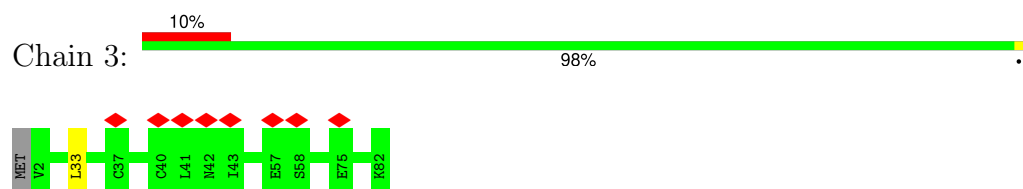
- Molecule 2: 40S ribosomal protein S25-A



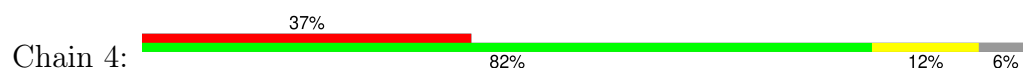
- Molecule 3: 40S ribosomal protein S26

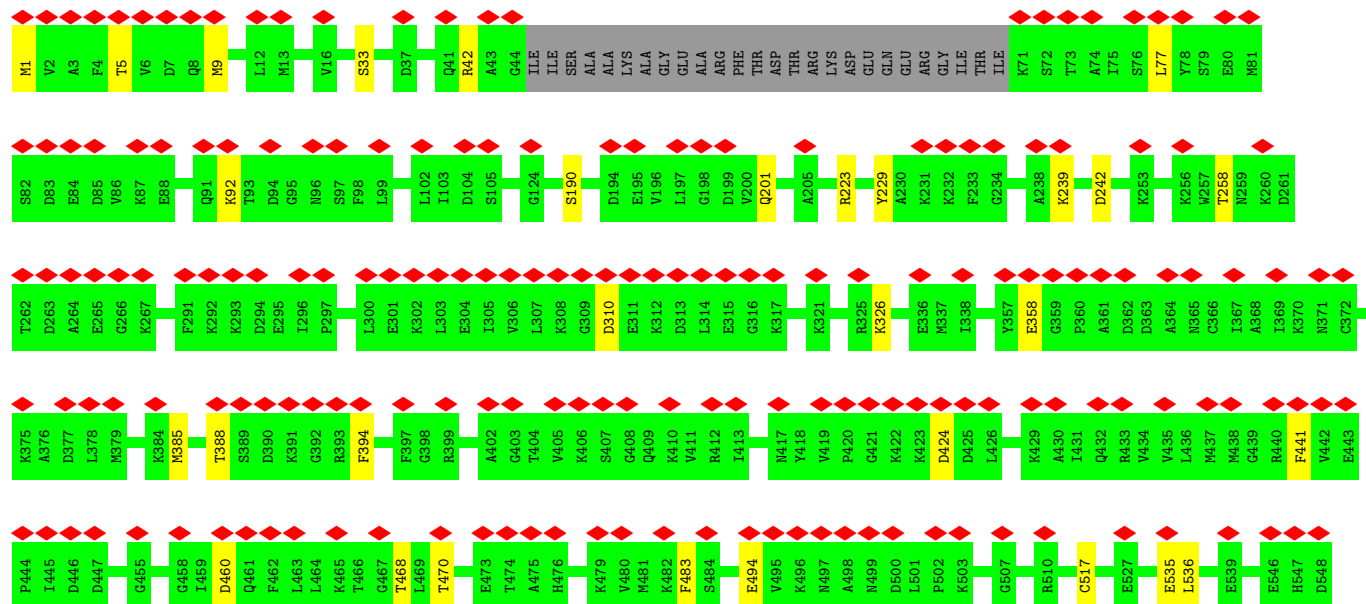


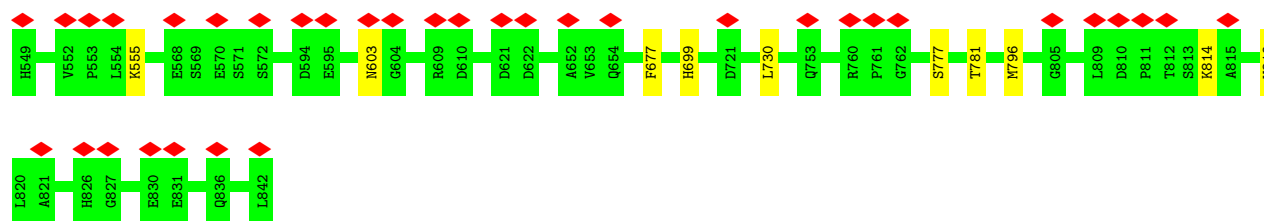
- Molecule 4: 40S ribosomal protein S27-A



- Molecule 5: 40S ribosomal protein S28-A

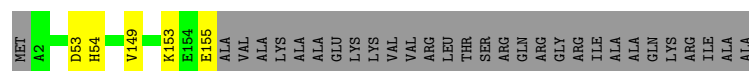






- Molecule 13: 60S ribosomal protein L17-A

Chain B: 81% 16%



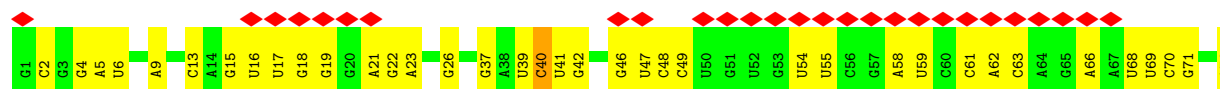
- Molecule 14: 5S ribosomal RNA

Chain BB: 93% 7%



- Molecule 15: Transfer RNA Phe

Chain Bb: 36% 51% 47%



- Molecule 16: 60S ribosomal protein L18-A

Chain C: 98% 2%



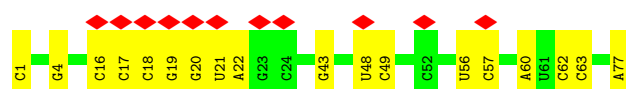
- Molecule 17: 5.8S ribosomal RNA

Chain CC: 87% 13%



- Molecule 18: Transfer RNA fMet

Chain Cc: 14% 77% 23%

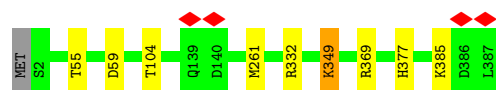




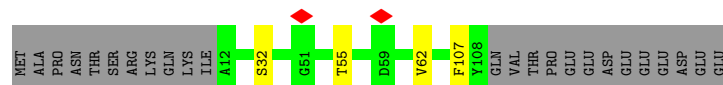
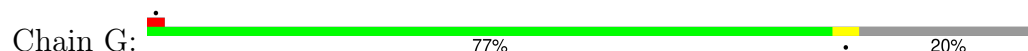
- Molecule 25: 60S ribosomal protein L21-A



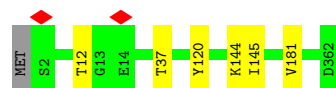
- Molecule 26: 60S ribosomal protein L3



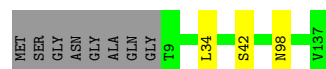
- Molecule 27: 60S ribosomal protein L22-A



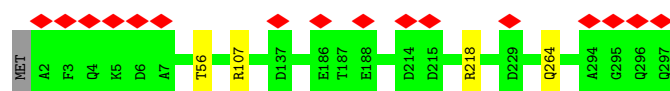
- Molecule 28: 60S ribosomal protein L4-A



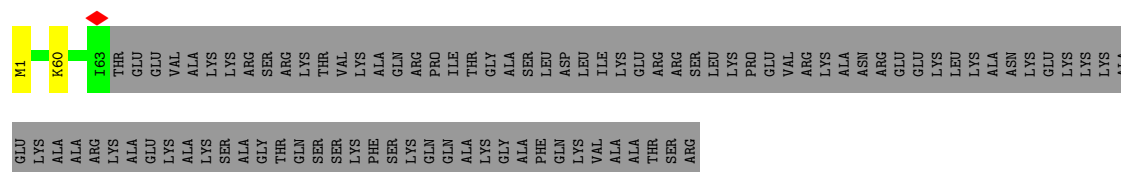
- Molecule 29: 60S ribosomal protein L23-A



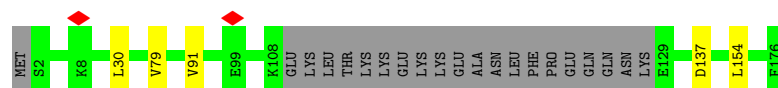
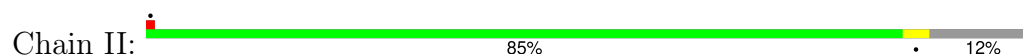
- Molecule 30: 60S ribosomal protein L5



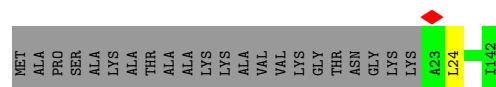
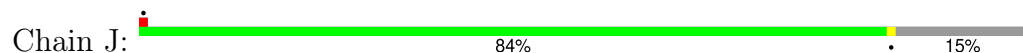
- Molecule 31: 60S ribosomal protein L24-A



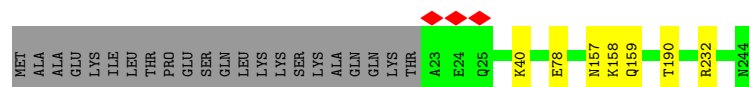
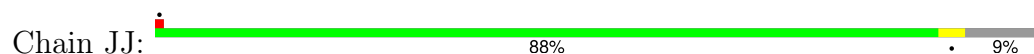
- Molecule 32: 60S ribosomal protein L6-A



- Molecule 33: 60S ribosomal protein L25



- Molecule 34: 60S ribosomal protein L7-A

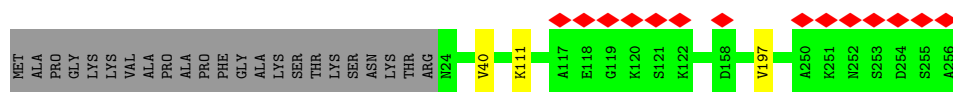


- Molecule 35: 60S ribosomal protein L26-A



- Molecule 36: 60S ribosomal protein L8-A





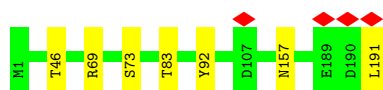
- Molecule 37: 60S ribosomal protein L27-A

Chain L: 96%



- Molecule 38: RPL9A isoform 1

Chain LL: 96%



- Molecule 39: 60S ribosomal protein L28

Chain M: 93% 6%



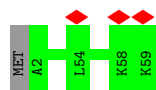
- Molecule 40: 60S ribosomal protein L10

Chain MM: 95%



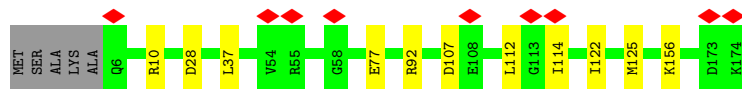
- Molecule 41: 60S ribosomal protein L29

Chain N: 5% 98%



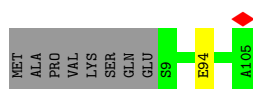
- Molecule 42: 60S ribosomal protein L11-A

Chain NN: 5% 91% 6%



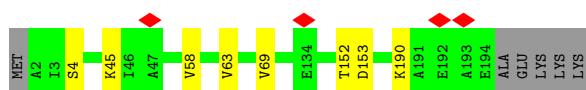
- Molecule 43: 60S ribosomal protein L30

Chain O:  91% 8%



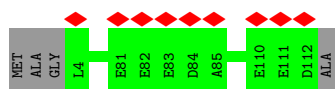
- Molecule 44: 60S ribosomal protein L13-A

Chain OO:  93%



- Molecule 45: 60S ribosomal protein L31-A

Chain P:  8% 96%



- Molecule 46: 60S ribosomal protein L14-A

Chain PP:  95%



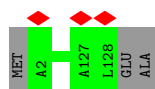
- Molecule 47: Polypeptide

Chain Pp:  50% 50%



- Molecule 48: 60S ribosomal protein L32

Chain Q:  98%



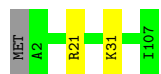
- Molecule 49: 60S ribosomal protein L15-A

Chain QQ:  99%



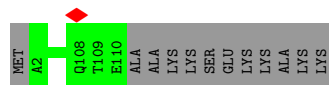
- Molecule 50: 60S ribosomal protein L33-A

Chain R:  97% ..



- Molecule 51: 60S ribosomal protein L34-A

Chain S:  90% 10%



- Molecule 52: 60S ribosomal protein L35-A

Chain T:  96% ..



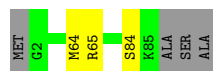
- Molecule 53: 60S ribosomal protein L36-A

Chain U:  94% 5% .



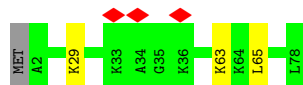
- Molecule 54: 60S ribosomal protein L37-A

Chain V:  92% 5%



- Molecule 55: 60S ribosomal protein L38

Chain W:  95% ..

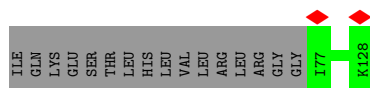
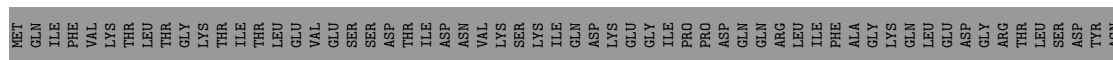


- Molecule 56: 60S ribosomal protein L39

Chain X:  98% .



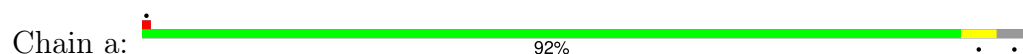
- Molecule 57: Ubiquitin-60S ribosomal protein L40



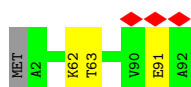
- Molecule 58: 60S ribosomal protein L41



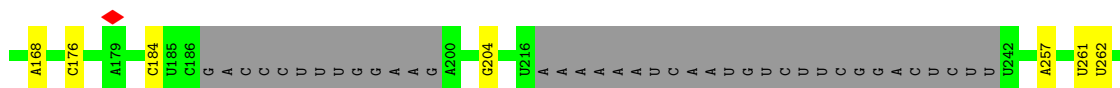
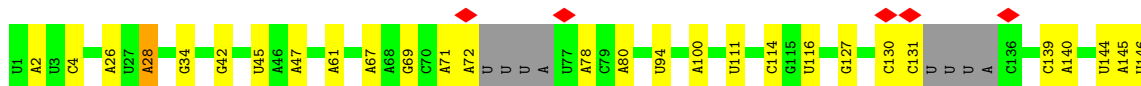
- Molecule 59: 60S ribosomal protein L42-A

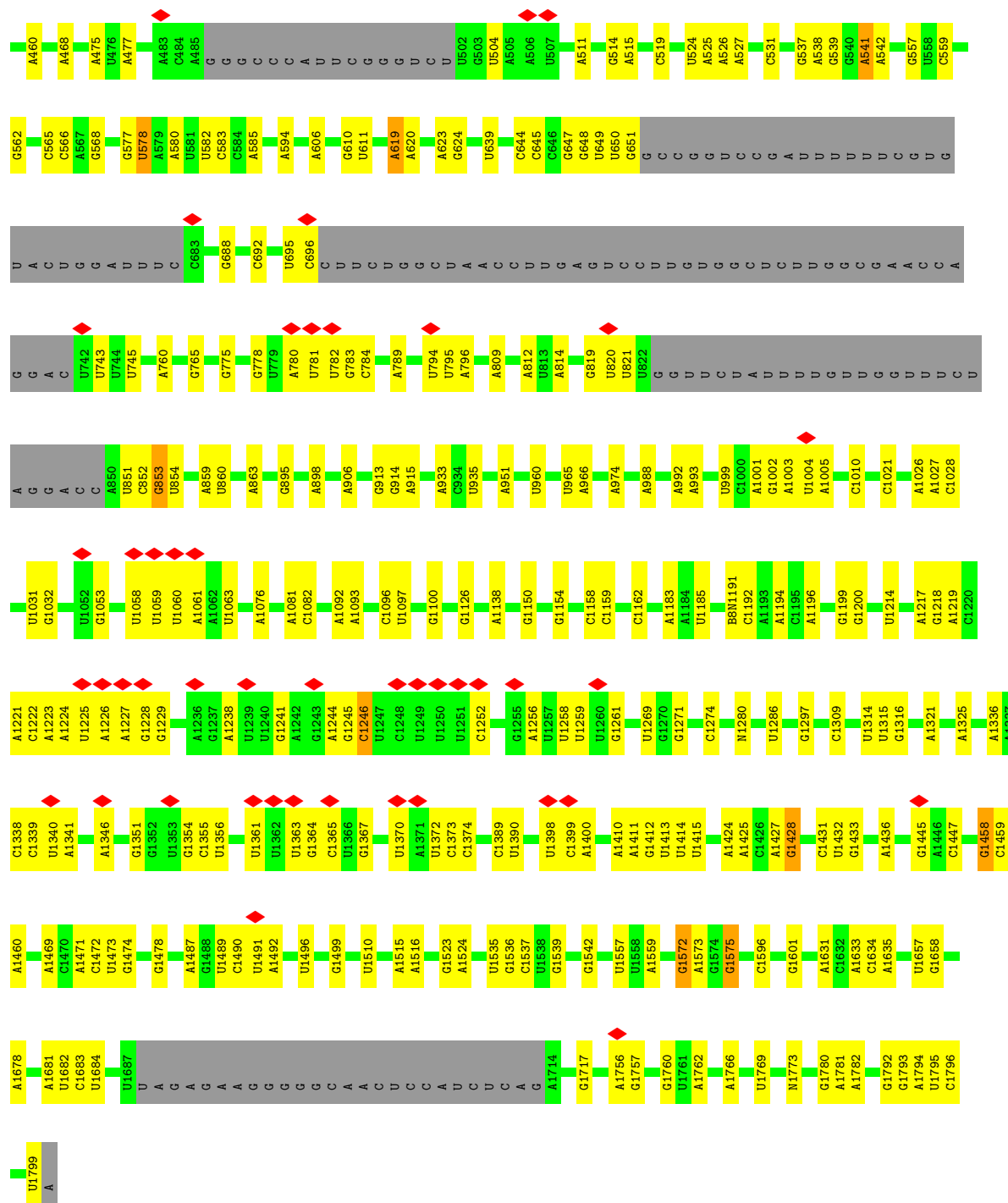


- Molecule 60: 60S ribosomal protein L43-A



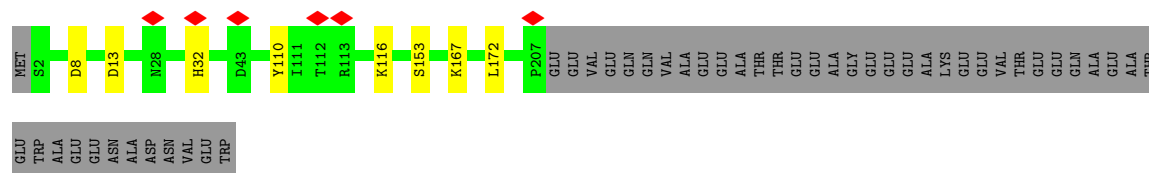
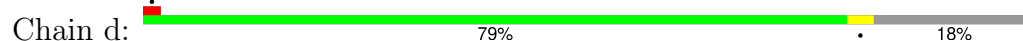
- Molecule 61: 18S ribosomal RNA






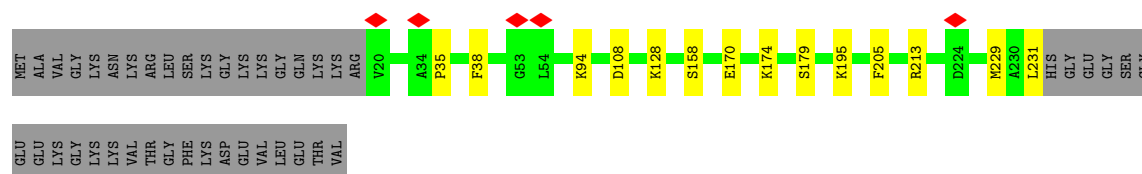
• Molecule 62: 40S ribosomal protein S0-A

Chain d:




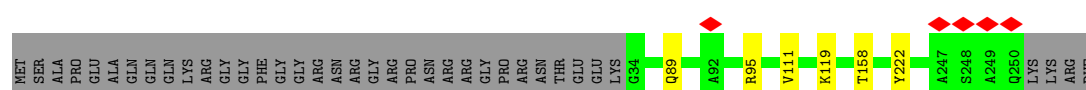
- Molecule 63: 40S ribosomal protein S1-A

Chain e:  78% 5% 17%



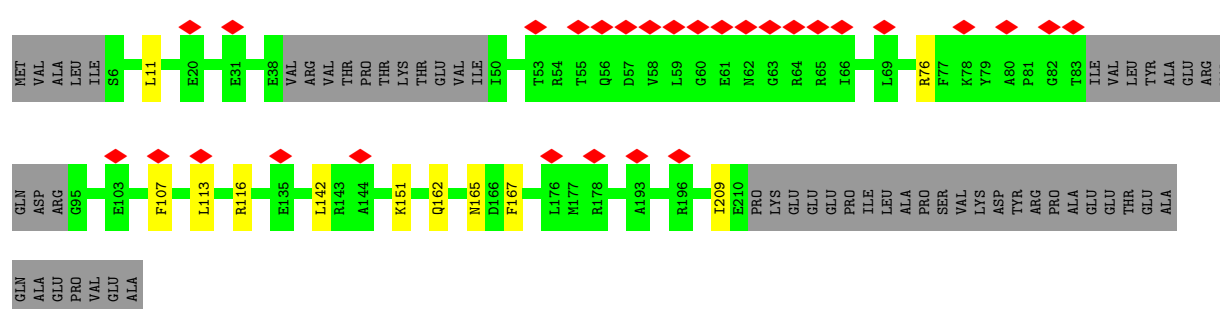
- Molecule 64: 40S ribosomal protein S2

Chain f:  83% 15%



- Molecule 65: RPS3 isoform 1

Chain g:  12% 72% 5% 24%




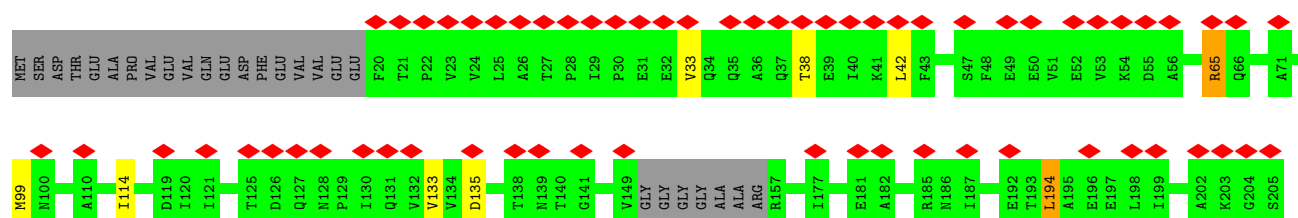
- Molecule 66: 40S ribosomal protein S4-A

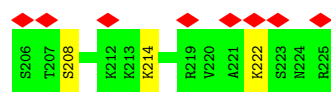
Chain h:  93% 6%



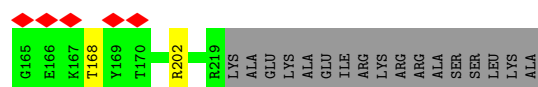
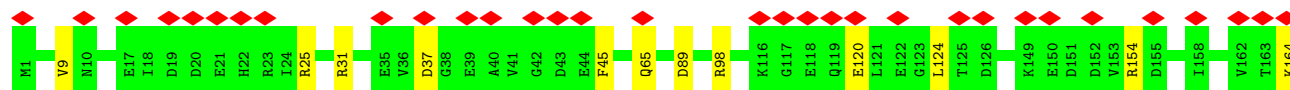
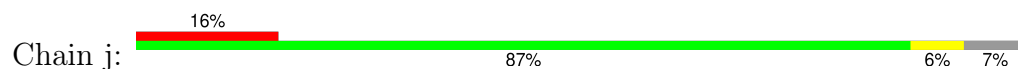
- Molecule 67: 40S ribosomal protein S5

Chain i:  32% 83% 12%

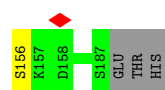
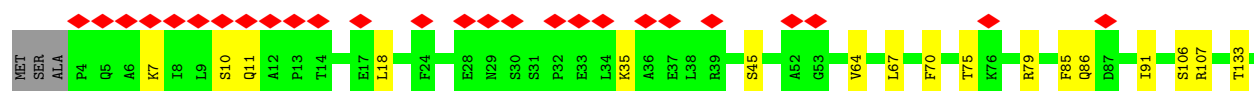
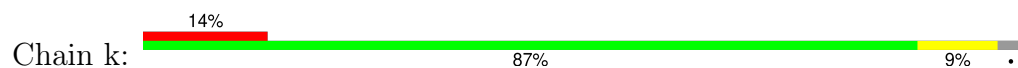




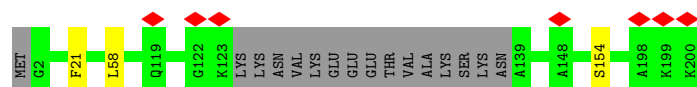
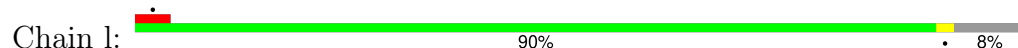
- Molecule 68: 40S ribosomal protein S6-A



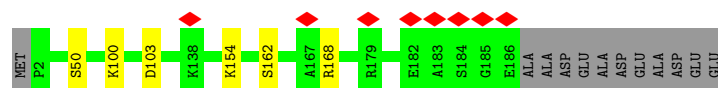
- Molecule 69: 40S ribosomal protein S7-A



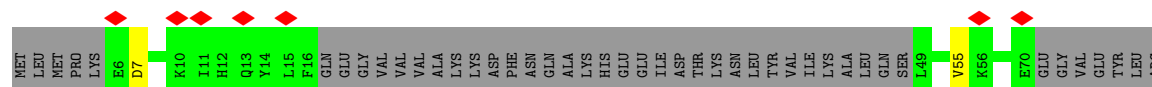
- Molecule 70: 40S ribosomal protein S8-B



- Molecule 71: 40S ribosomal protein S9-A




- Molecule 72: 40S ribosomal protein S10-A



GLU
TYR
LEU
ASN
LEU
PRO
GLU
HIS
ILE
VAL
PRO
GLY
THR
TYR
ILE
GLN
GLU
ARG
ASN
PRO
THR
GLN
ARG
GLN
ARG
TYR

- Molecule 73: 40S ribosomal protein S11-A

Chain o:  5% 88% 9%


MET SER THR E4 L5 T6 V7 K26 T27 S28 K29 R30 T31 R67 S132 A144 A145 ALA GLY LYS ALA ASN LYS GLN PHE ALA LYS PHE

- Molecule 74: 40S ribosomal protein S13

Chain p:  97%

MET G2 V60 T61 Q62 E103 N151

- Molecule 75: 40S ribosomal protein S14-A

Chain q:  91% 7%

MET SER ASN VAL VAL GLN ALA ARG ASP ASN S11 V30 V79 D124 L137


- Molecule 76: 40S ribosomal protein S15

Chain r:  25% 58% 6% 36%

MET SER GLN ALA VAL ASN ALA LYS LYS ARG VAL PHE THR HIS S16 Y17 R18 G19 V20 ASP LEU GLU LYS LEU LEU GLU MET SER THR GUJ D32 F33 L36 A37 V41 R42 R43 R44 F45 ALA ARG GLY MET THR LYS PRO ALA GLY PHE M57 K58 K59 A62 A63 K64

L65 A66 A67 P68 E69 N70 E71 K72 P73 A74 M83 P87 E88 M89 I90 G91 V94 A101 F102 N103 Q104 V105 E106 I107 R108 P109 V126 R127 H128 GLY ARG ALA GLY ALA THR SER ARG PHE ILE PRO LEU LYS

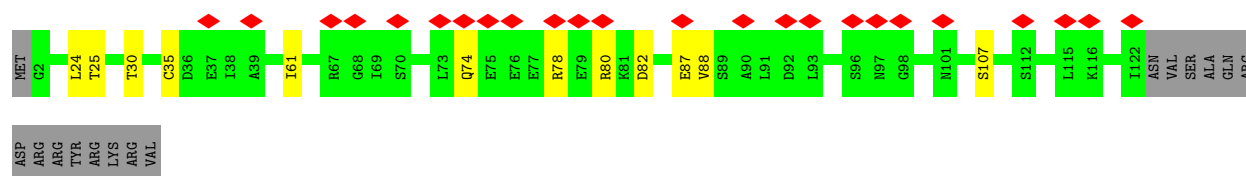
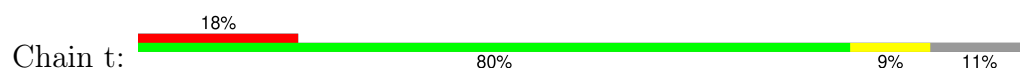
- Molecule 77: 40S ribosomal protein S16-A

Chain s:  18% 85% 10%

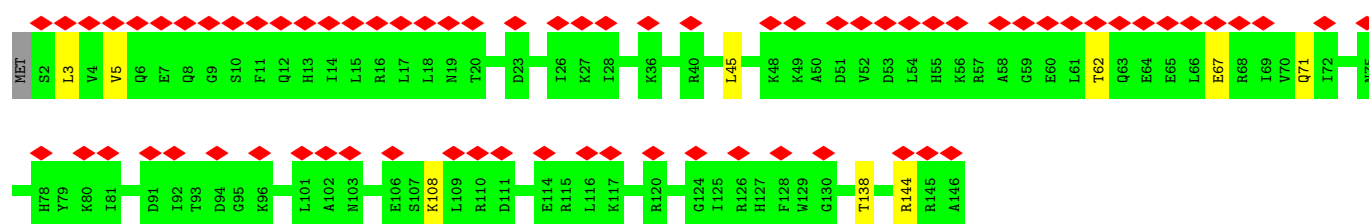
MET SER VAL PRO SER V7 Q8 G11 V19 A24 L28 V31 N32 I36 T37 L38 V39 E40 R45 F46 E50 L54 V55 G56 L57 D58 K59 F60 S61 D64 I65 R68 V69 T70 D98 E99 K102 L105 K106 K107 T110 R114 T115

D120 S136 R143

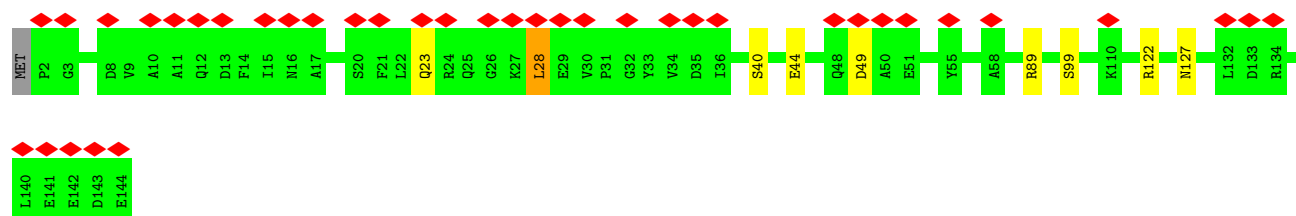
- Molecule 78: 40S ribosomal protein S17-A



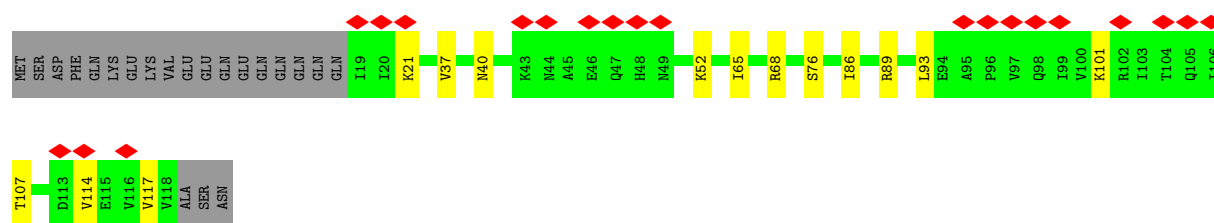
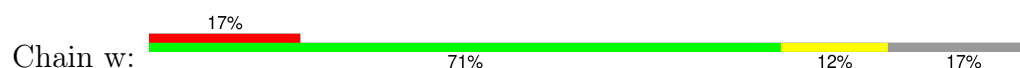
- Molecule 79: 40S ribosomal protein S18-A



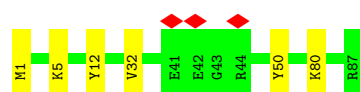
- Molecule 80: 40S ribosomal protein S19-A



- Molecule 81: 40S ribosomal protein S20



- Molecule 82: 40S ribosomal protein S21-A



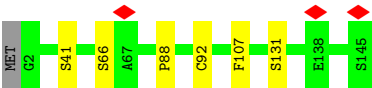
- Molecule 83: 40S ribosomal protein S22-A

Chain y:  96% ..



• Molecule 84: 40S ribosomal protein S23-A

Chain z:  95% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58351	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	270000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.697	Depositor
Minimum map value	-0.518	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.161	Depositor
Map size (Å)	540.0, 540.0, 540.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO1, DDE, GDP, A2M, OMU, PO4, G7M, 1MA, OMG, ZN, OMC, YYG, 5MC, B8N, UR3, MA6, K, 4AC, MG, SPD

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	0	0.28	0/1087	0.59	1/1449 (0.1%)
2	1	0.24	0/571	0.57	0/768
3	2	0.27	0/782	0.59	0/1047
4	3	0.27	0/620	0.56	0/838
5	4	0.27	0/499	0.63	0/670
6	5	0.27	0/412	0.61	0/544
7	6	0.26	0/433	0.65	0/575
8	7	0.26	0/2489	0.56	0/3389
9	8	0.23	0/279	0.52	0/369
10	A	0.29	0/1585	0.53	0/2128
11	AA	0.63	6/75545 (0.0%)	0.81	44/117782 (0.0%)
12	Aa	0.26	0/6470	0.53	0/8759
13	B	0.29	0/1245	0.53	0/1676
14	BB	0.34	0/2883	0.75	0/4491
15	Bb	0.26	0/1788	0.90	1/2786 (0.0%)
16	C	0.29	0/1465	0.56	0/1965
17	CC	0.39	0/3746	0.77	0/5832
18	Cc	0.34	1/1836 (0.1%)	0.78	0/2859
19	D	0.25	0/1440	0.56	0/1921
20	DD	0.26	0/1558	0.51	0/2107
21	Dd	0.24	0/138	0.76	0/212
22	E	0.29	0/1481	0.57	0/1990
23	EE	0.30	0/1948	0.57	0/2617
24	Ee	0.64	2/1210 (0.2%)	0.80	2/1627 (0.1%)
25	F	0.28	0/1300	0.52	0/1743
26	FF	0.29	0/3146	0.55	0/4228
27	G	0.28	0/786	0.52	0/1065
28	GG	0.27	0/2800	0.53	0/3790
29	H	0.29	0/978	0.56	0/1316
30	HH	0.28	0/2425	0.52	0/3271
31	I	0.29	0/533	0.52	0/707

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	II	0.28	0/1251	0.53	0/1682
33	J	0.29	0/974	0.52	0/1314
34	JJ	0.29	0/1821	0.53	1/2451 (0.0%)
35	K	0.27	0/1004	0.55	0/1341
36	KK	0.27	0/1836	0.48	0/2481
37	L	0.29	0/1118	0.49	0/1497
38	LL	0.28	0/1539	0.52	0/2073
39	M	0.28	0/1204	0.54	0/1612
40	MM	0.28	0/1779	0.55	0/2386
41	N	0.27	0/473	0.48	0/629
42	NN	0.27	0/1374	0.58	0/1842
43	O	0.28	0/750	0.46	0/1008
44	OO	0.27	0/1568	0.57	0/2106
45	P	0.27	0/897	0.56	0/1205
46	PP	0.27	0/1068	0.51	0/1438
47	Pp	0.35	0/19	0.71	0/23
48	Q	0.27	0/1041	0.51	0/1394
49	QQ	0.30	0/1757	0.58	0/2354
50	R	0.31	0/868	0.56	0/1168
51	S	0.28	0/871	0.57	0/1164
52	T	0.27	0/978	0.51	0/1301
53	U	0.26	0/778	0.59	0/1034
54	V	0.28	0/680	0.62	0/901
55	W	0.29	0/618	0.59	0/826
56	X	0.27	0/443	0.64	0/588
57	Y	0.26	0/423	0.54	0/562
58	Z	0.26	0/234	0.69	0/300
59	a	0.29	0/831	0.58	0/1097
60	b	0.27	0/701	0.57	0/934
61	c	0.31	0/37760	0.80	22/58811 (0.0%)
62	d	0.27	0/1623	0.52	0/2222
63	e	0.27	0/1714	0.55	0/2308
64	f	0.28	0/1665	0.55	0/2263
65	g	0.27	0/1429	0.58	0/1913
66	h	0.27	0/2097	0.55	0/2823
67	i	0.26	0/1591	0.60	1/2151 (0.0%)
68	j	0.25	0/1790	0.58	1/2393 (0.0%)
69	k	0.27	0/1506	0.60	1/2028 (0.0%)
70	l	0.27	0/1482	0.58	0/1980
71	m	0.26	0/1519	0.54	0/2035
72	n	0.26	0/309	0.48	0/416
73	o	0.28	0/1172	0.55	0/1580
74	p	0.27	0/1215	0.52	0/1638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	q	0.26	0/901	0.61	0/1217
76	r	0.26	0/747	0.59	0/1002
77	s	0.27	0/1099	0.54	0/1473
78	t	0.25	0/971	0.57	0/1303
79	u	0.24	0/1211	0.57	0/1628
80	v	0.26	0/1130	0.58	1/1517 (0.1%)
81	w	0.26	0/810	0.54	0/1095
82	x	0.28	0/693	0.55	0/935
83	y	0.29	0/1038	0.56	0/1395
84	z	0.26	0/1139	0.55	0/1518
All	All	0.44	9/218987 (0.0%)	0.72	75/320876 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
19	D	0	1
26	FF	0	1
34	JJ	0	2
37	L	0	2
54	V	0	1
59	a	0	1
63	e	0	2
67	i	0	1
69	k	0	3
77	s	0	1
84	z	0	1
All	All	0	16

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	1236	G	N3-C4	73.32	1.86	1.35
11	AA	1236	G	C2-N3	65.52	1.85	1.32
11	AA	1236	G	C6-N1	53.02	1.76	1.39
11	AA	1236	G	N1-C2	47.08	1.75	1.37
11	AA	1236	G	C5-C4	45.13	1.70	1.38
11	AA	1236	G	C5-C6	34.97	1.77	1.42
24	Ee	16	ARG	CD-NE	15.32	1.72	1.46
24	Ee	16	ARG	NE-CZ	13.00	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Cc	1	C	OP3-P	-10.60	1.48	1.61

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	1236	G	C2-N3-C4	25.38	124.59	111.90
11	AA	1236	G	N3-C4-C5	-23.48	116.86	128.60
11	AA	1236	G	N3-C4-N9	21.57	138.94	126.00
24	Ee	16	ARG	CD-NE-CZ	21.19	153.26	123.60
11	AA	1236	G	N1-C2-N3	-21.09	111.24	123.90
11	AA	1236	G	C5-C6-N1	17.71	120.36	111.50
11	AA	1236	G	C4-C5-N7	-17.51	103.79	110.80
11	AA	1236	G	N7-C8-N9	14.37	120.29	113.10
61	c	94	U	C2-N3-C4	13.87	135.32	127.00
11	AA	1236	G	N3-C2-N2	9.40	126.48	119.90
61	c	853	G	O4'-C1'-N9	8.26	114.81	108.20
11	AA	1236	G	N1-C6-O6	-7.96	115.12	119.90
11	AA	406	G	O4'-C1'-N9	7.85	114.48	108.20
11	AA	3278	C	N1-C2-O2	7.73	123.54	118.90
11	AA	1236	G	C6-C5-N7	7.53	134.92	130.40
61	c	1096	C	N1-C2-O2	7.49	123.39	118.90
11	AA	3278	C	C2-N1-C1'	7.24	126.77	118.80
11	AA	620	U	C2-N1-C1'	7.08	126.19	117.70
61	c	1096	C	C2-N1-C1'	6.95	126.45	118.80
61	c	1596	C	C2-N1-C1'	6.87	126.36	118.80
11	AA	1283	C	N3-C2-O2	-6.81	117.13	121.90
34	JJ	157	ASN	C-N-CA	6.80	138.71	121.70
11	AA	1236	G	C5-C6-O6	-6.80	124.52	128.60
61	c	94	U	N3-C4-C5	6.79	118.67	114.60
61	c	1389	C	C2-N1-C1'	6.77	126.25	118.80
11	AA	1236	G	N1-C2-N2	6.75	122.27	116.20
61	c	1365	C	N1-C2-O2	6.74	122.94	118.90
11	AA	3278	C	N3-C2-O2	-6.56	117.31	121.90
67	i	194	LEU	CA-CB-CG	6.56	130.39	115.30
61	c	1473	U	C2-N1-C1'	6.44	125.43	117.70
61	c	1596	C	N1-C2-O2	6.38	122.73	118.90
11	AA	922	U	C2-N1-C1'	6.35	125.32	117.70
61	c	94	U	N1-C2-N3	6.29	118.68	114.90
11	AA	2495	C	C2-N1-C1'	6.17	125.58	118.80
69	k	18	LEU	CA-CB-CG	6.14	129.42	115.30
68	j	124	LEU	CA-CB-CG	6.12	129.37	115.30
11	AA	620	U	N1-C2-O2	6.09	127.06	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	2490	C	C2-N1-C1'	6.07	125.47	118.80
80	v	28	LEU	CA-CB-CG	5.93	128.94	115.30
11	AA	2983	C	C2-N1-C1'	5.88	125.27	118.80
15	Bb	40	C	C2-N1-C1'	5.87	125.26	118.80
61	c	531	C	C2-N1-C1'	5.86	125.24	118.80
11	AA	1031	C	C2-N1-C1'	5.85	125.24	118.80
61	c	965	U	C2-N1-C1'	5.82	124.68	117.70
61	c	1096	C	N3-C2-O2	-5.81	117.83	121.90
11	AA	1496	C	C2-N1-C1'	5.70	125.06	118.80
61	c	1473	U	N1-C2-O2	5.68	126.78	122.80
11	AA	620	U	N3-C2-O2	-5.66	118.24	122.20
61	c	1365	C	N3-C2-O2	-5.62	117.96	121.90
11	AA	2836	C	C6-N1-C2	-5.60	118.06	120.30
11	AA	835	G	O4'-C1'-N9	5.59	112.67	108.20
11	AA	1222	G	O4'-C1'-N9	5.56	112.65	108.20
1	0	40	LEU	CA-CB-CG	5.53	128.01	115.30
11	AA	3058	U	C2-N1-C1'	5.51	124.31	117.70
11	AA	2836	C	C2-N1-C1'	5.50	124.85	118.80
11	AA	1283	C	N1-C2-O2	5.44	122.16	118.90
11	AA	2836	C	N3-C2-O2	-5.43	118.10	121.90
24	Ee	16	ARG	NE-CZ-NH1	5.42	123.01	120.30
11	AA	2490	C	N1-C2-O2	5.41	122.15	118.90
61	c	1596	C	N3-C2-O2	-5.40	118.12	121.90
11	AA	922	U	N1-C2-O2	5.36	126.55	122.80
61	c	1246	C	C2-N1-C1'	5.32	124.65	118.80
11	AA	2971	A	P-O3'-C3'	5.29	126.04	119.70
11	AA	2846	U	C2-N1-C1'	5.28	124.04	117.70
11	AA	1724	U	O4'-C1'-N1	5.25	112.40	108.20
61	c	1389	C	C6-N1-C2	-5.24	118.20	120.30
61	c	1458	G	C4-N9-C1'	5.21	133.28	126.50
11	AA	3057	U	N3-C2-O2	-5.21	118.55	122.20
11	AA	3181	C	N1-C2-O2	5.20	122.02	118.90
11	AA	2772	C	N1-C2-O2	5.16	122.00	118.90
61	c	1389	C	N1-C2-O2	5.14	121.98	118.90
11	AA	895	A	N9-C4-C5	-5.11	103.75	105.80
11	AA	895	A	C6-C5-N7	-5.07	128.75	132.30
61	c	610	G	C4-N9-C1'	5.05	133.06	126.50
11	AA	2846	U	N3-C2-O2	-5.01	118.69	122.20

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	D	130	ASN	Peptide
26	FF	349	LYS	Peptide
34	JJ	158	LYS	Peptide
34	JJ	232	ARG	Peptide
37	L	101	PHE	Peptide
37	L	102	GLU	Peptide
54	V	64	MET	Peptide
59	a	7	THR	Peptide
63	e	35	PRO	Peptide
63	e	38	PHE	Peptide
67	i	65	ARG	Peptide
69	k	10	SER	Peptide
69	k	11	GLN	Peptide
69	k	64	VAL	Peptide
77	s	40	GLU	Peptide
84	z	88	PRO	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	0	132/135 (98%)	127 (96%)	5 (4%)	0	100	100
2	1	68/108 (63%)	62 (91%)	6 (9%)	0	100	100
3	2	95/119 (80%)	88 (93%)	6 (6%)	1 (1%)	12	5
4	3	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
5	4	61/67 (91%)	61 (100%)	0	0	100	100
6	5	47/56 (84%)	47 (100%)	0	0	100	100
7	6	51/63 (81%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7	316/319 (99%)	297 (94%)	19 (6%)	0	100	100
9	8	32/152 (21%)	20 (62%)	12 (38%)	0	100	100
10	A	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
12	Aa	811/842 (96%)	787 (97%)	24 (3%)	0	100	100
13	B	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
16	C	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
19	D	174/189 (92%)	170 (98%)	3 (2%)	1 (1%)	22	13
20	DD	195/312 (62%)	194 (100%)	1 (0%)	0	100	100
22	E	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
23	EE	250/254 (98%)	245 (98%)	5 (2%)	0	100	100
24	Ee	156/165 (94%)	154 (99%)	2 (1%)	0	100	100
25	F	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
26	FF	384/387 (99%)	375 (98%)	9 (2%)	0	100	100
27	G	95/121 (78%)	94 (99%)	1 (1%)	0	100	100
28	GG	359/362 (99%)	344 (96%)	15 (4%)	0	100	100
29	H	127/137 (93%)	125 (98%)	2 (2%)	0	100	100
30	HH	294/297 (99%)	287 (98%)	7 (2%)	0	100	100
31	I	61/155 (39%)	61 (100%)	0	0	100	100
32	II	151/176 (86%)	146 (97%)	5 (3%)	0	100	100
33	J	118/142 (83%)	115 (98%)	3 (2%)	0	100	100
34	JJ	220/244 (90%)	212 (96%)	7 (3%)	1 (0%)	25	17
35	K	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
36	KK	231/256 (90%)	226 (98%)	5 (2%)	0	100	100
37	L	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
38	LL	189/191 (99%)	181 (96%)	8 (4%)	0	100	100
39	M	146/149 (98%)	139 (95%)	6 (4%)	1 (1%)	19	11
40	MM	213/221 (96%)	206 (97%)	7 (3%)	0	100	100
41	N	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
42	NN	167/174 (96%)	158 (95%)	9 (5%)	0	100	100
43	O	95/105 (90%)	95 (100%)	0	0	100	100
44	OO	191/199 (96%)	176 (92%)	14 (7%)	1 (0%)	25	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	P	107/113 (95%)	103 (96%)	4 (4%)	0	100	100
46	PP	134/138 (97%)	132 (98%)	2 (2%)	0	100	100
48	Q	125/130 (96%)	125 (100%)	0	0	100	100
49	QQ	201/204 (98%)	194 (96%)	7 (4%)	0	100	100
50	R	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
51	S	107/121 (88%)	106 (99%)	1 (1%)	0	100	100
52	T	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
53	U	97/100 (97%)	89 (92%)	8 (8%)	0	100	100
54	V	82/88 (93%)	77 (94%)	4 (5%)	1 (1%)	11	4
55	W	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
56	X	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
57	Y	50/128 (39%)	50 (100%)	0	0	100	100
58	Z	23/25 (92%)	23 (100%)	0	0	100	100
59	a	100/106 (94%)	95 (95%)	5 (5%)	0	100	100
60	b	89/92 (97%)	89 (100%)	0	0	100	100
62	d	204/252 (81%)	193 (95%)	11 (5%)	0	100	100
63	e	210/255 (82%)	199 (95%)	11 (5%)	0	100	100
64	f	215/254 (85%)	204 (95%)	11 (5%)	0	100	100
65	g	177/240 (74%)	168 (95%)	9 (5%)	0	100	100
66	h	256/261 (98%)	247 (96%)	9 (4%)	0	100	100
67	i	195/225 (87%)	186 (95%)	9 (5%)	0	100	100
68	j	217/236 (92%)	207 (95%)	10 (5%)	0	100	100
69	k	182/190 (96%)	172 (94%)	10 (6%)	0	100	100
70	l	180/200 (90%)	169 (94%)	11 (6%)	0	100	100
71	m	183/197 (93%)	176 (96%)	7 (4%)	0	100	100
72	n	29/105 (28%)	25 (86%)	4 (14%)	0	100	100
73	o	140/156 (90%)	132 (94%)	8 (6%)	0	100	100
74	p	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
75	q	125/137 (91%)	115 (92%)	10 (8%)	0	100	100
76	r	85/142 (60%)	84 (99%)	1 (1%)	0	100	100
77	s	135/143 (94%)	127 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	t	119/136 (88%)	112 (94%)	7 (6%)	0	100	100
79	u	143/146 (98%)	135 (94%)	8 (6%)	0	100	100
80	v	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
81	w	98/121 (81%)	98 (100%)	0	0	100	100
82	x	85/87 (98%)	76 (89%)	9 (11%)	0	100	100
83	y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
84	z	142/145 (98%)	129 (91%)	13 (9%)	0	100	100
All	All	11673/13056 (89%)	11237 (96%)	430 (4%)	6 (0%)	50	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	JJ	159	GLN
39	M	78	LEU
44	OO	63	VAL
54	V	65	ARG
3	2	47	ALA
19	D	131	ALA

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	0	112/113 (99%)	105 (94%)	7 (6%)	15	8
2	1	61/89 (68%)	53 (87%)	8 (13%)	3	1
3	2	83/101 (82%)	78 (94%)	5 (6%)	16	9
4	3	70/71 (99%)	69 (99%)	1 (1%)	62	63
5	4	56/60 (93%)	48 (86%)	8 (14%)	2	0
6	5	43/49 (88%)	39 (91%)	4 (9%)	7	3
7	6	46/54 (85%)	39 (85%)	7 (15%)	2	0
8	7	259/262 (99%)	237 (92%)	22 (8%)	8	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	8	30/135 (22%)	25 (83%)	5 (17%)	2	0
10	A	160/162 (99%)	158 (99%)	2 (1%)	65	66
12	Aa	694/714 (97%)	655 (94%)	39 (6%)	17	11
13	B	125/146 (86%)	120 (96%)	5 (4%)	27	21
16	C	150/151 (99%)	148 (99%)	2 (1%)	65	66
19	D	143/154 (93%)	139 (97%)	4 (3%)	38	34
20	DD	167/254 (66%)	157 (94%)	10 (6%)	16	9
22	E	156/156 (100%)	150 (96%)	6 (4%)	28	22
23	EE	193/196 (98%)	189 (98%)	4 (2%)	48	45
24	Ee	129/136 (95%)	114 (88%)	15 (12%)	4	1
25	F	136/137 (99%)	130 (96%)	6 (4%)	24	18
26	FF	320/323 (99%)	311 (97%)	9 (3%)	38	34
27	G	84/107 (78%)	80 (95%)	4 (5%)	21	15
28	GG	288/289 (100%)	282 (98%)	6 (2%)	48	45
29	H	101/105 (96%)	98 (97%)	3 (3%)	36	31
30	HH	244/245 (100%)	240 (98%)	4 (2%)	58	57
31	I	55/129 (43%)	53 (96%)	2 (4%)	30	25
32	II	133/153 (87%)	128 (96%)	5 (4%)	28	22
33	J	104/118 (88%)	103 (99%)	1 (1%)	73	74
34	JJ	186/205 (91%)	183 (98%)	3 (2%)	58	57
35	K	109/110 (99%)	105 (96%)	4 (4%)	29	23
36	KK	187/208 (90%)	184 (98%)	3 (2%)	58	57
37	L	115/116 (99%)	111 (96%)	4 (4%)	31	25
38	LL	171/171 (100%)	164 (96%)	7 (4%)	26	20
39	M	118/119 (99%)	110 (93%)	8 (7%)	13	7
40	MM	184/187 (98%)	179 (97%)	5 (3%)	40	35
41	N	46/47 (98%)	46 (100%)	0	100	100
42	NN	147/150 (98%)	136 (92%)	11 (8%)	11	5
43	O	81/88 (92%)	80 (99%)	1 (1%)	67	68
44	OO	154/159 (97%)	147 (96%)	7 (4%)	23	17
45	P	94/97 (97%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	PP	107/109 (98%)	102 (95%)	5 (5%)	22	16
47	Pp	2/2 (100%)	1 (50%)	1 (50%)	0	0
48	Q	109/111 (98%)	109 (100%)	0	100	100
49	QQ	175/176 (99%)	173 (99%)	2 (1%)	70	71
50	R	90/91 (99%)	88 (98%)	2 (2%)	47	43
51	S	94/103 (91%)	94 (100%)	0	100	100
52	T	104/105 (99%)	100 (96%)	4 (4%)	28	22
53	U	81/82 (99%)	76 (94%)	5 (6%)	15	8
54	V	69/71 (97%)	68 (99%)	1 (1%)	62	63
55	W	68/69 (99%)	65 (96%)	3 (4%)	24	18
56	X	45/46 (98%)	45 (100%)	0	100	100
57	Y	47/116 (40%)	47 (100%)	0	100	100
58	Z	23/23 (100%)	21 (91%)	2 (9%)	8	3
59	a	87/91 (96%)	84 (97%)	3 (3%)	32	26
60	b	71/72 (99%)	68 (96%)	3 (4%)	25	20
62	d	165/210 (79%)	157 (95%)	8 (5%)	21	15
63	e	189/224 (84%)	177 (94%)	12 (6%)	15	8
64	f	176/205 (86%)	170 (97%)	6 (3%)	32	26
65	g	145/195 (74%)	134 (92%)	11 (8%)	11	5
66	h	220/222 (99%)	204 (93%)	16 (7%)	11	5
67	i	172/191 (90%)	160 (93%)	12 (7%)	12	6
68	j	188/201 (94%)	175 (93%)	13 (7%)	13	7
69	k	165/170 (97%)	151 (92%)	14 (8%)	8	4
70	l	146/161 (91%)	143 (98%)	3 (2%)	48	45
71	m	158/166 (95%)	152 (96%)	6 (4%)	28	22
72	n	32/98 (33%)	30 (94%)	2 (6%)	15	8
73	o	127/137 (93%)	123 (97%)	4 (3%)	35	30
74	p	127/128 (99%)	124 (98%)	3 (2%)	44	40
75	q	81/105 (77%)	79 (98%)	2 (2%)	42	38
76	r	77/118 (65%)	68 (88%)	9 (12%)	4	1
77	s	114/119 (96%)	100 (88%)	14 (12%)	4	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	t	105/124 (85%)	93 (89%)	12 (11%)	4	1
79	u	128/129 (99%)	119 (93%)	9 (7%)	12	6
80	v	115/116 (99%)	106 (92%)	9 (8%)	10	4
81	w	94/114 (82%)	80 (85%)	14 (15%)	2	0
82	x	74/74 (100%)	68 (92%)	6 (8%)	9	4
83	y	110/111 (99%)	106 (96%)	4 (4%)	30	25
84	z	119/120 (99%)	114 (96%)	5 (4%)	25	20
All	All	9933/10971 (90%)	9461 (95%)	472 (5%)	24	15

All (472) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	3	ASP
1	0	25	VAL
1	0	38	ASP
1	0	49	LYS
1	0	52	LYS
1	0	105	ARG
1	0	112	LYS
2	1	47	TYR
2	1	51	LEU
2	1	52	LYS
2	1	53	GLU
2	1	56	THR
2	1	61	SER
2	1	90	LYS
2	1	100	ILE
3	2	15	ARG
3	2	30	ILE
3	2	52	ASP
3	2	64	LEU
3	2	84	VAL
4	3	33	LEU
5	4	12	VAL
5	4	22	ARG
5	4	29	ARG
5	4	30	VAL
5	4	41	VAL
5	4	49	ARG
5	4	61	ARG

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Mol	Chain	Res	Type
5	4	64	ARG
6	5	19	ARG
6	5	26	SER
6	5	42	CYS
6	5	56	ARG
7	6	18	THR
7	6	22	GLU
7	6	23	LYS
7	6	26	LYS
7	6	31	LYS
7	6	49	LEU
7	6	57	ASN
8	7	16	HIS
8	7	20	VAL
8	7	25	THR
8	7	41	THR
8	7	45	TRP
8	7	54	PHE
8	7	67	ILE
8	7	76	ASP
8	7	109	ASP
8	7	130	THR
8	7	137	LYS
8	7	157	VAL
8	7	167	VAL
8	7	177	MET
8	7	202	LEU
8	7	217	ASP
8	7	221	MET
8	7	225	LEU
8	7	231	MET
8	7	243	LEU
8	7	249	ARG
8	7	316	MET
9	8	98	VAL
9	8	121	CYS
9	8	132	LEU
9	8	136	LYS
9	8	137	ASP
10	A	56	ASP
10	A	184	THR
12	Aa	1	MET

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Mol	Chain	Res	Type
12	Aa	5	THR
12	Aa	9	MET
12	Aa	33	SER
12	Aa	42	ARG
12	Aa	77	LEU
12	Aa	92	LYS
12	Aa	190	SER
12	Aa	201	GLN
12	Aa	223	ARG
12	Aa	229	TYR
12	Aa	239	LYS
12	Aa	242	ASP
12	Aa	258	THR
12	Aa	310	ASP
12	Aa	326	LYS
12	Aa	358	GLU
12	Aa	385	MET
12	Aa	388	THR
12	Aa	394	PHE
12	Aa	424	ASP
12	Aa	441	PHE
12	Aa	460	ASP
12	Aa	468	THR
12	Aa	470	THR
12	Aa	483	PHE
12	Aa	494	GLU
12	Aa	517	CYS
12	Aa	535	GLU
12	Aa	536	LEU
12	Aa	555	LYS
12	Aa	603	ASN
12	Aa	677	PHE
12	Aa	730	LEU
12	Aa	777	SER
12	Aa	781	THR
12	Aa	796	MET
12	Aa	814	LYS
12	Aa	819	VAL
13	B	53	ASP
13	B	54	HIS
13	B	149	VAL
13	B	153	LYS

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Mol	Chain	Res	Type
13	B	155	GLU
16	C	8	LYS
16	C	41	ASP
19	D	43	LYS
19	D	150	GLN
19	D	175	GLN
19	D	176	ARG
20	DD	38	MET
20	DD	42	ARG
20	DD	52	LEU
20	DD	64	ARG
20	DD	122	ARG
20	DD	144	LYS
20	DD	155	ASP
20	DD	160	ASP
20	DD	164	LYS
20	DD	190	VAL
22	E	1	MET
22	E	45	LEU
22	E	95	ARG
22	E	96	ASP
22	E	132	THR
22	E	172	TYR
23	EE	72	ARG
23	EE	191	LEU
23	EE	202	VAL
23	EE	249	SER
24	Ee	10	VAL
24	Ee	11	LYS
24	Ee	13	LEU
24	Ee	18	VAL
24	Ee	41	LYS
24	Ee	52	GLU
24	Ee	56	ILE
24	Ee	57	LYS
24	Ee	67	ARG
24	Ee	86	LYS
24	Ee	96	LYS
24	Ee	118	ASP
24	Ee	123	ARG
24	Ee	150	ASP
24	Ee	164	GLU

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Mol	Chain	Res	Type
25	F	9	SER
25	F	14	MET
25	F	19	PHE
25	F	26	HIS
25	F	83	ARG
25	F	102	ARG
26	FF	55	THR
26	FF	59	ASP
26	FF	104	THR
26	FF	261	MET
26	FF	332	ARG
26	FF	349	LYS
26	FF	369	ARG
26	FF	377	HIS
26	FF	385	LYS
27	G	32	SER
27	G	55	THR
27	G	62	VAL
27	G	107	PHE
28	GG	12	THR
28	GG	37	THR
28	GG	120	TYR
28	GG	144	LYS
28	GG	145	ILE
28	GG	181	VAL
29	H	34	LEU
29	H	42	SER
29	H	98	ASN
30	HH	56	THR
30	HH	107	ARG
30	HH	218	ARG
30	HH	264	GLN
31	I	1	MET
31	I	60	LYS
32	II	30	LEU
32	II	79	VAL
32	II	91	VAL
32	II	137	ASP
32	II	154	LEU
33	J	24	LEU
34	JJ	40	LYS
34	JJ	78	GLU

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Mol	Chain	Res	Type
34	JJ	190	THR
35	K	3	LYS
35	K	7	ASP
35	K	74	TYR
35	K	125	LYS
36	KK	40	VAL
36	KK	111	LYS
36	KK	197	VAL
37	L	6	LYS
37	L	61	LYS
37	L	95	VAL
37	L	102	GLU
38	LL	46	THR
38	LL	69	ARG
38	LL	73	SER
38	LL	83	THR
38	LL	92	TYR
38	LL	157	ASN
38	LL	191	LEU
39	M	8	THR
39	M	60	TYR
39	M	88	ASP
39	M	92	LYS
39	M	93	SER
39	M	96	LYS
39	M	120	ASN
39	M	121	VAL
40	MM	4	ARG
40	MM	101	LYS
40	MM	110	ARG
40	MM	111	LEU
40	MM	138	VAL
42	NN	10	ARG
42	NN	28	ASP
42	NN	37	LEU
42	NN	77	GLU
42	NN	92	ARG
42	NN	107	ASP
42	NN	112	LEU
42	NN	114	ILE
42	NN	122	ILE
42	NN	125	MET

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Mol	Chain	Res	Type
42	NN	156	LYS
43	O	94	GLU
44	OO	4	SER
44	OO	45	LYS
44	OO	58	VAL
44	OO	69	VAL
44	OO	152	THR
44	OO	153	ASP
44	OO	190	LYS
46	PP	5	SER
46	PP	25	LYS
46	PP	63	VAL
46	PP	106	ARG
46	PP	137	LYS
47	Pp	1	MET
49	QQ	18	VAL
49	QQ	99	ARG
50	R	21	ARG
50	R	31	LYS
52	T	23	ASP
52	T	37	SER
52	T	40	SER
52	T	119	LYS
53	U	17	VAL
53	U	30	LYS
53	U	81	THR
53	U	97	SER
53	U	98	ARG
54	V	84	SER
55	W	29	LYS
55	W	63	LYS
55	W	65	LEU
58	Z	15	ARG
58	Z	24	SER
59	a	15	LYS
59	a	22	GLN
59	a	80	ARG
60	b	62	LYS
60	b	63	THR
60	b	91	GLU
62	d	8	ASP
62	d	13	ASP

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Mol	Chain	Res	Type
62	d	32	HIS
62	d	110	TYR
62	d	116	LYS
62	d	153	SER
62	d	167	LYS
62	d	172	LEU
63	e	94	LYS
63	e	108	ASP
63	e	128	LYS
63	e	158	SER
63	e	170	GLU
63	e	174	LYS
63	e	179	SER
63	e	195	LYS
63	e	205	PHE
63	e	213	ARG
63	e	229	MET
63	e	231	LEU
64	f	89	GLN
64	f	95	ARG
64	f	111	VAL
64	f	119	LYS
64	f	158	THR
64	f	222	TYR
65	g	11	LEU
65	g	76	ARG
65	g	107	PHE
65	g	113	LEU
65	g	116	ARG
65	g	142	LEU
65	g	151	LYS
65	g	162	GLN
65	g	165	ASN
65	g	167	PHE
65	g	209	ILE
66	h	11	ARG
66	h	17	HIS
66	h	32	SER
66	h	37	LYS
66	h	41	SER
66	h	105	VAL
66	h	108	ARG

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Mol	Chain	Res	Type
66	h	116	ASP
66	h	118	GLU
66	h	120	SER
66	h	146	THR
66	h	173	ILE
66	h	182	TYR
66	h	206	ASP
66	h	251	GLU
66	h	255	ARG
67	i	33	VAL
67	i	38	THR
67	i	42	LEU
67	i	65	ARG
67	i	99	MET
67	i	114	ILE
67	i	133	VAL
67	i	135	ASP
67	i	194	LEU
67	i	208	SER
67	i	214	LYS
67	i	222	LYS
68	j	9	VAL
68	j	25	ARG
68	j	31	ARG
68	j	37	ASP
68	j	45	PHE
68	j	65	GLN
68	j	89	ASP
68	j	98	ARG
68	j	120	GLU
68	j	154	ARG
68	j	164	LYS
68	j	168	THR
68	j	202	ARG
69	k	7	LYS
69	k	35	LYS
69	k	45	SER
69	k	67	LEU
69	k	70	PHE
69	k	75	THR
69	k	79	ARG
69	k	85	PHE

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Mol	Chain	Res	Type
69	k	86	GLN
69	k	91	ILE
69	k	106	SER
69	k	107	ARG
69	k	133	THR
69	k	156	SER
70	l	21	PHE
70	l	58	LEU
70	l	154	SER
71	m	50	SER
71	m	100	LYS
71	m	103	ASP
71	m	154	LYS
71	m	162	SER
71	m	168	ARG
72	n	7	ASP
72	n	55	VAL
73	o	7	VAL
73	o	31	THR
73	o	67	ARG
73	o	132	SER
74	p	60	VAL
74	p	62	GLN
74	p	103	GLU
75	q	30	VAL
75	q	79	VAL
76	r	17	TYR
76	r	36	LEU
76	r	41	VAL
76	r	43	ARG
76	r	45	PHE
76	r	57	MET
76	r	58	LYS
76	r	64	LYS
76	r	83	MET
77	s	8	GLN
77	s	19	VAL
77	s	28	LEU
77	s	45	ARG
77	s	46	PHE
77	s	58	ASP
77	s	65	ILE

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Mol	Chain	Res	Type
77	s	70	THR
77	s	99	GLU
77	s	102	LYS
77	s	107	LYS
77	s	115	THR
77	s	120	ASP
77	s	136	SER
78	t	24	LEU
78	t	25	THR
78	t	30	THR
78	t	35	CYS
78	t	61	ILE
78	t	74	GLN
78	t	78	ARG
78	t	80	ARG
78	t	82	ASP
78	t	87	GLU
78	t	88	VAL
78	t	107	SER
79	u	3	LEU
79	u	5	VAL
79	u	45	LEU
79	u	62	THR
79	u	67	GLU
79	u	71	GLN
79	u	108	LYS
79	u	138	THR
79	u	144	ARG
80	v	23	GLN
80	v	28	LEU
80	v	40	SER
80	v	44	GLU
80	v	49	ASP
80	v	89	ARG
80	v	99	SER
80	v	122	ARG
80	v	127	ASN
81	w	21	LYS
81	w	37	VAL
81	w	40	ASN
81	w	52	LYS
81	w	65	ILE

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Mol	Chain	Res	Type
81	w	68	ARG
81	w	76	SER
81	w	86	ILE
81	w	89	ARG
81	w	93	LEU
81	w	101	LYS
81	w	107	THR
81	w	114	VAL
81	w	117	VAL
82	x	1	MET
82	x	5	LYS
82	x	12	TYR
82	x	32	VAL
82	x	50	TYR
82	x	80	LYS
83	y	30	SER
83	y	58	SER
83	y	106	THR
83	y	117	ARG
84	z	41	SER
84	z	66	SER
84	z	92	CYS
84	z	107	PHE
84	z	131	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
19	D	144	GLN
23	EE	132	ASN
26	FF	212	ASN
42	NN	7	ASN
56	X	33	ASN
65	g	111	ASN
65	g	162	GLN
66	h	157	ASN
68	j	65	GLN
69	k	5	GLN
69	k	29	ASN
74	p	49	GLN
78	t	42	GLN
78	t	48	ASN

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Mol	Chain	Res	Type
78	t	74	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	3193/3396 (94%)	472 (14%)	24 (0%)
14	BB	120/121 (99%)	8 (6%)	1 (0%)
15	Bb	75/76 (98%)	36 (48%)	0
17	CC	157/158 (99%)	20 (12%)	0
18	Cc	76/77 (98%)	17 (22%)	0
21	Dd	5/39 (12%)	0	0
61	c	1593/1800 (88%)	320 (20%)	0
All	All	5219/5667 (92%)	873 (16%)	25 (0%)

All (873) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	AA	4	U
11	AA	6	A
11	AA	14	U
11	AA	26	A
11	AA	40	A
11	AA	43	A
11	AA	49	A
11	AA	59	G
11	AA	60	A
11	AA	65	A
11	AA	66	A
11	AA	92	G
11	AA	99	A
11	AA	110	G
11	AA	111	C
11	AA	122	A
11	AA	135	C
11	AA	136	G
11	AA	156	G
11	AA	157	A
11	AA	165	A
11	AA	172	G
11	AA	190	U
11	AA	200	C

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Mol	Chain	Res	Type
11	AA	219	A
11	AA	241	G
11	AA	242	C
11	AA	243	G
11	AA	247	C
11	AA	248	U
11	AA	249	U
11	AA	251	G
11	AA	252	U
11	AA	253	A
11	AA	269	G
11	AA	286	U
11	AA	295	A
11	AA	305	U
11	AA	329	U
11	AA	376	G
11	AA	390	G
11	AA	398	A
11	AA	399	A
11	AA	401	U
11	AA	402	A
11	AA	403	C
11	AA	420	G
11	AA	421	G
11	AA	422	A
11	AA	498	A
11	AA	520	U
11	AA	521	A
11	AA	532	A
11	AA	533	A
11	AA	534	U
11	AA	546	C
11	AA	548	G
11	AA	557	A
11	AA	559	A
11	AA	560	G
11	AA	589	A
11	AA	592	A
11	AA	601	U
11	AA	602	A
11	AA	603	A
11	AA	604	G

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Mol	Chain	Res	Type
11	AA	607	A
11	AA	611	A
11	AA	612	U
11	AA	620	U
11	AA	621	A
11	AA	636	C
11	AA	649	A2M
11	AA	660	A
11	AA	667	C
11	AA	677	A
11	AA	678	G
11	AA	681	U
11	AA	691	A
11	AA	705	A
11	AA	712	G
11	AA	715	A
11	AA	719	U
11	AA	758	C
11	AA	766	U
11	AA	767	U
11	AA	774	G
11	AA	780	A
11	AA	781	G
11	AA	785	G
11	AA	786	A
11	AA	799	G
11	AA	817	A2M
11	AA	830	A
11	AA	861	C
11	AA	867	OMG
11	AA	874	U
11	AA	879	U
11	AA	880	G
11	AA	890	C
11	AA	896	A
11	AA	907	G
11	AA	908	OMG
11	AA	914	A
11	AA	916	G
11	AA	917	A
11	AA	921	A
11	AA	923	C

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Mol	Chain	Res	Type
11	AA	924	G
11	AA	925	A
11	AA	937	G
11	AA	944	C
11	AA	959	C
11	AA	960	U
11	AA	961	C
11	AA	964	G
11	AA	974	G
11	AA	979	U
11	AA	980	A
11	AA	991	G
11	AA	994	G
11	AA	995	U
11	AA	1006	A
11	AA	1012	G
11	AA	1013	G
11	AA	1015	U
11	AA	1017	C
11	AA	1018	G
11	AA	1019	G
11	AA	1020	G
11	AA	1023	C
11	AA	1027	A
11	AA	1028	U
11	AA	1029	G
11	AA	1031	C
11	AA	1032	C
11	AA	1034	U
11	AA	1036	A
11	AA	1037	C
11	AA	1038	C
11	AA	1047	A
11	AA	1064	A
11	AA	1072	G
11	AA	1081	U
11	AA	1087	G
11	AA	1096	U
11	AA	1097	G
11	AA	1098	A
11	AA	1103	A
11	AA	1117	G

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Mol	Chain	Res	Type
11	AA	1131	G
11	AA	1144	U
11	AA	1153	A
11	AA	1159	A
11	AA	1160	C
11	AA	1180	A
11	AA	1181	U
11	AA	1182	A
11	AA	1191	U
11	AA	1192	C
11	AA	1193	A
11	AA	1196	C
11	AA	1201	C
11	AA	1208	U
11	AA	1209	G
11	AA	1222	G
11	AA	1235	U
11	AA	1236	G
11	AA	1240	A
11	AA	1241	U
11	AA	1242	G
11	AA	1245	A
11	AA	1258	U
11	AA	1262	G
11	AA	1263	A
11	AA	1265	U
11	AA	1272	C
11	AA	1302	A
11	AA	1307	G
11	AA	1308	A
11	AA	1309	U
11	AA	1345	G
11	AA	1348	U
11	AA	1349	G
11	AA	1351	U
11	AA	1352	A
11	AA	1353	U
11	AA	1355	A
11	AA	1356	U
11	AA	1357	G
11	AA	1386	A
11	AA	1392	G

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Mol	Chain	Res	Type
11	AA	1399	A
11	AA	1400	G
11	AA	1425	U
11	AA	1434	G
11	AA	1437	OMC
11	AA	1443	G
11	AA	1446	A
11	AA	1450	OMG
11	AA	1468	A
11	AA	1481	A
11	AA	1483	G
11	AA	1487	G
11	AA	1508	C
11	AA	1527	C
11	AA	1536	G
11	AA	1539	A
11	AA	1555	U
11	AA	1556	C
11	AA	1560	G
11	AA	1562	C
11	AA	1563	C
11	AA	1568	U
11	AA	1569	U
11	AA	1570	U
11	AA	1571	A
11	AA	1573	G
11	AA	1579	C
11	AA	1581	C
11	AA	1583	A
11	AA	1589	A
11	AA	1593	A
11	AA	1605	A
11	AA	1629	U
11	AA	1630	U
11	AA	1643	A
11	AA	1657	C
11	AA	1724	U
11	AA	1741	A
11	AA	1750	A
11	AA	1751	G
11	AA	1762	C
11	AA	1763	U

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Mol	Chain	Res	Type
11	AA	1765	U
11	AA	1767	C
11	AA	1769	G
11	AA	1796	G
11	AA	1797	A
11	AA	1815	U
11	AA	1816	A
11	AA	1817	G
11	AA	1820	U
11	AA	1821	U
11	AA	1842	A
11	AA	1866	C
11	AA	1867	A
11	AA	1878	G
11	AA	1879	A
11	AA	1880	U
11	AA	1893	A
11	AA	1906	G
11	AA	1935	G
11	AA	2102	U
11	AA	2112	U
11	AA	2114	C
11	AA	2122	G
11	AA	2131	A
11	AA	2140	U
11	AA	2144	A
11	AA	2158	A
11	AA	2168	A
11	AA	2169	G
11	AA	2170	U
11	AA	2171	G
11	AA	2188	A
11	AA	2206	G
11	AA	2208	A
11	AA	2223	A
11	AA	2244	A
11	AA	2249	G
11	AA	2258	U
11	AA	2265	C
11	AA	2272	G
11	AA	2273	G
11	AA	2281	A2M

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Mol	Chain	Res	Type
11	AA	2307	G
11	AA	2308	C
11	AA	2310	U
11	AA	2313	A
11	AA	2315	G
11	AA	2334	U
11	AA	2335	G
11	AA	2336	U
11	AA	2363	A
11	AA	2373	A
11	AA	2374	C
11	AA	2375	G
11	AA	2388	U
11	AA	2393	G
11	AA	2397	A
11	AA	2402	A
11	AA	2403	G
11	AA	2404	A
11	AA	2411	U
11	AA	2418	G
11	AA	2419	A
11	AA	2435	G
11	AA	2437	G
11	AA	2444	C
11	AA	2446	U
11	AA	2447	A
11	AA	2448	G
11	AA	2449	A
11	AA	2450	G
11	AA	2453	U
11	AA	2454	G
11	AA	2458	A
11	AA	2459	A
11	AA	2460	U
11	AA	2461	A
11	AA	2462	A
11	AA	2464	U
11	AA	2465	G
11	AA	2466	G
11	AA	2467	G
11	AA	2468	A
11	AA	2470	C

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Mol	Chain	Res	Type
11	AA	2471	U
11	AA	2472	U
11	AA	2473	C
11	AA	2474	G
11	AA	2475	G
11	AA	2477	G
11	AA	2478	C
11	AA	2479	C
11	AA	2480	A
11	AA	2481	G
11	AA	2486	A
11	AA	2487	U
11	AA	2488	A
11	AA	2489	C
11	AA	2490	C
11	AA	2491	A
11	AA	2492	C
11	AA	2494	A
11	AA	2495	C
11	AA	2496	C
11	AA	2499	U
11	AA	2500	A
11	AA	2501	U
11	AA	2502	A
11	AA	2505	U
11	AA	2511	A
11	AA	2514	U
11	AA	2515	A
11	AA	2522	G
11	AA	2523	A
11	AA	2534	G
11	AA	2536	A
11	AA	2539	C
11	AA	2541	U
11	AA	2542	U
11	AA	2549	G
11	AA	2552	C
11	AA	2554	A
11	AA	2560	C
11	AA	2561	A
11	AA	2569	A
11	AA	2570	U

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Mol	Chain	Res	Type
11	AA	2571	U
11	AA	2572	C
11	AA	2573	G
11	AA	2585	G
11	AA	2593	A
11	AA	2606	G
11	AA	2607	G
11	AA	2614	G
11	AA	2652	U
11	AA	2656	A
11	AA	2672	G
11	AA	2674	A
11	AA	2677	G
11	AA	2681	U
11	AA	2689	A
11	AA	2691	A
11	AA	2696	A
11	AA	2704	A
11	AA	2705	A
11	AA	2728	G
11	AA	2737	C
11	AA	2753	G
11	AA	2755	C
11	AA	2772	C
11	AA	2773	C
11	AA	2777	G
11	AA	2778	G
11	AA	2795	U
11	AA	2796	G
11	AA	2799	A
11	AA	2800	G
11	AA	2801	A
11	AA	2802	A
11	AA	2808	A
11	AA	2810	C
11	AA	2814	G
11	AA	2817	A
11	AA	2844	C
11	AA	2845	A
11	AA	2867	C
11	AA	2871	G
11	AA	2872	A

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Mol	Chain	Res	Type
11	AA	2887	A
11	AA	2898	G
11	AA	2899	C
11	AA	2910	A
11	AA	2914	G
11	AA	2922	OMG
11	AA	2923	U
11	AA	2935	U
11	AA	2936	A
11	AA	2938	G
11	AA	2942	C
11	AA	2947	G
11	AA	2971	A
11	AA	2972	G
11	AA	2977	G
11	AA	2983	C
11	AA	2990	G
11	AA	2997	G
11	AA	3012	A
11	AA	3056	U
11	AA	3059	G
11	AA	3078	U
11	AA	3080	G
11	AA	3092	C
11	AA	3101	G
11	AA	3104	U
11	AA	3116	G
11	AA	3122	A
11	AA	3130	A
11	AA	3131	U
11	AA	3142	A
11	AA	3143	C
11	AA	3153	U
11	AA	3154	C
11	AA	3155	U
11	AA	3156	U
11	AA	3157	U
11	AA	3168	A
11	AA	3170	A
11	AA	3172	A
11	AA	3173	G
11	AA	3176	G

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Mol	Chain	Res	Type
11	AA	3179	U
11	AA	3181	C
11	AA	3187	A
11	AA	3206	C
11	AA	3207	U
11	AA	3217	C
11	AA	3218	A
11	AA	3219	G
11	AA	3224	G
11	AA	3243	A
11	AA	3270	U
11	AA	3276	G
11	AA	3277	U
11	AA	3281	U
11	AA	3288	G
11	AA	3294	A
11	AA	3304	U
11	AA	3313	U
11	AA	3316	A
11	AA	3320	A
11	AA	3341	U
11	AA	3345	G
11	AA	3351	U
11	AA	3352	U
11	AA	3353	G
11	AA	3369	G
11	AA	3378	C
11	AA	3389	U
14	BB	7	G
14	BB	42	A
14	BB	54	U
14	BB	55	A
14	BB	65	G
14	BB	73	C
14	BB	76	A
14	BB	112	G
15	Bb	2	C
15	Bb	4	G
15	Bb	5	A
15	Bb	6	U
15	Bb	9	A
15	Bb	13	C

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Mol	Chain	Res	Type
15	Bb	15	G
15	Bb	16	U
15	Bb	17	U
15	Bb	18	G
15	Bb	19	G
15	Bb	21	A
15	Bb	22	G
15	Bb	23	A
15	Bb	26	G
15	Bb	39	U
15	Bb	40	C
15	Bb	41	U
15	Bb	42	G
15	Bb	46	G
15	Bb	47	U
15	Bb	48	C
15	Bb	49	C
15	Bb	54	U
15	Bb	55	U
15	Bb	58	A
15	Bb	59	U
15	Bb	61	C
15	Bb	62	A
15	Bb	63	C
15	Bb	66	A
15	Bb	68	U
15	Bb	69	U
15	Bb	70	C
15	Bb	71	G
15	Bb	76	A
17	CC	23	U
17	CC	34	U
17	CC	35	C
17	CC	52	A
17	CC	59	A
17	CC	62	C
17	CC	63	G
17	CC	82	U
17	CC	83	C
17	CC	84	C
17	CC	86	U
17	CC	87	G

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Mol	Chain	Res	Type
17	CC	91	C
17	CC	95	G
17	CC	104	A
17	CC	106	C
17	CC	113	U
17	CC	125	U
17	CC	126	A
17	CC	152	G
18	Cc	4	G
18	Cc	16	C
18	Cc	17	C
18	Cc	18	C
18	Cc	19	G
18	Cc	20	G
18	Cc	21	U
18	Cc	22	A
18	Cc	43	G
18	Cc	48	U
18	Cc	49	C
18	Cc	56	U
18	Cc	57	C
18	Cc	60	A
18	Cc	62	C
18	Cc	63	C
18	Cc	77	A
61	c	2	A
61	c	4	C
61	c	26	A
61	c	28	A2M
61	c	34	G
61	c	42	G
61	c	45	U
61	c	47	A
61	c	61	A
61	c	67	A
61	c	69	G
61	c	71	A
61	c	72	A
61	c	78	A
61	c	80	A
61	c	111	U
61	c	114	C

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Mol	Chain	Res	Type
61	c	116	U
61	c	127	G
61	c	130	C
61	c	131	C
61	c	139	C
61	c	140	A
61	c	144	U
61	c	145	A
61	c	146	U
61	c	168	A
61	c	176	C
61	c	184	C
61	c	204	G
61	c	257	A
61	c	261	U
61	c	262	U
61	c	272	U
61	c	277	U
61	c	278	U
61	c	279	G
61	c	285	G
61	c	287	G
61	c	299	A
61	c	309	C
61	c	314	C
61	c	316	A
61	c	320	U
61	c	321	C
61	c	322	G
61	c	337	G
61	c	338	C
61	c	361	C
61	c	390	G
61	c	400	A
61	c	401	A
61	c	402	C
61	c	404	G
61	c	417	A
61	c	422	G
61	c	423	G
61	c	424	C
61	c	426	G

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Mol	Chain	Res	Type
61	c	434	G
61	c	439	U
61	c	444	C
61	c	448	C
61	c	452	A
61	c	454	U
61	c	455	C
61	c	460	A
61	c	468	A
61	c	475	A
61	c	477	A
61	c	504	U
61	c	511	A
61	c	514	G
61	c	515	A
61	c	519	C
61	c	524	U
61	c	525	A
61	c	526	A
61	c	527	A
61	c	537	G
61	c	538	A
61	c	539	G
61	c	541	A2M
61	c	542	A
61	c	557	G
61	c	559	C
61	c	565	C
61	c	566	C
61	c	568	G
61	c	577	G
61	c	578	OMU
61	c	580	A
61	c	582	U
61	c	583	C
61	c	585	A
61	c	594	A
61	c	606	A
61	c	611	U
61	c	619	A2M
61	c	620	A
61	c	623	A

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Mol	Chain	Res	Type
61	c	624	G
61	c	639	U
61	c	644	C
61	c	645	C
61	c	647	G
61	c	648	G
61	c	649	U
61	c	650	U
61	c	651	G
61	c	688	G
61	c	692	C
61	c	695	U
61	c	696	C
61	c	743	U
61	c	745	U
61	c	760	A
61	c	765	G
61	c	775	G
61	c	778	G
61	c	780	A
61	c	781	U
61	c	782	U
61	c	783	G
61	c	784	C
61	c	789	A
61	c	794	U
61	c	795	U
61	c	809	A
61	c	812	A
61	c	814	A
61	c	819	G
61	c	820	U
61	c	821	U
61	c	851	U
61	c	852	C
61	c	853	G
61	c	854	U
61	c	859	A
61	c	860	U
61	c	863	A
61	c	895	G
61	c	898	A

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Mol	Chain	Res	Type
61	c	906	A
61	c	913	G
61	c	914	G
61	c	915	A
61	c	933	A
61	c	935	U
61	c	951	A
61	c	960	U
61	c	966	A
61	c	988	A
61	c	992	A
61	c	993	A
61	c	999	U
61	c	1001	A
61	c	1002	G
61	c	1003	A
61	c	1004	U
61	c	1005	A
61	c	1010	C
61	c	1021	C
61	c	1026	A
61	c	1027	A
61	c	1028	C
61	c	1031	U
61	c	1032	G
61	c	1053	G
61	c	1058	U
61	c	1059	U
61	c	1060	U
61	c	1061	A
61	c	1063	U
61	c	1076	A
61	c	1081	A
61	c	1082	C
61	c	1092	A
61	c	1093	A
61	c	1097	U
61	c	1100	G
61	c	1138	A
61	c	1150	G
61	c	1154	G
61	c	1158	C

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Mol	Chain	Res	Type
61	c	1159	C
61	c	1162	C
61	c	1183	A
61	c	1185	U
61	c	1192	C
61	c	1194	A
61	c	1196	A
61	c	1199	G
61	c	1200	G
61	c	1214	U
61	c	1217	A
61	c	1218	G
61	c	1219	A
61	c	1221	A
61	c	1222	C
61	c	1223	A
61	c	1224	A
61	c	1225	U
61	c	1226	A
61	c	1227	A
61	c	1228	G
61	c	1229	G
61	c	1238	A
61	c	1241	G
61	c	1244	A
61	c	1245	G
61	c	1246	C
61	c	1252	C
61	c	1256	A
61	c	1258	U
61	c	1259	U
61	c	1261	G
61	c	1274	C
61	c	1286	U
61	c	1297	G
61	c	1309	C
61	c	1314	U
61	c	1315	U
61	c	1316	G
61	c	1321	A
61	c	1325	A
61	c	1336	A

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Mol	Chain	Res	Type
61	c	1338	C
61	c	1339	C
61	c	1340	U
61	c	1341	A
61	c	1346	A
61	c	1351	G
61	c	1354	G
61	c	1355	C
61	c	1356	U
61	c	1361	U
61	c	1363	U
61	c	1364	G
61	c	1367	G
61	c	1370	U
61	c	1372	U
61	c	1373	C
61	c	1374	C
61	c	1390	U
61	c	1398	U
61	c	1399	C
61	c	1400	A
61	c	1410	A
61	c	1411	A
61	c	1412	G
61	c	1413	U
61	c	1414	U
61	c	1415	U
61	c	1424	A
61	c	1425	A
61	c	1427	A
61	c	1428	OMG
61	c	1431	C
61	c	1432	U
61	c	1433	G
61	c	1436	A
61	c	1445	G
61	c	1447	C
61	c	1458	G
61	c	1459	C
61	c	1460	A
61	c	1469	A
61	c	1471	A

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Mol	Chain	Res	Type
61	c	1472	C
61	c	1474	G
61	c	1478	G
61	c	1487	A
61	c	1489	U
61	c	1490	C
61	c	1491	U
61	c	1492	A
61	c	1496	U
61	c	1499	G
61	c	1510	U
61	c	1515	A
61	c	1516	A
61	c	1523	G
61	c	1524	A
61	c	1535	U
61	c	1536	G
61	c	1537	C
61	c	1539	G
61	c	1542	G
61	c	1557	U
61	c	1559	A
61	c	1572	OMG
61	c	1573	A
61	c	1575	G7M
61	c	1601	G
61	c	1631	A
61	c	1633	A
61	c	1634	C
61	c	1635	A
61	c	1657	U
61	c	1658	G
61	c	1678	A
61	c	1681	A
61	c	1682	U
61	c	1683	C
61	c	1684	U
61	c	1717	G
61	c	1756	A
61	c	1757	G
61	c	1760	G
61	c	1762	A

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Mol	Chain	Res	Type
61	c	1766	A
61	c	1769	U
61	c	1780	G
61	c	1792	G
61	c	1793	G
61	c	1794	A
61	c	1795	U
61	c	1796	C
61	c	1799	U

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	AA	601	U
11	AA	619	A
11	AA	873	C
11	AA	908	OMG
11	AA	916	G
11	AA	1016	C
11	AA	1033	U
11	AA	1235	U
11	AA	1562	C
11	AA	2101	C
11	AA	2372	A
11	AA	2418	G
11	AA	2458	A
11	AA	2467	G
11	AA	2487	U
11	AA	2490	C
11	AA	2500	A
11	AA	2501	U
11	AA	2535	A
11	AA	2870	5MC
11	AA	2922	OMG
11	AA	2971	A
11	AA	3121	U
11	AA	3206	C
14	BB	72	A

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

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$
61	OMU	c	578	61	19,22,23	3.14	8 (42%)	25,31,34	1.78	5 (20%)
11	OMC	AA	650	11	19,22,23	0.59	0	25,31,34	0.69	0
61	A2M	c	420	61	18,25,26	3.59	7 (38%)	20,36,39	3.31	5 (25%)
11	A2M	AA	1133	86,11	18,25,26	3.59	6 (33%)	20,36,39	3.48	6 (30%)
11	OMG	AA	1450	11	19,26,27	1.13	2 (10%)	21,38,41	0.77	1 (4%)
11	OMU	AA	2417	11	19,22,23	3.03	8 (42%)	25,31,34	1.81	5 (20%)
61	A2M	c	974	61	18,25,26	3.59	7 (38%)	20,36,39	3.32	4 (20%)
11	A2M	AA	876	11	18,25,26	3.58	7 (38%)	20,36,39	3.28	5 (25%)
61	MA6	c	1781	61	19,26,27	1.60	3 (15%)	18,38,41	3.35	3 (16%)
61	A2M	c	100	86,61	18,25,26	3.60	7 (38%)	20,36,39	3.29	5 (25%)
61	OMU	c	1269	61	19,22,23	3.15	8 (42%)	25,31,34	1.82	5 (20%)
11	A2M	AA	817	86,11	18,25,26	3.57	6 (33%)	20,36,39	3.45	4 (20%)
11	A2M	AA	2640	11	18,25,26	3.58	7 (38%)	20,36,39	3.25	5 (25%)
11	OMC	AA	2948	11	19,22,23	0.55	0	25,31,34	0.75	1 (4%)
11	OMG	AA	2619	11,15	19,26,27	1.19	2 (10%)	21,38,41	0.83	1 (4%)
61	OMG	c	1428	61	19,26,27	1.14	2 (10%)	21,38,41	0.79	1 (4%)
11	OMU	AA	1888	11	19,22,23	3.06	8 (42%)	25,31,34	1.94	6 (24%)
11	OMG	AA	805	11	19,26,27	1.19	2 (10%)	21,38,41	0.84	1 (4%)
11	OMU	AA	2724	11	19,22,23	3.04	8 (42%)	25,31,34	1.80	5 (20%)
11	OMG	AA	2288	11	19,26,27	1.18	2 (10%)	21,38,41	0.80	1 (4%)
11	OMU	AA	2921	86,11	19,22,23	3.08	8 (42%)	25,31,34	1.82	5 (20%)
61	A2M	c	28	61,84	18,25,26	3.57	7 (38%)	20,36,39	3.35	6 (30%)
11	1MA	AA	2142	86,11	17,25,26	1.04	2 (11%)	17,37,40	1.23	2 (11%)
61	OMC	c	1639	86,61	19,22,23	0.54	0	25,31,34	0.55	0
11	OMC	AA	2337	11	19,22,23	0.54	0	25,31,34	0.62	0
61	G7M	c	1575	61,18	20,26,27	2.41	6 (30%)	16,39,42	1.14	1 (6%)
11	A2M	AA	2220	11	18,25,26	3.58	7 (38%)	20,36,39	3.30	4 (20%)
11	OMU	AA	898	11	19,22,23	3.03	8 (42%)	25,31,34	1.80	5 (20%)
11	OMG	AA	867	11,87	19,26,27	1.19	2 (10%)	21,38,41	0.86	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	OMG	AA	908	11	19,26,27	1.27	2 (10%)	21,38,41	0.91	1 (4%)
11	A2M	AA	2280	11	18,25,26	3.58	7 (38%)	20,36,39	3.33	4 (20%)
11	OMG	AA	2791	11	19,26,27	1.16	2 (10%)	21,38,41	0.81	1 (4%)
11	OMC	AA	2959	86,11	19,22,23	0.56	0	25,31,34	0.68	0
61	A2M	c	541	61	18,25,26	3.58	7 (38%)	20,36,39	3.36	5 (25%)
11	UR3	AA	2634	11	19,22,23	2.87	6 (31%)	26,32,35	1.64	2 (7%)
61	MA6	c	1782	61	19,26,27	1.58	3 (15%)	18,38,41	3.42	3 (16%)
61	A2M	c	619	86,61	18,25,26	3.61	7 (38%)	20,36,39	3.38	4 (20%)
11	A2M	AA	807	11	18,25,26	3.60	7 (38%)	20,36,39	3.55	5 (25%)
61	OMG	c	1271	61	19,26,27	1.12	2 (10%)	21,38,41	0.83	1 (4%)
61	4AC	c	1280	61	21,24,25	3.54	10 (47%)	28,34,37	1.73	6 (21%)
61	A2M	c	436	61	18,25,26	3.60	7 (38%)	20,36,39	3.29	3 (15%)
11	OMG	AA	2922	11	19,26,27	1.19	2 (10%)	21,38,41	0.89	1 (4%)
61	OMG	c	1126	61	19,26,27	1.20	2 (10%)	21,38,41	0.83	1 (4%)
11	A2M	AA	2281	11	18,25,26	3.66	7 (38%)	20,36,39	3.90	6 (30%)
11	OMU	AA	2729	11	19,22,23	3.03	8 (42%)	25,31,34	1.74	5 (20%)
61	B8N	c	1191	61	25,29,30	3.39	7 (28%)	28,42,45	2.00	8 (28%)
11	A2M	AA	1449	86,11	18,25,26	3.59	7 (38%)	20,36,39	3.33	5 (25%)
15	YYG	Bb	37	15	30,42,43	2.28	8 (26%)	32,62,65	2.04	11 (34%)
11	A2M	AA	649	11	18,25,26	3.59	7 (38%)	20,36,39	3.27	4 (20%)
61	OMG	c	1572	61	19,26,27	1.13	2 (10%)	21,38,41	0.93	1 (4%)
11	OMC	AA	663	11	19,22,23	0.56	0	25,31,34	0.76	0
61	OMG	c	562	7,61	19,26,27	1.13	2 (10%)	21,38,41	0.82	1 (4%)
61	4AC	c	1773	61	21,24,25	3.36	10 (47%)	28,34,37	1.61	6 (21%)
11	OMG	AA	2815	11	19,26,27	1.17	2 (10%)	21,38,41	0.80	1 (4%)
11	5MC	AA	2278	86,11	19,22,23	0.55	0	26,32,35	0.66	0
11	OMU	AA	2347	11	19,22,23	3.09	8 (42%)	25,31,34	1.84	5 (20%)
11	5MC	AA	2870	11,87	19,22,23	0.67	0	26,32,35	0.62	0
11	OMG	AA	2793	11	19,26,27	1.19	3 (15%)	21,38,41	0.81	1 (4%)
61	A2M	c	796	61	18,25,26	3.61	7 (38%)	20,36,39	3.31	5 (25%)
11	OMU	AA	2421	11	19,22,23	3.06	8 (42%)	25,31,34	1.88	5 (20%)
11	OMC	AA	2197	11,87	19,22,23	0.55	0	25,31,34	0.57	0
61	OMC	c	414	61	19,22,23	0.52	0	25,31,34	0.67	0
61	OMC	c	1007	61	19,22,23	0.54	0	25,31,34	0.66	0
11	A2M	AA	2256	11	18,25,26	3.60	7 (38%)	20,36,39	3.71	7 (35%)
11	A2M	AA	2946	86,11	18,25,26	3.58	7 (38%)	20,36,39	3.36	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	OMC	AA	1437	86,11	19,22,23	0.57	0	25,31,34	0.90	1 (4%)
11	1MA	AA	645	86,11	17,25,26	0.97	2 (11%)	17,37,40	1.12	2 (11%)
12	DDE	Aa	699	12	15,20,21	0.98	1 (6%)	11,28,30	1.04	1 (9%)

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
61	OMU	c	578	61	-	2/9/27/28	0/2/2/2
11	OMC	AA	650	11	-	0/9/27/28	0/2/2/2
61	A2M	c	420	61	-	2/5/27/28	0/3/3/3
11	A2M	AA	1133	86,11	-	0/5/27/28	0/3/3/3
11	OMG	AA	1450	11	-	2/5/27/28	0/3/3/3
11	OMU	AA	2417	11	-	1/9/27/28	0/2/2/2
61	A2M	c	974	61	-	0/5/27/28	0/3/3/3
11	A2M	AA	876	11	-	0/5/27/28	0/3/3/3
61	MA6	c	1781	61	-	0/7/29/30	0/3/3/3
61	A2M	c	100	86,61	-	1/5/27/28	0/3/3/3
61	OMU	c	1269	61	-	3/9/27/28	0/2/2/2
11	A2M	AA	817	86,11	-	1/5/27/28	0/3/3/3
11	A2M	AA	2640	11	-	0/5/27/28	0/3/3/3
11	OMC	AA	2948	11	-	0/9/27/28	0/2/2/2
11	OMG	AA	2619	11,15	-	1/5/27/28	0/3/3/3
61	OMG	c	1428	61	-	1/5/27/28	0/3/3/3
11	OMU	AA	1888	11	-	0/9/27/28	0/2/2/2
11	OMG	AA	805	11	-	0/5/27/28	0/3/3/3
11	OMU	AA	2724	11	-	1/9/27/28	0/2/2/2
11	OMG	AA	2288	11	-	0/5/27/28	0/3/3/3
11	OMU	AA	2921	86,11	-	0/9/27/28	0/2/2/2
61	A2M	c	28	61,84	-	2/5/27/28	0/3/3/3
11	1MA	AA	2142	86,11	-	1/3/25/26	0/3/3/3
61	OMC	c	1639	86,61	-	0/9/27/28	0/2/2/2
11	OMC	AA	2337	11	-	0/9/27/28	0/2/2/2
61	G7M	c	1575	61,18	-	3/3/25/26	0/3/3/3
11	A2M	AA	2220	11	-	1/5/27/28	0/3/3/3
11	OMU	AA	898	11	-	0/9/27/28	0/2/2/2
11	OMG	AA	867	11,87	-	2/5/27/28	0/3/3/3
11	OMG	AA	908	11	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	A2M	AA	2280	11	-	0/5/27/28	0/3/3/3
11	OMG	AA	2791	11	-	0/5/27/28	0/3/3/3
11	OMC	AA	2959	86,11	-	0/9/27/28	0/2/2/2
61	A2M	c	541	61	-	3/5/27/28	0/3/3/3
11	UR3	AA	2634	11	-	0/7/25/26	0/2/2/2
61	MA6	c	1782	61	-	2/7/29/30	0/3/3/3
61	A2M	c	619	86,61	-	3/5/27/28	0/3/3/3
11	A2M	AA	807	11	-	1/5/27/28	0/3/3/3
61	OMG	c	1271	61	-	1/5/27/28	0/3/3/3
61	4AC	c	1280	61	-	4/11/29/30	0/2/2/2
61	A2M	c	436	61	-	0/5/27/28	0/3/3/3
11	OMG	AA	2922	11	-	2/5/27/28	0/3/3/3
61	OMG	c	1126	61	-	0/5/27/28	0/3/3/3
11	A2M	AA	2281	11	-	3/5/27/28	0/3/3/3
11	OMU	AA	2729	11	-	0/9/27/28	0/2/2/2
61	B8N	c	1191	61	-	5/16/34/35	0/2/2/2
11	A2M	AA	1449	86,11	-	0/5/27/28	0/3/3/3
15	YYG	Bb	37	15	-	14/20/42/43	0/3/4/4
11	A2M	AA	649	11	-	1/5/27/28	0/3/3/3
61	OMG	c	1572	61	-	3/5/27/28	0/3/3/3
11	OMC	AA	663	11	-	1/9/27/28	0/2/2/2
61	OMG	c	562	7,61	-	1/5/27/28	0/3/3/3
61	4AC	c	1773	61	-	2/11/29/30	0/2/2/2
11	OMG	AA	2815	11	-	0/5/27/28	0/3/3/3
11	5MC	AA	2278	86,11	-	0/7/25/26	0/2/2/2
11	OMU	AA	2347	11	-	0/9/27/28	0/2/2/2
11	5MC	AA	2870	11,87	-	4/7/25/26	0/2/2/2
11	OMG	AA	2793	11	-	1/5/27/28	0/3/3/3
61	A2M	c	796	61	-	0/5/27/28	0/3/3/3
11	OMU	AA	2421	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2197	11,87	-	4/9/27/28	0/2/2/2
61	OMC	c	414	61	-	1/9/27/28	0/2/2/2
61	OMC	c	1007	61	-	0/9/27/28	0/2/2/2
11	A2M	AA	2256	11	-	1/5/27/28	0/3/3/3
11	A2M	AA	2946	86,11	-	0/5/27/28	0/3/3/3
11	OMC	AA	1437	86,11	-	1/9/27/28	0/2/2/2
11	1MA	AA	645	86,11	-	0/3/25/26	0/3/3/3
12	DDE	Aa	699	12	-	4/20/21/23	0/1/1/1

All (307) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	28	A2M	C3'-C4'	-9.14	1.29	1.53
11	AA	807	A2M	C3'-C4'	-8.96	1.30	1.53
61	c	541	A2M	C3'-C4'	-8.93	1.30	1.53
11	AA	2280	A2M	C3'-C4'	-8.93	1.30	1.53
61	c	619	A2M	C3'-C4'	-8.92	1.30	1.53
61	c	974	A2M	C3'-C4'	-8.92	1.30	1.53
61	c	796	A2M	C3'-C4'	-8.92	1.30	1.53
61	c	100	A2M	C3'-C4'	-8.91	1.30	1.53
11	AA	1133	A2M	C3'-C4'	-8.90	1.30	1.53
61	c	420	A2M	C3'-C4'	-8.90	1.30	1.53
11	AA	876	A2M	C3'-C4'	-8.87	1.30	1.53
11	AA	2220	A2M	C3'-C4'	-8.86	1.30	1.53
61	c	436	A2M	C3'-C4'	-8.85	1.30	1.53
11	AA	2640	A2M	C3'-C4'	-8.84	1.30	1.53
11	AA	649	A2M	C3'-C4'	-8.83	1.30	1.53
11	AA	2946	A2M	C3'-C4'	-8.81	1.30	1.53
11	AA	817	A2M	C3'-C4'	-8.80	1.30	1.53
11	AA	1449	A2M	C3'-C4'	-8.77	1.30	1.53
11	AA	2256	A2M	C3'-C4'	-8.52	1.31	1.53
11	AA	2281	A2M	O4'-C1'	-8.48	1.29	1.40
11	AA	2281	A2M	C3'-C4'	-8.47	1.31	1.53
61	c	1191	B8N	C6-N1	8.04	1.56	1.36
11	AA	2256	A2M	O4'-C4'	8.02	1.62	1.45
61	c	619	A2M	O4'-C1'	-7.89	1.30	1.40
61	c	796	A2M	O4'-C4'	7.77	1.62	1.45
61	c	1280	4AC	C4-N3	7.75	1.45	1.32
61	c	1191	B8N	C4-N3	-7.73	1.26	1.40
11	AA	807	A2M	O4'-C1'	-7.72	1.30	1.40
11	AA	2946	A2M	O4'-C4'	7.71	1.62	1.45
11	AA	1133	A2M	O4'-C4'	7.70	1.62	1.45
11	AA	2220	A2M	O4'-C4'	7.69	1.62	1.45
61	c	1191	B8N	C4-C5	7.68	1.65	1.47
11	AA	1449	A2M	O4'-C4'	7.68	1.62	1.45
11	AA	649	A2M	O4'-C1'	-7.65	1.30	1.40
11	AA	2256	A2M	O4'-C1'	-7.64	1.30	1.40
61	c	420	A2M	O4'-C4'	7.63	1.61	1.45
61	c	436	A2M	O4'-C4'	7.62	1.61	1.45
61	c	974	A2M	O4'-C4'	7.60	1.61	1.45
11	AA	876	A2M	O4'-C4'	7.60	1.61	1.45
11	AA	2640	A2M	O4'-C4'	7.59	1.61	1.45
11	AA	2281	A2M	O4'-C4'	7.58	1.61	1.45
61	c	100	A2M	O4'-C4'	7.56	1.61	1.45
61	c	541	A2M	O4'-C4'	7.56	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	436	A2M	O4'-C1'	-7.54	1.31	1.40
11	AA	649	A2M	O4'-C4'	7.52	1.61	1.45
61	c	28	A2M	O4'-C4'	7.50	1.61	1.45
11	AA	1449	A2M	O4'-C1'	-7.49	1.31	1.40
11	AA	817	A2M	O4'-C1'	-7.49	1.31	1.40
61	c	1269	OMU	C2-N1	7.48	1.50	1.38
61	c	100	A2M	O4'-C1'	-7.48	1.31	1.40
11	AA	2280	A2M	O4'-C1'	-7.47	1.31	1.40
11	AA	2640	A2M	O4'-C1'	-7.47	1.31	1.40
11	AA	2280	A2M	O4'-C4'	7.45	1.61	1.45
11	AA	817	A2M	O4'-C4'	7.45	1.61	1.45
61	c	420	A2M	O4'-C1'	-7.44	1.31	1.40
11	AA	876	A2M	O4'-C1'	-7.43	1.31	1.40
11	AA	1133	A2M	O4'-C1'	-7.42	1.31	1.40
11	AA	2347	OMU	C2-N1	7.40	1.50	1.38
61	c	578	OMU	C2-N1	7.37	1.50	1.38
61	c	974	A2M	O4'-C1'	-7.37	1.31	1.40
11	AA	2946	A2M	O4'-C1'	-7.37	1.31	1.40
61	c	796	A2M	O4'-C1'	-7.37	1.31	1.40
61	c	541	A2M	O4'-C1'	-7.33	1.31	1.40
11	AA	2220	A2M	O4'-C1'	-7.30	1.31	1.40
61	c	1773	4AC	C4-N3	7.30	1.45	1.32
11	AA	807	A2M	O4'-C4'	7.30	1.61	1.45
61	c	619	A2M	O4'-C4'	7.27	1.61	1.45
11	AA	1888	OMU	C2-N1	7.23	1.49	1.38
11	AA	2921	OMU	C2-N1	7.23	1.49	1.38
11	AA	2421	OMU	C2-N1	7.17	1.49	1.38
61	c	28	A2M	O4'-C1'	-7.14	1.31	1.40
15	Bb	37	YYG	C21-N20	7.13	1.52	1.34
11	AA	2724	OMU	C2-N1	7.10	1.49	1.38
61	c	578	OMU	C2-N3	7.07	1.50	1.38
11	AA	898	OMU	C2-N1	7.07	1.49	1.38
11	AA	2417	OMU	C2-N1	6.96	1.49	1.38
61	c	1269	OMU	C2-N3	6.95	1.50	1.38
61	c	1773	4AC	C6-C5	6.89	1.51	1.35
11	AA	2634	UR3	C2-N1	6.87	1.48	1.38
11	AA	2347	OMU	C2-N3	6.87	1.49	1.38
11	AA	2729	OMU	C2-N1	6.84	1.49	1.38
11	AA	2921	OMU	C2-N3	6.82	1.49	1.38
11	AA	2729	OMU	C2-N3	6.80	1.49	1.38
11	AA	2724	OMU	C2-N3	6.80	1.49	1.38
11	AA	2421	OMU	C2-N3	6.76	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2417	OMU	C2-N3	6.75	1.49	1.38
11	AA	2634	UR3	C6-C5	6.72	1.50	1.35
11	AA	898	OMU	C2-N3	6.72	1.49	1.38
11	AA	1888	OMU	C2-N3	6.71	1.49	1.38
61	c	1280	4AC	C6-C5	6.70	1.50	1.35
61	c	1191	B8N	C2-N1	5.94	1.56	1.39
61	c	578	OMU	C6-C5	5.80	1.48	1.35
61	c	1269	OMU	C6-C5	5.76	1.48	1.35
15	Bb	37	YYG	O23-C21	5.71	1.43	1.34
11	AA	2921	OMU	C6-C5	5.71	1.48	1.35
11	AA	2729	OMU	C6-C5	5.69	1.48	1.35
11	AA	1888	OMU	C6-C5	5.67	1.48	1.35
11	AA	2417	OMU	C6-C5	5.65	1.48	1.35
11	AA	898	OMU	C6-C5	5.65	1.48	1.35
11	AA	2421	OMU	C6-C5	5.63	1.48	1.35
11	AA	2724	OMU	C6-C5	5.59	1.48	1.35
11	AA	2347	OMU	C6-C5	5.57	1.48	1.35
11	AA	2634	UR3	C2-N3	5.52	1.49	1.39
61	c	1280	4AC	C2-N1	5.46	1.51	1.40
61	c	1575	G7M	C2-N3	5.39	1.46	1.33
61	c	1191	B8N	C6-C5	5.35	1.42	1.35
61	c	1280	4AC	C2-N3	5.32	1.46	1.36
61	c	1280	4AC	C7-N4	5.23	1.47	1.37
61	c	1773	4AC	C2-N1	5.01	1.50	1.40
61	c	1280	4AC	C4-N4	4.97	1.47	1.39
61	c	1575	G7M	C4-N3	4.92	1.49	1.37
61	c	1773	4AC	C7-N4	4.81	1.47	1.37
61	c	1575	G7M	C2-N2	4.75	1.45	1.34
61	c	1773	4AC	C2-N3	4.75	1.45	1.36
61	c	1773	4AC	C4-N4	4.64	1.46	1.39
61	c	578	OMU	C4-N3	4.51	1.46	1.38
61	c	1269	OMU	C4-N3	4.45	1.46	1.38
61	c	1781	MA6	C6-N6	4.38	1.47	1.37
11	AA	2724	OMU	C4-N3	4.28	1.45	1.38
61	c	1782	MA6	C6-N6	4.28	1.47	1.37
11	AA	2347	OMU	C4-N3	4.25	1.45	1.38
11	AA	2417	OMU	C4-N3	4.24	1.45	1.38
11	AA	1888	OMU	C4-N3	4.23	1.45	1.38
11	AA	2729	OMU	C4-N3	4.20	1.45	1.38
11	AA	2921	OMU	C4-N3	4.20	1.45	1.38
61	c	1280	4AC	CM7-C7	4.20	1.59	1.50
11	AA	2421	OMU	C4-N3	4.18	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	898	OMU	C4-N3	4.17	1.45	1.38
61	c	1781	MA6	C6-C5	-4.13	1.38	1.44
61	c	1191	B8N	C1'-C5	4.11	1.59	1.50
61	c	1782	MA6	C6-C5	-4.10	1.38	1.44
15	Bb	37	YYG	O18-C16	3.95	1.42	1.33
61	c	1773	4AC	C5-C4	3.86	1.49	1.41
61	c	1280	4AC	C5-C4	3.79	1.49	1.41
15	Bb	37	YYG	C13-C12	3.78	1.58	1.50
61	c	1773	4AC	CM7-C7	3.71	1.58	1.50
61	c	1575	G7M	C6-N1	3.62	1.43	1.37
11	AA	2634	UR3	C6-N1	3.35	1.46	1.38
15	Bb	37	YYG	C4-N3	-3.28	1.35	1.40
11	AA	908	OMG	C8-N7	-3.25	1.29	1.34
11	AA	2256	A2M	C6-N6	3.20	1.45	1.34
61	c	541	A2M	C6-N6	3.19	1.45	1.34
61	c	28	A2M	C6-N6	3.18	1.45	1.34
61	c	420	A2M	C6-N6	3.18	1.45	1.34
61	c	436	A2M	C6-N6	3.17	1.45	1.34
11	AA	2640	A2M	C6-N6	3.17	1.45	1.34
11	AA	2220	A2M	C6-N6	3.17	1.45	1.34
61	c	1575	G7M	C5-C6	3.16	1.53	1.45
11	AA	2280	A2M	C6-N6	3.16	1.45	1.34
61	c	796	A2M	C6-N6	3.16	1.45	1.34
61	c	100	A2M	C6-N6	3.16	1.45	1.34
61	c	619	A2M	C6-N6	3.16	1.45	1.34
11	AA	2288	OMG	C8-N7	-3.16	1.29	1.34
11	AA	807	A2M	C6-N6	3.15	1.45	1.34
61	c	974	A2M	C6-N6	3.14	1.45	1.34
11	AA	876	A2M	C6-N6	3.14	1.45	1.34
11	AA	2421	OMU	O4-C4	-3.13	1.18	1.24
11	AA	867	OMG	C8-N7	-3.13	1.29	1.34
11	AA	2922	OMG	C8-N7	-3.12	1.29	1.34
11	AA	649	A2M	C6-N6	3.12	1.45	1.34
11	AA	1449	A2M	C6-N6	3.12	1.45	1.34
11	AA	2946	A2M	C6-N6	3.11	1.45	1.34
11	AA	1133	A2M	C6-N6	3.10	1.45	1.34
11	AA	2619	OMG	C8-N7	-3.09	1.30	1.34
11	AA	2417	OMU	O4-C4	-3.09	1.18	1.24
11	AA	817	A2M	C6-N6	3.09	1.45	1.34
11	AA	2729	OMU	O4-C4	-3.08	1.18	1.24
11	AA	898	OMU	O4-C4	-3.07	1.18	1.24
11	AA	2724	OMU	O4-C4	-3.06	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2921	OMU	O4-C4	-3.06	1.18	1.24
61	c	1126	OMG	C8-N7	-3.05	1.30	1.34
11	AA	2815	OMG	C8-N7	-3.04	1.30	1.34
11	AA	805	OMG	C8-N7	-3.03	1.30	1.34
11	AA	1888	OMU	O4-C4	-3.02	1.18	1.24
11	AA	2793	OMG	C8-N7	-3.02	1.30	1.34
11	AA	2791	OMG	C8-N7	-3.02	1.30	1.34
11	AA	2347	OMU	O4-C4	-3.01	1.18	1.24
61	c	1269	OMU	C6-N1	3.00	1.45	1.38
11	AA	2281	A2M	C6-N6	2.98	1.44	1.34
61	c	1428	OMG	C8-N7	-2.96	1.30	1.34
61	c	578	OMU	C6-N1	2.93	1.45	1.38
61	c	1269	OMU	O4-C4	-2.89	1.18	1.24
11	AA	2729	OMU	C6-N1	2.87	1.44	1.38
11	AA	2417	OMU	C6-N1	2.87	1.44	1.38
11	AA	2142	1MA	C8-N7	-2.86	1.30	1.34
11	AA	1888	OMU	C6-N1	2.84	1.44	1.38
61	c	562	OMG	C8-N7	-2.83	1.30	1.34
61	c	578	OMU	O4-C4	-2.83	1.19	1.24
11	AA	1449	A2M	O3'-C3'	2.81	1.49	1.43
11	AA	1450	OMG	C8-N7	-2.81	1.30	1.34
61	c	796	A2M	O2'-C2'	-2.80	1.35	1.42
11	AA	807	A2M	O2'-C2'	-2.79	1.35	1.42
61	c	1271	OMG	C8-N7	-2.79	1.30	1.34
11	AA	817	A2M	O3'-C3'	2.78	1.49	1.43
61	c	436	A2M	O3'-C3'	2.78	1.49	1.43
61	c	974	A2M	O2'-C2'	-2.78	1.35	1.42
11	AA	2421	OMU	C6-N1	2.78	1.44	1.38
11	AA	876	A2M	O2'-C2'	-2.78	1.35	1.42
61	c	1575	G7M	C2-N1	2.78	1.44	1.37
11	AA	2946	A2M	O2'-C2'	-2.78	1.35	1.42
11	AA	2281	A2M	O3'-C3'	2.78	1.49	1.43
11	AA	2921	OMU	C6-N1	2.76	1.44	1.38
15	Bb	37	YYG	C10-C11	2.76	1.54	1.50
11	AA	817	A2M	O2'-C2'	-2.76	1.35	1.42
11	AA	1449	A2M	O2'-C2'	-2.75	1.35	1.42
11	AA	2256	A2M	O3'-C3'	2.75	1.49	1.43
61	c	619	A2M	O3'-C3'	2.75	1.49	1.43
11	AA	2724	OMU	C6-N1	2.75	1.44	1.38
11	AA	2281	A2M	O2'-C2'	-2.74	1.35	1.42
11	AA	2347	OMU	C6-N1	2.74	1.44	1.38
61	c	100	A2M	O2'-C2'	-2.73	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	436	A2M	O2'-C2'	-2.73	1.35	1.42
11	AA	898	OMU	C6-N1	2.73	1.44	1.38
11	AA	2640	A2M	O2'-C2'	-2.73	1.35	1.42
61	c	100	A2M	O3'-C3'	2.72	1.49	1.43
11	AA	2280	A2M	O2'-C2'	-2.72	1.35	1.42
11	AA	1133	A2M	O2'-C2'	-2.72	1.35	1.42
61	c	1572	OMG	C8-N7	-2.72	1.30	1.34
11	AA	2220	A2M	O2'-C2'	-2.70	1.36	1.42
61	c	541	A2M	O3'-C3'	2.70	1.49	1.43
61	c	420	A2M	O3'-C3'	2.69	1.49	1.43
11	AA	2640	A2M	O3'-C3'	2.68	1.49	1.43
11	AA	649	A2M	O2'-C2'	-2.67	1.36	1.42
61	c	541	A2M	O2'-C2'	-2.67	1.36	1.42
11	AA	2946	A2M	O3'-C3'	2.66	1.49	1.43
11	AA	1133	A2M	O3'-C3'	2.65	1.49	1.43
61	c	420	A2M	O2'-C2'	-2.65	1.36	1.42
61	c	796	A2M	O3'-C3'	2.64	1.49	1.43
11	AA	2220	A2M	O3'-C3'	2.64	1.49	1.43
11	AA	645	1MA	C8-N7	-2.64	1.30	1.34
11	AA	898	OMU	O2-C2	-2.63	1.18	1.23
11	AA	2347	OMU	O2-C2	-2.63	1.18	1.23
11	AA	876	A2M	O3'-C3'	2.63	1.49	1.43
61	c	1126	OMG	C5-C6	-2.62	1.42	1.47
11	AA	807	A2M	O3'-C3'	2.62	1.49	1.43
11	AA	2921	OMU	O2-C2	-2.62	1.18	1.23
61	c	974	A2M	O3'-C3'	2.61	1.49	1.43
61	c	28	A2M	O2'-C2'	-2.60	1.36	1.42
11	AA	649	A2M	O3'-C3'	2.60	1.49	1.43
11	AA	2421	OMU	O2-C2	-2.59	1.18	1.23
11	AA	2280	A2M	O3'-C3'	2.58	1.49	1.43
61	c	1773	4AC	C6-N1	2.58	1.44	1.38
11	AA	2634	UR3	C4-N3	2.58	1.45	1.40
11	AA	908	OMG	C5-C6	-2.58	1.42	1.47
11	AA	2922	OMG	C5-C6	-2.58	1.42	1.47
61	c	619	A2M	O2'-C2'	-2.57	1.36	1.42
11	AA	2288	OMG	C5-C6	-2.57	1.42	1.47
15	Bb	37	YYG	C2-N1	-2.57	1.32	1.37
11	AA	2619	OMG	C5-C6	-2.56	1.42	1.47
11	AA	2793	OMG	C5-C6	-2.55	1.42	1.47
11	AA	2729	OMU	O2-C2	-2.55	1.18	1.23
11	AA	2815	OMG	C5-C6	-2.54	1.42	1.47
61	c	1280	4AC	C6-N1	2.53	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	867	OMG	C5-C6	-2.53	1.42	1.47
11	AA	805	OMG	C5-C6	-2.52	1.42	1.47
61	c	578	OMU	C5-C4	2.51	1.49	1.43
61	c	1269	OMU	O2-C2	-2.51	1.18	1.23
61	c	28	A2M	O3'-C3'	2.51	1.49	1.43
11	AA	2724	OMU	O2-C2	-2.51	1.18	1.23
11	AA	2417	OMU	O2-C2	-2.51	1.18	1.23
11	AA	1888	OMU	C5-C4	2.49	1.49	1.43
61	c	1269	OMU	C5-C4	2.49	1.49	1.43
11	AA	1888	OMU	O2-C2	-2.46	1.18	1.23
61	c	1428	OMG	C5-C6	-2.46	1.42	1.47
11	AA	1450	OMG	C5-C6	-2.45	1.42	1.47
61	c	1782	MA6	C2-N3	2.45	1.35	1.32
11	AA	2421	OMU	C5-C4	2.44	1.49	1.43
11	AA	2791	OMG	C5-C6	-2.43	1.42	1.47
61	c	1781	MA6	C2-N3	2.42	1.35	1.32
61	c	1271	OMG	C5-C6	-2.42	1.42	1.47
11	AA	2729	OMU	C5-C4	2.42	1.48	1.43
11	AA	2417	OMU	C5-C4	2.39	1.48	1.43
11	AA	2921	OMU	C5-C4	2.39	1.48	1.43
61	c	562	OMG	C5-C6	-2.38	1.42	1.47
61	c	1572	OMG	C5-C6	-2.38	1.42	1.47
11	AA	645	1MA	C5-C4	-2.37	1.37	1.43
61	c	578	OMU	O2-C2	-2.37	1.18	1.23
11	AA	2142	1MA	C5-C4	-2.37	1.37	1.43
11	AA	898	OMU	C5-C4	2.36	1.48	1.43
61	c	1773	4AC	O7-C7	-2.34	1.18	1.23
11	AA	2634	UR3	C5-C4	2.32	1.49	1.43
11	AA	2724	OMU	C5-C4	2.30	1.48	1.43
11	AA	2256	A2M	C2-N3	2.29	1.35	1.32
61	c	1280	4AC	O7-C7	-2.29	1.18	1.23
11	AA	2256	A2M	O2'-C2'	-2.28	1.37	1.42
61	c	541	A2M	C2-N3	2.26	1.35	1.32
61	c	28	A2M	C2-N3	2.24	1.35	1.32
11	AA	2347	OMU	C5-C4	2.23	1.48	1.43
61	c	420	A2M	C2-N3	2.22	1.35	1.32
61	c	436	A2M	C2-N3	2.20	1.35	1.32
61	c	100	A2M	C2-N3	2.18	1.35	1.32
11	AA	2640	A2M	C2-N3	2.16	1.35	1.32
11	AA	2280	A2M	C2-N3	2.14	1.35	1.32
61	c	796	A2M	C2-N3	2.14	1.35	1.32
61	c	1191	B8N	O4-C4	-2.13	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2220	A2M	C2-N3	2.12	1.35	1.32
11	AA	649	A2M	C2-N3	2.12	1.35	1.32
11	AA	876	A2M	C2-N3	2.12	1.35	1.32
12	Aa	699	DDE	CD2-NE2	2.09	1.39	1.36
11	AA	807	A2M	C2-N3	2.09	1.35	1.32
11	AA	2281	A2M	C2-N3	2.08	1.35	1.32
11	AA	1449	A2M	C2-N3	2.08	1.35	1.32
61	c	619	A2M	C2-N3	2.06	1.35	1.32
61	c	974	A2M	C2-N3	2.06	1.35	1.32
11	AA	2946	A2M	C2-N3	2.05	1.35	1.32
11	AA	2793	OMG	C5-C4	-2.01	1.38	1.43
15	Bb	37	YYG	O6-C6	-2.01	1.18	1.23

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	c	1782	MA6	N1-C6-N6	-12.46	102.43	116.83
61	c	1781	MA6	N1-C6-N6	-12.04	102.92	116.83
11	AA	817	A2M	C5-C6-N6	11.19	137.36	120.31
11	AA	1133	A2M	C5-C6-N6	10.82	136.79	120.31
11	AA	1449	A2M	C5-C6-N6	10.69	136.59	120.31
11	AA	2220	A2M	C5-C6-N6	10.65	136.53	120.31
61	c	420	A2M	C5-C6-N6	10.63	136.51	120.31
61	c	619	A2M	C5-C6-N6	10.61	136.47	120.31
11	AA	807	A2M	C5-C6-N6	10.61	136.47	120.31
61	c	436	A2M	C5-C6-N6	10.58	136.43	120.31
61	c	796	A2M	C5-C6-N6	10.58	136.42	120.31
11	AA	2280	A2M	C5-C6-N6	10.53	136.36	120.31
61	c	28	A2M	C5-C6-N6	10.52	136.34	120.31
61	c	974	A2M	C5-C6-N6	10.52	136.33	120.31
11	AA	876	A2M	C5-C6-N6	10.51	136.33	120.31
61	c	100	A2M	C5-C6-N6	10.49	136.30	120.31
11	AA	2256	A2M	C5-C6-N6	10.48	136.28	120.31
11	AA	649	A2M	C5-C6-N6	10.47	136.25	120.31
11	AA	2640	A2M	C5-C6-N6	10.45	136.23	120.31
11	AA	2946	A2M	C5-C6-N6	10.32	136.04	120.31
61	c	541	A2M	C5-C6-N6	10.26	135.94	120.31
11	AA	2281	A2M	C5-C6-N6	10.17	135.81	120.31
11	AA	2281	A2M	C4'-O4'-C1'	-8.98	101.70	109.92
11	AA	817	A2M	N6-C6-N1	-7.28	102.78	118.33
11	AA	1449	A2M	N6-C6-N1	-6.96	103.47	118.33
61	c	436	A2M	N6-C6-N1	-6.95	103.49	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	1133	A2M	N6-C6-N1	-6.92	103.55	118.33
61	c	420	A2M	N6-C6-N1	-6.91	103.57	118.33
11	AA	2256	A2M	N6-C6-N1	-6.87	103.65	118.33
11	AA	2280	A2M	N6-C6-N1	-6.87	103.66	118.33
11	AA	2220	A2M	N6-C6-N1	-6.86	103.67	118.33
11	AA	807	A2M	N6-C6-N1	-6.86	103.68	118.33
61	c	796	A2M	N6-C6-N1	-6.86	103.68	118.33
61	c	619	A2M	N6-C6-N1	-6.84	103.72	118.33
61	c	28	A2M	N6-C6-N1	-6.83	103.73	118.33
61	c	100	A2M	N6-C6-N1	-6.82	103.77	118.33
61	c	974	A2M	N6-C6-N1	-6.78	103.84	118.33
11	AA	649	A2M	N6-C6-N1	-6.78	103.84	118.33
11	AA	2281	A2M	N6-C6-N1	-6.76	103.89	118.33
11	AA	876	A2M	N6-C6-N1	-6.74	103.92	118.33
11	AA	2640	A2M	N6-C6-N1	-6.74	103.94	118.33
11	AA	1133	A2M	N3-C2-N1	-6.72	119.55	128.67
61	c	974	A2M	N3-C2-N1	-6.72	119.55	128.67
11	AA	2946	A2M	N6-C6-N1	-6.71	104.00	118.33
61	c	541	A2M	N6-C6-N1	-6.63	104.16	118.33
61	c	619	A2M	N3-C2-N1	-6.60	119.71	128.67
11	AA	649	A2M	N3-C2-N1	-6.60	119.72	128.67
61	c	28	A2M	N3-C2-N1	-6.59	119.73	128.67
11	AA	2256	A2M	N3-C2-N1	-6.57	119.76	128.67
11	AA	2946	A2M	N3-C2-N1	-6.55	119.79	128.67
11	AA	2281	A2M	N3-C2-N1	-6.52	119.82	128.67
11	AA	817	A2M	N3-C2-N1	-6.51	119.83	128.67
11	AA	2220	A2M	N3-C2-N1	-6.48	119.87	128.67
11	AA	1449	A2M	N3-C2-N1	-6.47	119.89	128.67
11	AA	876	A2M	N3-C2-N1	-6.43	119.94	128.67
61	c	436	A2M	N3-C2-N1	-6.43	119.94	128.67
61	c	100	A2M	N3-C2-N1	-6.40	119.98	128.67
11	AA	807	A2M	C4'-O4'-C1'	-6.37	104.09	109.92
61	c	420	A2M	N3-C2-N1	-6.36	120.04	128.67
61	c	1781	MA6	N3-C2-N1	-6.35	120.06	128.67
11	AA	2280	A2M	N3-C2-N1	-6.32	120.09	128.67
61	c	796	A2M	N3-C2-N1	-6.32	120.10	128.67
11	AA	807	A2M	N3-C2-N1	-6.27	120.16	128.67
11	AA	2640	A2M	N3-C2-N1	-6.27	120.17	128.67
61	c	541	A2M	N3-C2-N1	-6.25	120.18	128.67
61	c	1782	MA6	N3-C2-N1	-6.23	120.22	128.67
61	c	1280	4AC	CM7-C7-N4	6.17	125.22	115.27
11	AA	2634	UR3	C4-N3-C2	-6.02	119.73	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	2421	OMU	C4-N3-C2	-5.92	119.26	126.61
11	AA	1888	OMU	C4-N3-C2	-5.88	119.31	126.61
11	AA	2256	A2M	C4'-O4'-C1'	-5.79	104.62	109.92
11	AA	898	OMU	C4-N3-C2	-5.66	119.58	126.61
61	c	1773	4AC	CM7-C7-N4	5.66	124.40	115.27
11	AA	2921	OMU	C4-N3-C2	-5.65	119.60	126.61
11	AA	2417	OMU	C4-N3-C2	-5.61	119.64	126.61
11	AA	2347	OMU	C4-N3-C2	-5.57	119.70	126.61
61	c	578	OMU	C4-N3-C2	-5.51	119.77	126.61
11	AA	2724	OMU	C4-N3-C2	-5.48	119.81	126.61
61	c	1269	OMU	C4-N3-C2	-5.43	119.87	126.61
11	AA	2729	OMU	C4-N3-C2	-5.36	119.96	126.61
15	Bb	37	YYG	O23-C21-N20	5.25	119.60	110.77
61	c	1191	B8N	C5-C4-N3	5.15	125.51	116.15
61	c	1191	B8N	C4-N3-C2	-4.51	120.06	125.62
61	c	541	A2M	C4'-O4'-C1'	-4.22	106.06	109.92
11	AA	2421	OMU	N3-C2-N1	4.16	120.30	114.89
11	AA	1888	OMU	N3-C2-N1	4.12	120.26	114.89
11	AA	2921	OMU	N3-C2-N1	3.98	120.08	114.89
61	c	1269	OMU	N3-C2-N1	3.95	120.03	114.89
11	AA	2417	OMU	N3-C2-N1	3.89	119.96	114.89
11	AA	898	OMU	N3-C2-N1	3.88	119.94	114.89
15	Bb	37	YYG	C13-C12-N1	3.86	129.49	122.55
11	AA	2724	OMU	N3-C2-N1	3.82	119.87	114.89
61	c	578	OMU	N3-C2-N1	3.82	119.86	114.89
11	AA	2347	OMU	N3-C2-N1	3.78	119.82	114.89
11	AA	2634	UR3	C5-C4-N3	3.78	120.02	115.04
11	AA	2946	A2M	C4'-O4'-C1'	-3.73	106.51	109.92
11	AA	2421	OMU	C5-C4-N3	3.68	119.95	114.80
11	AA	898	OMU	C5-C4-N3	3.65	119.91	114.80
11	AA	2347	OMU	C5-C4-N3	3.64	119.90	114.80
11	AA	2417	OMU	C5-C4-N3	3.64	119.90	114.80
11	AA	1888	OMU	C5-C4-N3	3.64	119.89	114.80
11	AA	2724	OMU	C5-C4-N3	3.63	119.88	114.80
61	c	619	A2M	C4'-O4'-C1'	-3.63	106.60	109.92
11	AA	2256	A2M	O2'-C2'-C1'	3.60	115.97	109.00
11	AA	2280	A2M	C4'-O4'-C1'	-3.59	106.64	109.92
11	AA	2921	OMU	C5-C4-N3	3.57	119.81	114.80
11	AA	2729	OMU	C5-C4-N3	3.57	119.80	114.80
61	c	1191	B8N	N3-C2-N1	3.56	121.07	116.72
11	AA	2729	OMU	N3-C2-N1	3.55	119.51	114.89
61	c	1781	MA6	C2-N1-C6	3.55	120.32	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Bb	37	YYG	C8-N7-C5	3.49	108.49	102.55
61	c	578	OMU	C5-C4-N3	3.46	119.65	114.80
61	c	1269	OMU	C5-C4-N3	3.45	119.64	114.80
11	AA	2281	A2M	O4'-C1'-N9	3.44	113.31	108.75
61	c	1191	B8N	C1'-C5-C4	3.35	122.69	117.61
61	c	974	A2M	C4'-O4'-C1'	-3.32	106.88	109.92
15	Bb	37	YYG	O18-C16-C15	3.28	119.84	111.49
11	AA	1133	A2M	C4'-O4'-C1'	-3.28	106.92	109.92
61	c	1782	MA6	C2-N1-C6	3.26	120.03	116.84
15	Bb	37	YYG	C5-C6-N1	3.25	118.61	114.00
61	c	1191	B8N	C31-N3-C4	3.20	121.71	117.18
15	Bb	37	YYG	O23-C21-O22	-3.14	120.05	124.62
61	c	420	A2M	C4'-O4'-C1'	-3.09	107.09	109.92
11	AA	2347	OMU	O4-C4-C5	-3.09	119.84	125.16
61	c	541	A2M	C1'-N9-C4	3.04	131.99	126.64
61	c	1575	G7M	C2-N1-C6	-3.04	119.55	125.11
61	c	100	A2M	C4'-O4'-C1'	-3.04	107.14	109.92
11	AA	2921	OMU	O4-C4-C5	-2.99	120.01	125.16
61	c	1280	4AC	O7-C7-N4	-2.96	117.23	121.90
61	c	28	A2M	C4'-O4'-C1'	-2.96	107.21	109.92
11	AA	2724	OMU	O4-C4-C5	-2.91	120.14	125.16
61	c	578	OMU	O4-C4-C5	-2.90	120.15	125.16
11	AA	1133	A2M	C2'-C1'-N9	-2.89	106.15	112.56
61	c	796	A2M	C4'-O4'-C1'	-2.86	107.31	109.92
11	AA	2256	A2M	O4'-C1'-C2'	-2.84	101.76	106.61
11	AA	1888	OMU	O4-C4-C5	-2.82	120.29	125.16
11	AA	2417	OMU	O4-C4-C5	-2.82	120.30	125.16
61	c	1280	4AC	C6-C5-C4	2.81	120.39	117.00
11	AA	898	OMU	O4-C4-C5	-2.80	120.33	125.16
11	AA	2729	OMU	O4-C4-C5	-2.79	120.34	125.16
61	c	1269	OMU	O4-C4-C5	-2.79	120.36	125.16
15	Bb	37	YYG	O22-C21-N20	-2.75	120.35	124.86
11	AA	2421	OMU	O4-C4-C5	-2.74	120.43	125.16
15	Bb	37	YYG	C14-C13-C12	2.73	118.44	112.94
11	AA	1449	A2M	C4'-O4'-C1'	-2.69	107.46	109.92
11	AA	2220	A2M	C4'-O4'-C1'	-2.69	107.46	109.92
61	c	1280	4AC	C5-C4-N3	-2.68	118.41	122.60
61	c	1773	4AC	C5-C4-N3	-2.65	118.46	122.60
15	Bb	37	YYG	C3-N3-C4	2.64	120.75	116.76
11	AA	2142	1MA	N1-C6-N6	2.63	126.31	119.71
11	AA	2281	A2M	O4'-C1'-C2'	-2.62	102.13	106.61
11	AA	2256	A2M	O4'-C1'-N9	2.61	112.20	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	c	1191	B8N	O4-C4-C5	-2.59	118.11	122.58
11	AA	817	A2M	C4'-O4'-C1'	-2.58	107.56	109.92
11	AA	876	A2M	C4'-O4'-C1'	-2.58	107.56	109.92
11	AA	1437	OMC	C1'-N1-C2	2.58	124.14	118.44
11	AA	2640	A2M	C4'-O4'-C1'	-2.58	107.56	109.92
61	c	1773	4AC	O7-C7-N4	-2.56	117.86	121.90
61	c	1280	4AC	O7-C7-CM7	-2.53	117.55	122.05
11	AA	649	A2M	C4'-O4'-C1'	-2.52	107.61	109.92
15	Bb	37	YYG	O6-C6-C5	-2.51	120.02	124.16
11	AA	2142	1MA	C5-C6-N1	-2.50	110.37	113.95
11	AA	2417	OMU	O2-C2-N1	-2.49	119.56	122.80
11	AA	1888	OMU	O2-C2-N1	-2.46	119.60	122.80
12	Aa	699	DDE	CAU-CBW-CBI	-2.46	106.42	111.22
61	c	1773	4AC	C6-C5-C4	2.45	119.95	117.00
61	c	1773	4AC	O7-C7-CM7	-2.42	117.74	122.05
61	c	1271	OMG	O6-C6-C5	2.42	129.11	124.32
11	AA	2619	OMG	O6-C6-C5	2.39	129.06	124.32
61	c	1572	OMG	O6-C6-C5	2.38	129.05	124.32
11	AA	876	A2M	C1'-N9-C4	2.38	130.82	126.64
11	AA	645	1MA	N1-C6-N6	2.36	125.64	119.71
11	AA	2347	OMU	C1'-N1-C2	2.34	121.80	117.59
61	c	562	OMG	O6-C6-C5	2.34	128.96	124.32
11	AA	2946	A2M	C2'-C1'-N9	-2.33	107.39	112.56
11	AA	2421	OMU	O2-C2-N1	-2.31	119.79	122.80
11	AA	2922	OMG	O6-C6-C5	2.30	128.88	124.32
11	AA	2793	OMG	O6-C6-C5	2.29	128.87	124.32
11	AA	2791	OMG	O6-C6-C5	2.29	128.86	124.32
11	AA	2640	A2M	C1'-N9-C4	2.28	130.65	126.64
11	AA	908	OMG	O6-C6-C5	2.28	128.84	124.32
11	AA	2815	OMG	O6-C6-C5	2.28	128.83	124.32
11	AA	805	OMG	O6-C6-C5	2.27	128.82	124.32
61	c	1428	OMG	O6-C6-C5	2.26	128.81	124.32
11	AA	2946	A2M	O4'-C1'-N9	2.26	111.74	108.75
11	AA	2729	OMU	O2-C2-N1	-2.25	119.86	122.80
11	AA	867	OMG	O6-C6-C5	2.23	128.73	124.32
11	AA	1133	A2M	O4'-C1'-N9	2.22	111.69	108.75
61	c	1191	B8N	O4-C4-N3	-2.22	116.38	119.99
11	AA	1450	OMG	O6-C6-C5	2.22	128.73	124.32
61	c	1269	OMU	C1'-N1-C2	2.22	121.58	117.59
61	c	1126	OMG	O6-C6-C5	2.21	128.70	124.32
11	AA	2288	OMG	O6-C6-C5	2.19	128.67	124.32
11	AA	645	1MA	C5-C6-N1	-2.19	110.81	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	c	100	A2M	C1'-N9-C4	2.17	130.46	126.64
11	AA	2948	OMC	C1'-N1-C2	2.16	123.22	118.44
61	c	28	A2M	C1'-N9-C4	2.16	130.44	126.64
11	AA	1449	A2M	C1'-N9-C4	2.16	130.43	126.64
11	AA	898	OMU	O2-C2-N1	-2.15	119.99	122.80
61	c	578	OMU	O2-C2-N1	-2.13	120.02	122.80
15	Bb	37	YYG	C3-N3-C2	-2.12	118.13	120.09
11	AA	2724	OMU	O2-C2-N1	-2.12	120.03	122.80
61	c	28	A2M	C5'-C4'-C3'	-2.11	107.60	115.21
61	c	796	A2M	C1'-N9-C4	2.11	130.35	126.64
61	c	1773	4AC	C5-C4-N4	2.11	126.49	122.94
11	AA	807	A2M	C1'-N9-C4	2.09	130.31	126.64
11	AA	2921	OMU	O2-C2-N1	-2.09	120.08	122.80
11	AA	1888	OMU	C2'-C1'-N1	-2.07	110.31	114.24
61	c	1191	B8N	O4'-C1'-C2'	2.05	107.99	105.15
61	c	420	A2M	C1'-N9-C4	2.05	130.25	126.64
61	c	1280	4AC	O2-C2-N3	-2.04	119.11	122.33

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AA	649	A2M	C1'-C2'-O2'-CM'
11	AA	663	OMC	C1'-C2'-O2'-CM2
11	AA	1437	OMC	C1'-C2'-O2'-CM2
11	AA	1450	OMG	O4'-C4'-C5'-O5'
11	AA	2197	OMC	C2'-C1'-N1-C6
11	AA	2220	A2M	C1'-C2'-O2'-CM'
11	AA	2256	A2M	C1'-C2'-O2'-CM'
11	AA	2417	OMU	C1'-C2'-O2'-CM2
11	AA	2421	OMU	C1'-C2'-O2'-CM2
11	AA	2619	OMG	C1'-C2'-O2'-CM2
11	AA	2724	OMU	C1'-C2'-O2'-CM2
12	Aa	699	DDE	CAU-CAT-CE1-NE2
15	Bb	37	YYG	N1-C12-C13-C14
15	Bb	37	YYG	C11-C12-C13-C14
15	Bb	37	YYG	C12-C13-C14-C15
15	Bb	37	YYG	O22-C21-N20-C15
15	Bb	37	YYG	O23-C21-N20-C15
15	Bb	37	YYG	N20-C21-O23-C24
15	Bb	37	YYG	O22-C21-O23-C24
61	c	414	OMC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
61	c	420	A2M	C1'-C2'-O2'-CM'
61	c	541	A2M	O4'-C4'-C5'-O5'
61	c	541	A2M	C3'-C4'-C5'-O5'
61	c	562	OMG	C1'-C2'-O2'-CM2
61	c	619	A2M	C1'-C2'-O2'-CM'
61	c	1191	B8N	C2'-C1'-C5-C4
61	c	1191	B8N	N34-C33-C34-O35
61	c	1271	OMG	C1'-C2'-O2'-CM2
61	c	1572	OMG	C1'-C2'-O2'-CM2
15	Bb	37	YYG	O17-C16-O18-C19
15	Bb	37	YYG	C15-C16-O18-C19
15	Bb	37	YYG	C13-C14-C15-N20
11	AA	2197	OMC	C2'-C1'-N1-C2
11	AA	867	OMG	C3'-C4'-C5'-O5'
61	c	28	A2M	O4'-C4'-C5'-O5'
61	c	28	A2M	C3'-C4'-C5'-O5'
61	c	1280	4AC	C3'-C4'-C5'-O5'
61	c	1572	OMG	O4'-C4'-C5'-O5'
15	Bb	37	YYG	C16-C15-N20-C21
15	Bb	37	YYG	C13-C14-C15-C16
11	AA	2922	OMG	C3'-C4'-C5'-O5'
61	c	578	OMU	C3'-C4'-C5'-O5'
61	c	578	OMU	O4'-C4'-C5'-O5'
61	c	1575	G7M	O4'-C4'-C5'-O5'
61	c	1575	G7M	C3'-C4'-C5'-O5'
61	c	1191	B8N	N34-C33-C34-O36
11	AA	2870	5MC	C2'-C1'-N1-C6
11	AA	1450	OMG	C3'-C4'-C5'-O5'
61	c	619	A2M	O4'-C4'-C5'-O5'
61	c	619	A2M	C3'-C4'-C5'-O5'
61	c	1572	OMG	C3'-C4'-C5'-O5'
61	c	1280	4AC	O4'-C4'-C5'-O5'
11	AA	2922	OMG	O4'-C4'-C5'-O5'
61	c	100	A2M	O4'-C4'-C5'-O5'
11	AA	867	OMG	O4'-C4'-C5'-O5'
61	c	1280	4AC	O7-C7-N4-C4
61	c	1280	4AC	CM7-C7-N4-C4
61	c	1773	4AC	O7-C7-N4-C4
61	c	1773	4AC	CM7-C7-N4-C4
15	Bb	37	YYG	N20-C15-C16-O18
11	AA	2870	5MC	O4'-C1'-N1-C6
15	Bb	37	YYG	N20-C15-C16-O17

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Mol	Chain	Res	Type	Atoms
11	AA	2870	5MC	C2'-C1'-N1-C2
11	AA	908	OMG	C3'-C2'-O2'-CM2
61	c	1191	B8N	N3-C31-C32-C33
61	c	1782	MA6	C5-C6-N6-C10
61	c	1575	G7M	C4'-C5'-O5'-P
11	AA	2281	A2M	O4'-C4'-C5'-O5'
11	AA	2197	OMC	O4'-C1'-N1-C2
11	AA	2870	5MC	O4'-C1'-N1-C2
11	AA	817	A2M	C4'-C5'-O5'-P
61	c	1191	B8N	O4'-C1'-C5-C4
11	AA	807	A2M	C3'-C4'-C5'-O5'
61	c	1428	OMG	C4'-C5'-O5'-P
11	AA	2197	OMC	O4'-C1'-N1-C6
61	c	420	A2M	O4'-C4'-C5'-O5'
61	c	1269	OMU	O4'-C1'-N1-C6
61	c	541	A2M	C4'-C5'-O5'-P
11	AA	2793	OMG	C3'-C2'-O2'-CM2
61	c	1782	MA6	C4'-C5'-O5'-P
12	Aa	699	DDE	CAU-CBW-NCB-CAB
11	AA	2281	A2M	C3'-C2'-O2'-CM'
11	AA	2281	A2M	C3'-C4'-C5'-O5'
61	c	1269	OMU	C2'-C1'-N1-C6
61	c	1269	OMU	O4'-C1'-N1-C2
12	Aa	699	DDE	CBI-CBW-NCB-CAB
12	Aa	699	DDE	CBI-CBW-NCB-CAC
11	AA	2142	1MA	C4'-C5'-O5'-P

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 297 ligands modelled in this entry, 291 are monoatomic - leaving 6 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	$\# Z > 2$
88	SPD	AA	3615	-	9,9,9	0.29	0	8,8,8	0.77	0
90	PO4	Aa	1002	86	4,4,4	1.06	0	6,6,6	0.54	0
89	GDP	Aa	1001	86	25,30,30	0.95	1 (4%)	30,47,47	1.12	3 (10%)
88	SPD	AA	3613	-	9,9,9	0.32	0	8,8,8	0.89	0
88	SPD	AA	3614	-	9,9,9	0.33	0	8,8,8	0.93	0
91	SO1	Aa	1003	-	34,39,39	1.19	3 (8%)	38,64,64	1.15	3 (7%)

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
88	SPD	AA	3615	-	-	3/7/7/7	-
89	GDP	Aa	1001	86	-	5/12/32/32	0/3/3/3
88	SPD	AA	3613	-	-	1/7/7/7	-
88	SPD	AA	3614	-	-	0/7/7/7	-
91	SO1	Aa	1003	-	-	10/21/104/104	0/7/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	Aa	1003	SO1	C2-C6	-4.05	1.49	1.55
91	Aa	1003	SO1	C16-C22	-2.44	1.50	1.54
89	Aa	1001	GDP	C6-N1	-2.29	1.34	1.37
91	Aa	1003	SO1	C3-C9	-2.16	1.51	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	Aa	1003	SO1	C52-O56-C56	-2.98	108.54	113.63
89	Aa	1001	GDP	C8-N7-C5	2.89	107.47	102.55
91	Aa	1003	SO1	C12-C6-C10	-2.68	105.82	107.92
89	Aa	1001	GDP	O4'-C1'-N9	2.10	111.53	108.75
91	Aa	1003	SO1	C53-C54-C55	2.09	114.43	109.68
89	Aa	1001	GDP	C5-C6-N1	2.04	117.97	114.07

There are no chirality outliers.

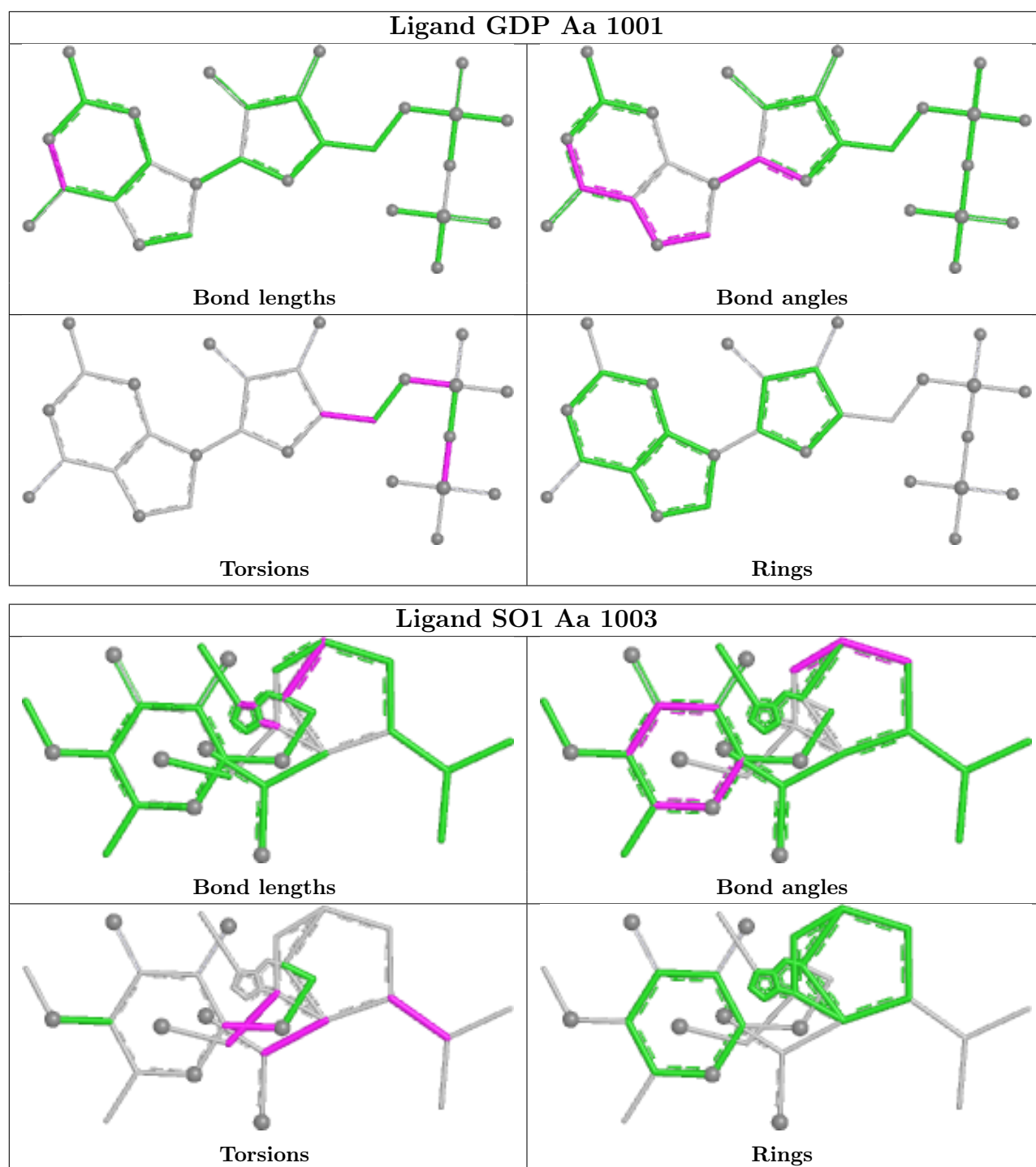
All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	Aa	1001	GDP	O4'-C4'-C5'-O5'
91	Aa	1003	SO1	C2-C1-C5-O14
91	Aa	1003	SO1	C2-C1-C5-O15
91	Aa	1003	SO1	C20-C13-C4-C1
91	Aa	1003	SO1	C21-C13-C4-C1
91	Aa	1003	SO1	C20-C13-C4-C12
91	Aa	1003	SO1	C21-C13-C4-C12
91	Aa	1003	SO1	O19-C11-C3-C10
88	AA	3615	SPD	C2-C3-C4-C5
89	Aa	1001	GDP	C3'-C4'-C5'-O5'
91	Aa	1003	SO1	O56-C52-O17-C8
88	AA	3615	SPD	C8-C7-N6-C5
89	Aa	1001	GDP	PA-O3A-PB-O2B
91	Aa	1003	SO1	O19-C11-C3-C9
89	Aa	1001	GDP	C5'-O5'-PA-O3A
89	Aa	1001	GDP	C5'-O5'-PA-O1A
88	AA	3615	SPD	C7-C8-C9-N10
88	AA	3613	SPD	N1-C2-C3-C4
91	Aa	1003	SO1	O19-C11-C3-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.

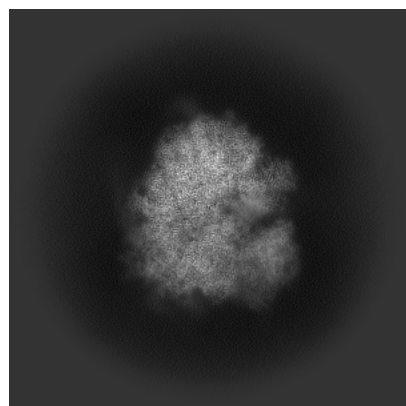
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16609. These allow visual inspection of the internal detail of the map and identification of artifacts.

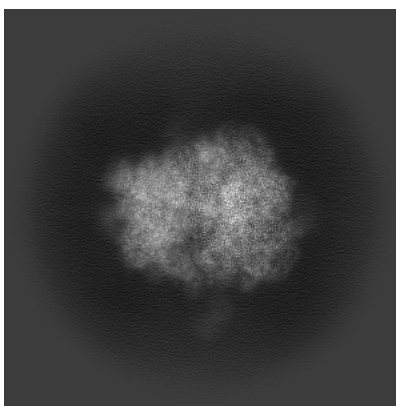
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

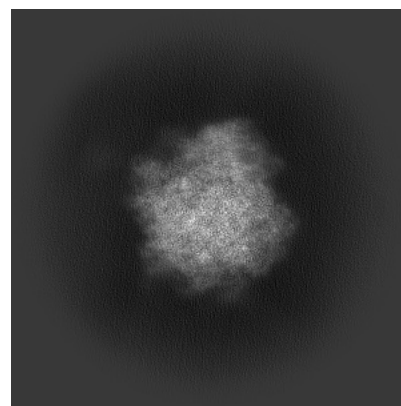
6.1.1 Primary map



X

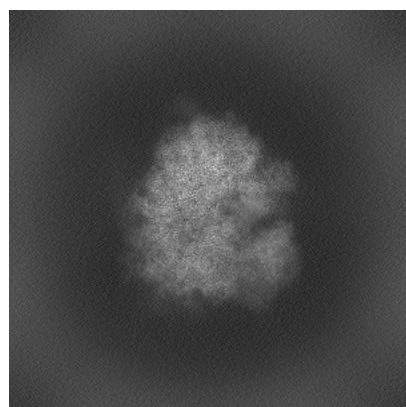


Y

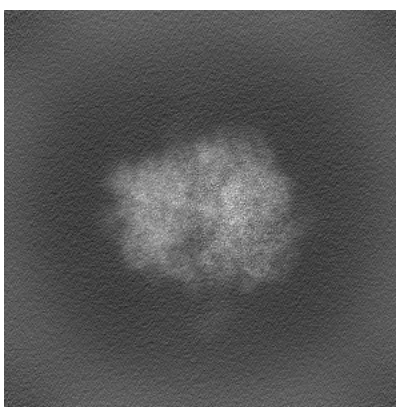


Z

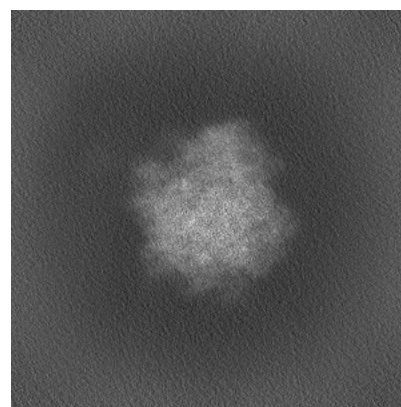
6.1.2 Raw map



X



Y

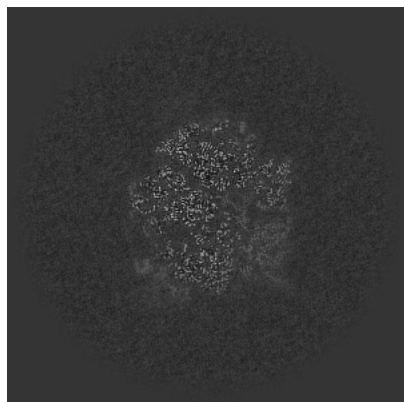


Z

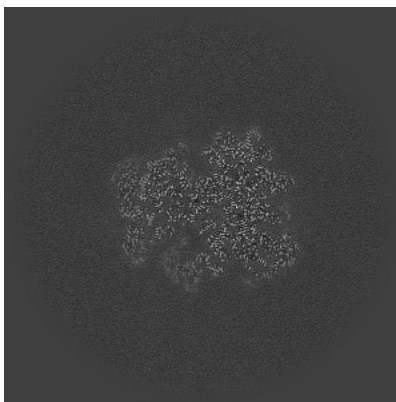
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

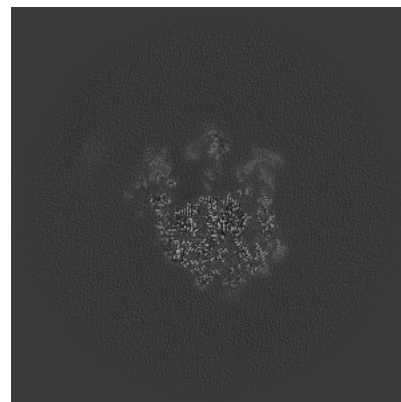
6.2.1 Primary map



X Index: 300

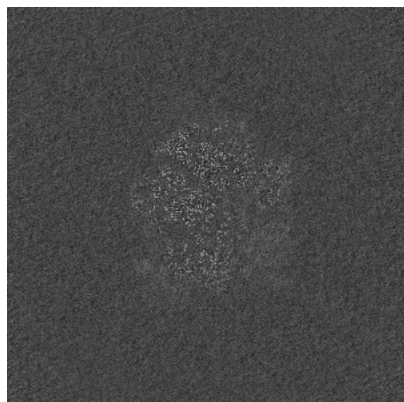


Y Index: 300

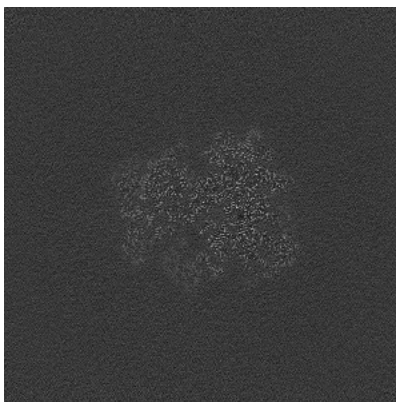


Z Index: 300

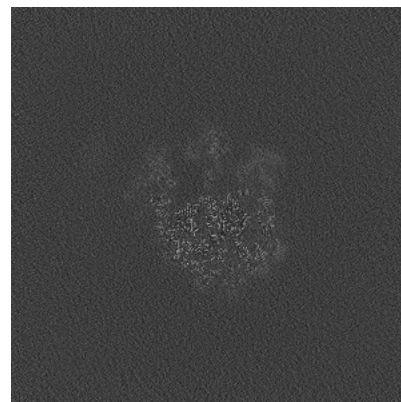
6.2.2 Raw map



X Index: 300



Y Index: 300

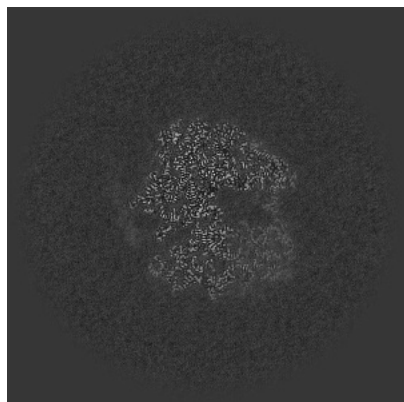


Z Index: 300

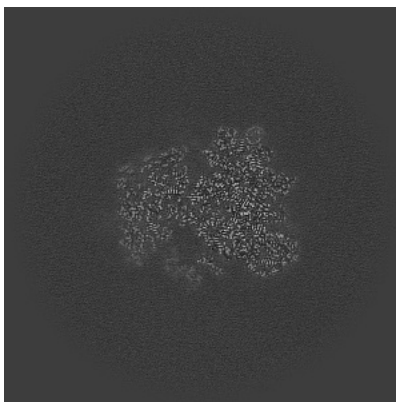
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

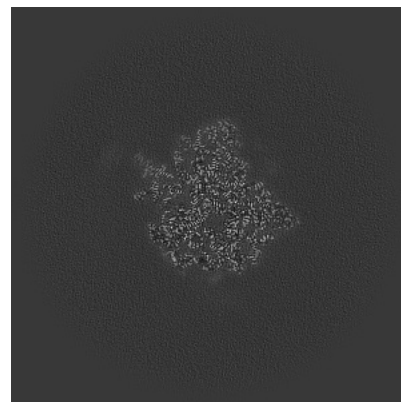
6.3.1 Primary map



X Index: 324

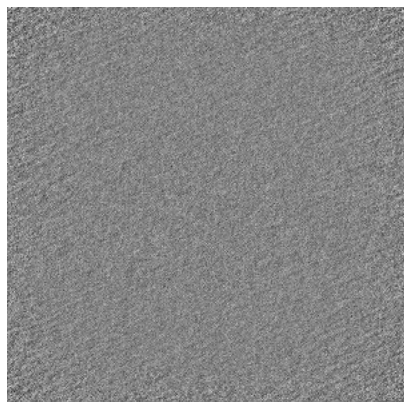


Y Index: 295

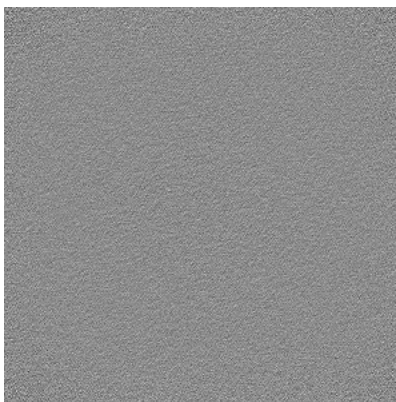


Z Index: 340

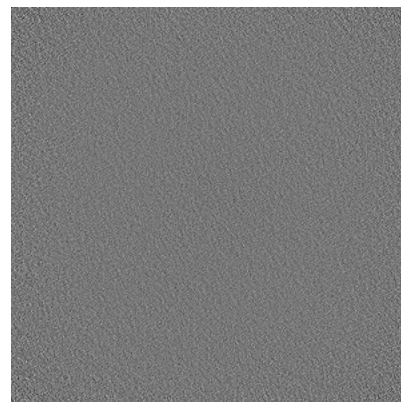
6.3.2 Raw map



X Index: 0



Y Index: 0

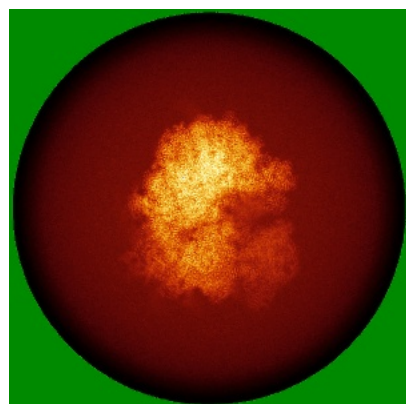


Z Index: 0

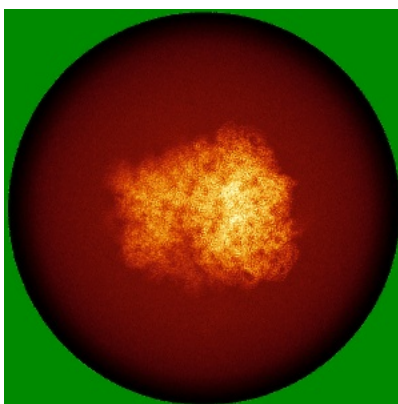
The images above show the largest variance slices of the map in three orthogonal directions.

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

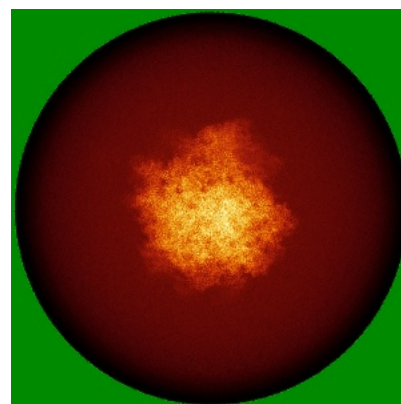
6.4.1 Primary map



X

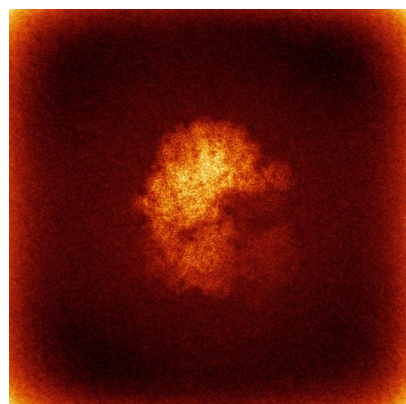


Y

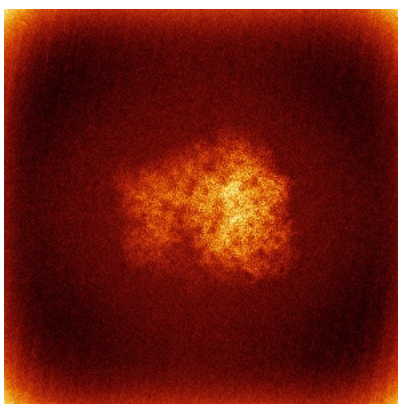


Z

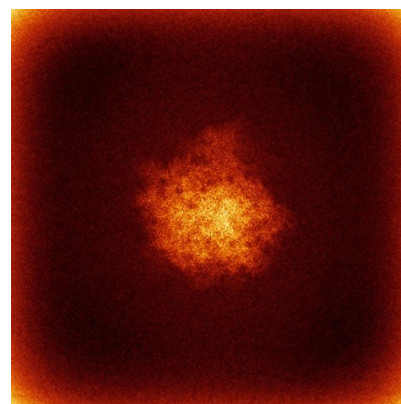
6.4.2 Raw map



X



Y

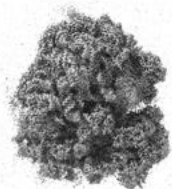


Z

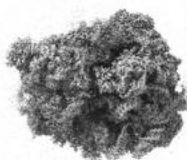
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

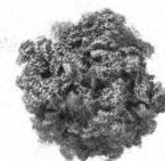
6.5.1 Primary map



X



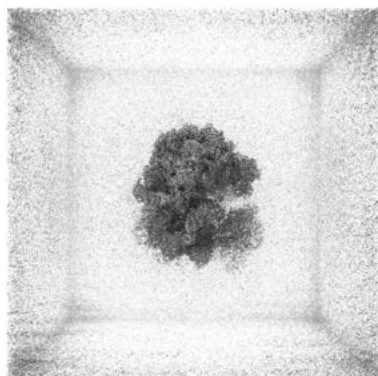
Y



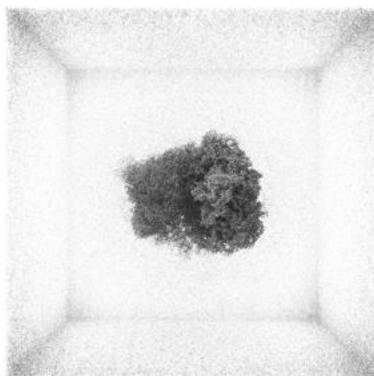
Z

The images above show the 3D surface view of the map at the recommended contour level 0.161. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

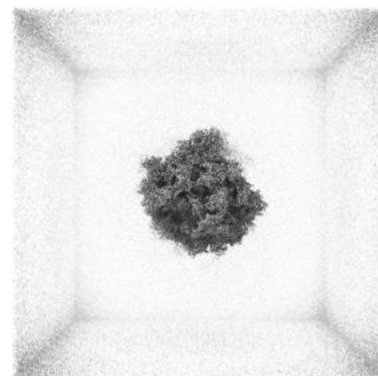
6.5.2 Raw map



X



Y



Z

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

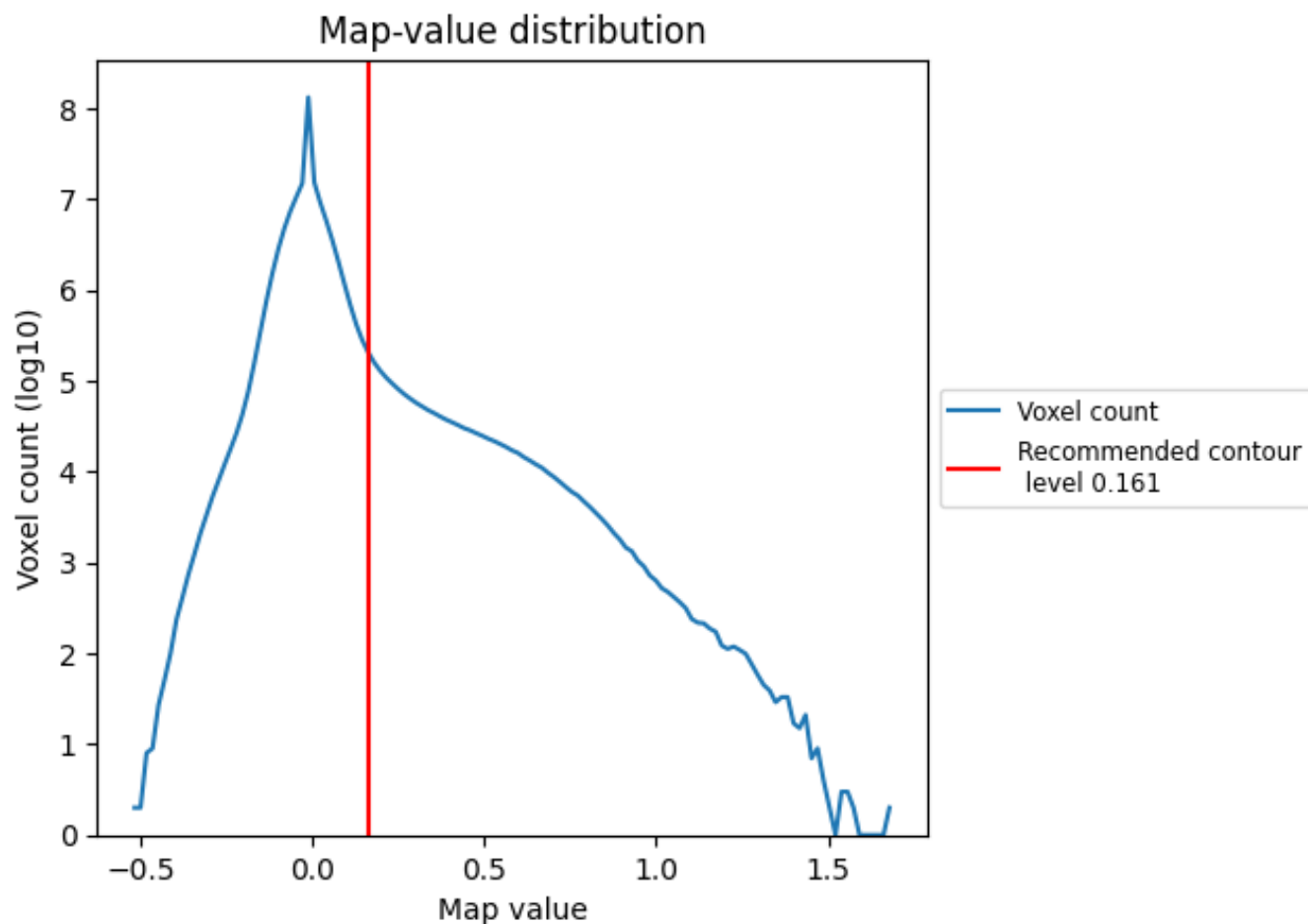
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

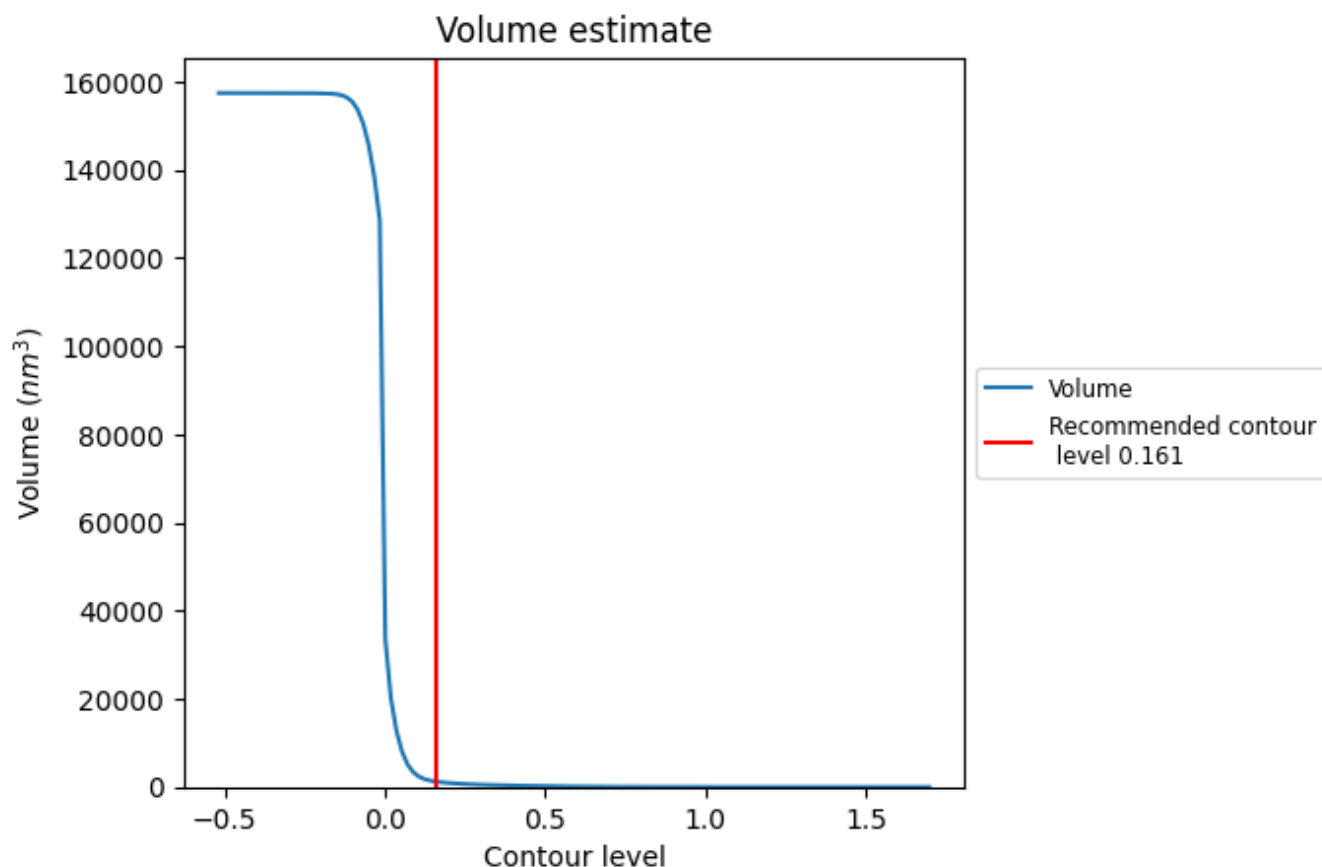
This section contains the results of statistical analysis of the map.

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.

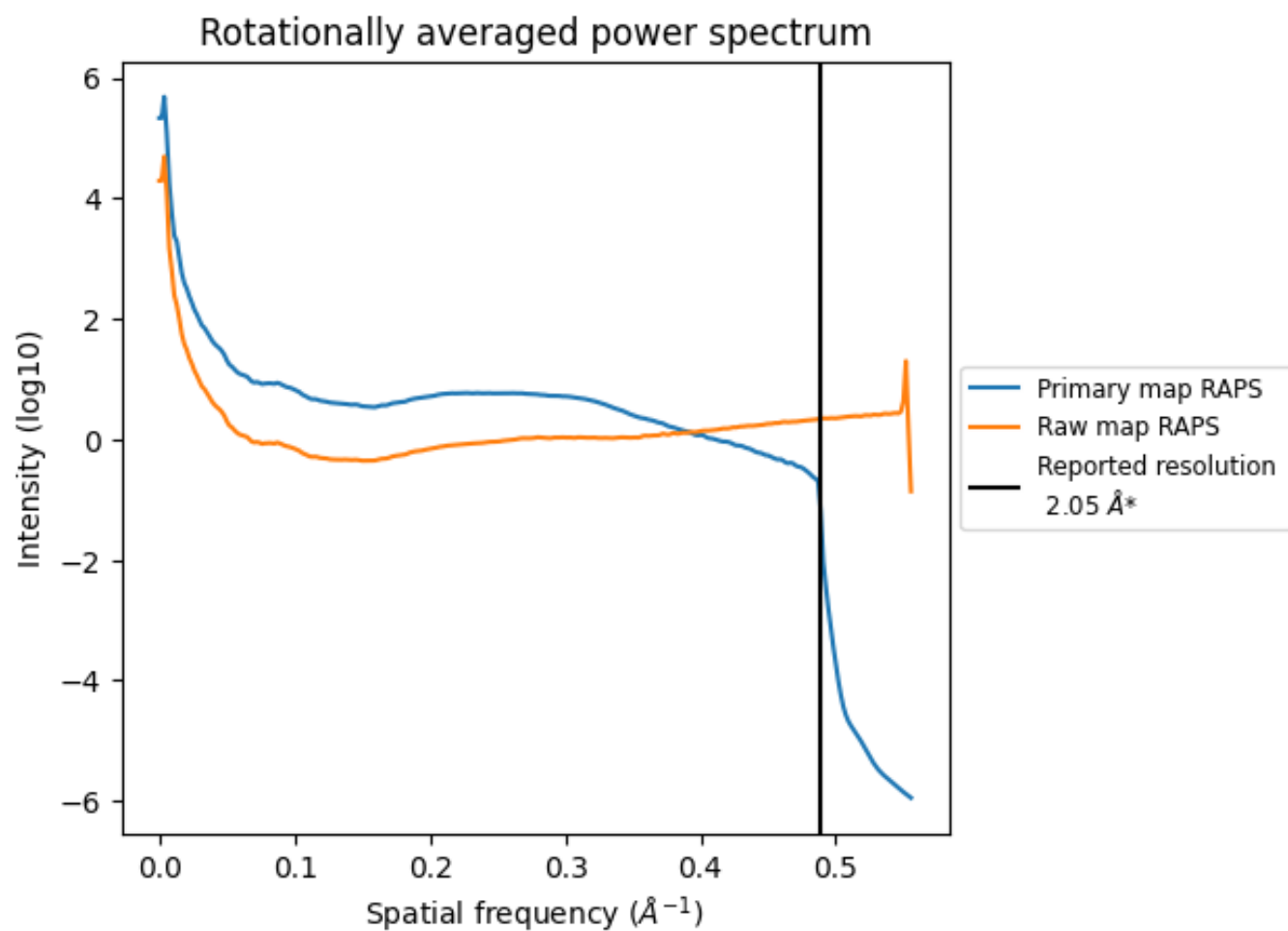
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1195 nm³; this corresponds to an approximate mass of 1079 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 ⓘ

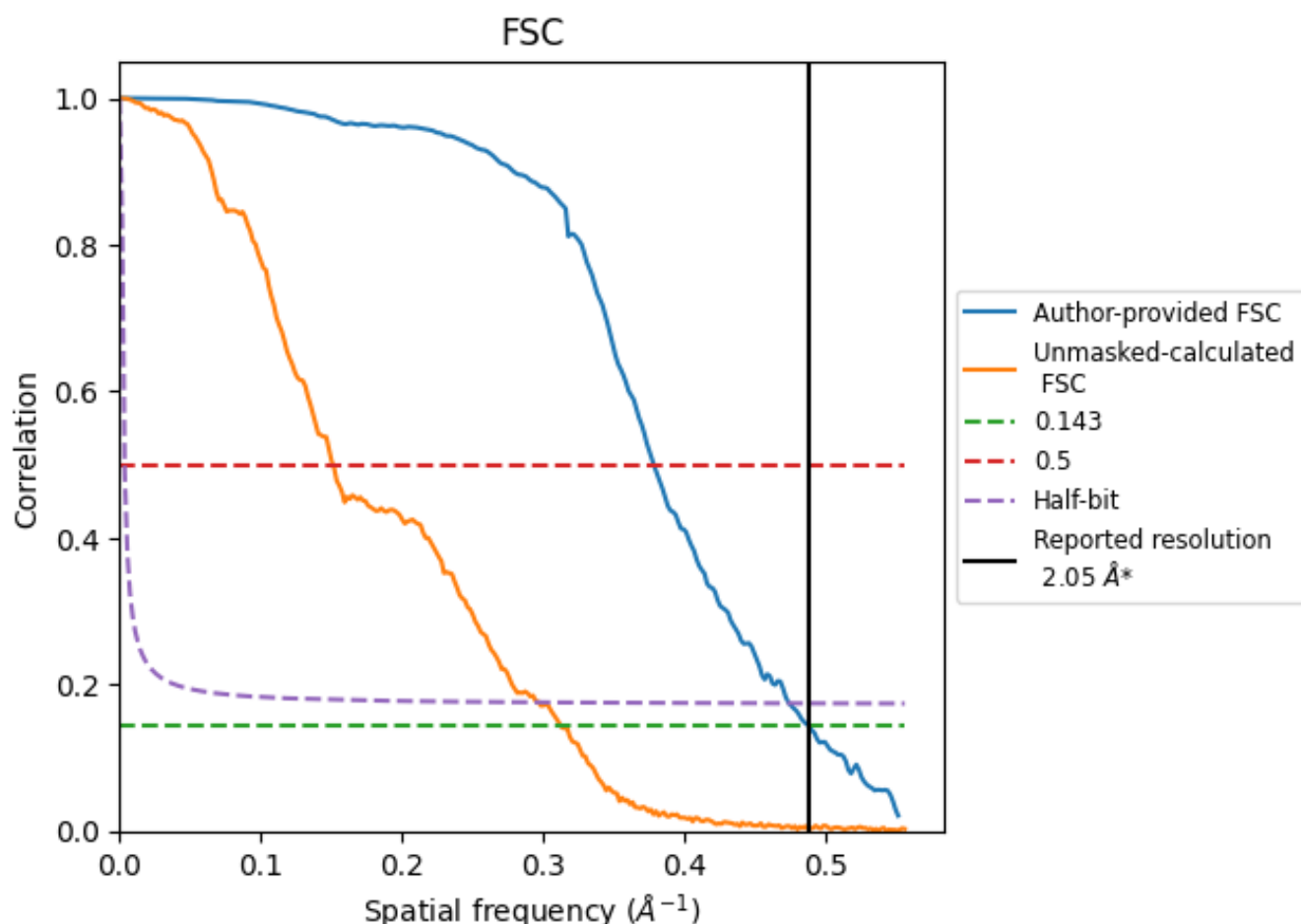


*Reported resolution corresponds to spatial frequency of 0.488 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.488 Å⁻¹

8.2 Resolution estimates [i](#)

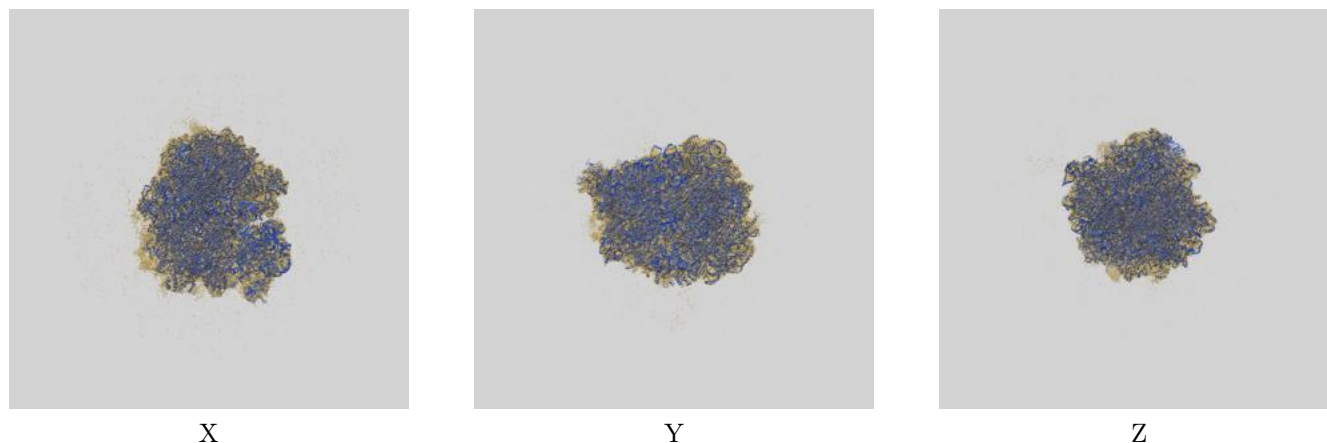
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.05	-	-
Author-provided FSC curve	2.05	2.65	2.11
Unmasked-calculated*	3.20	6.63	3.37

*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 3.20 differs from the reported value 2.05 by more than 10 %

9 Map-model fit [i](#)

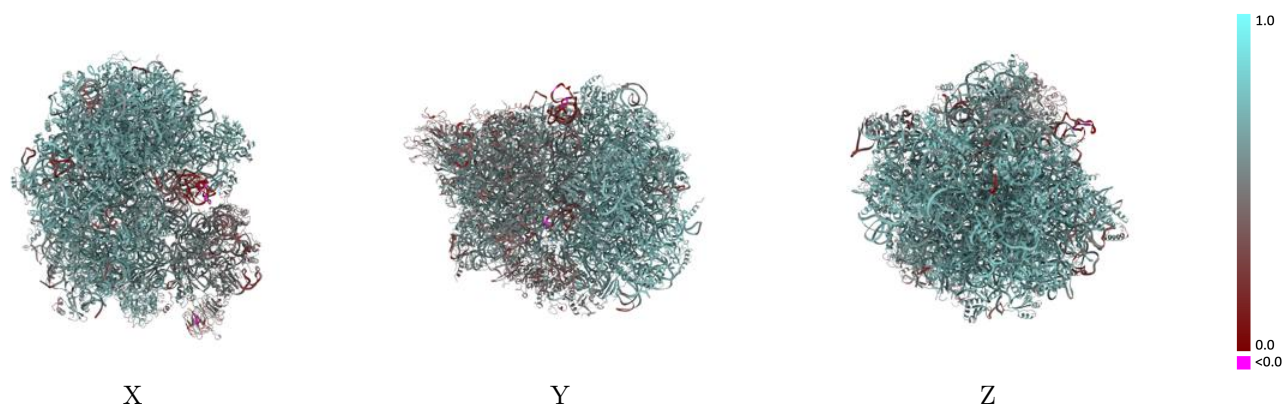
This section contains information regarding the fit between EMDB map EMD-16609 and PDB model 8CEH. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



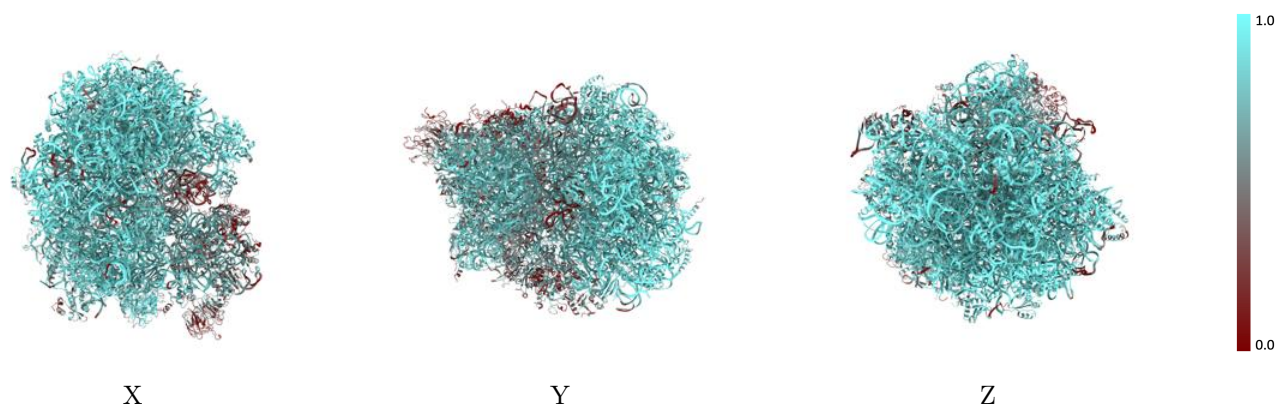
The images above show the 3D surface view of the map at the recommended contour level 0.161 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



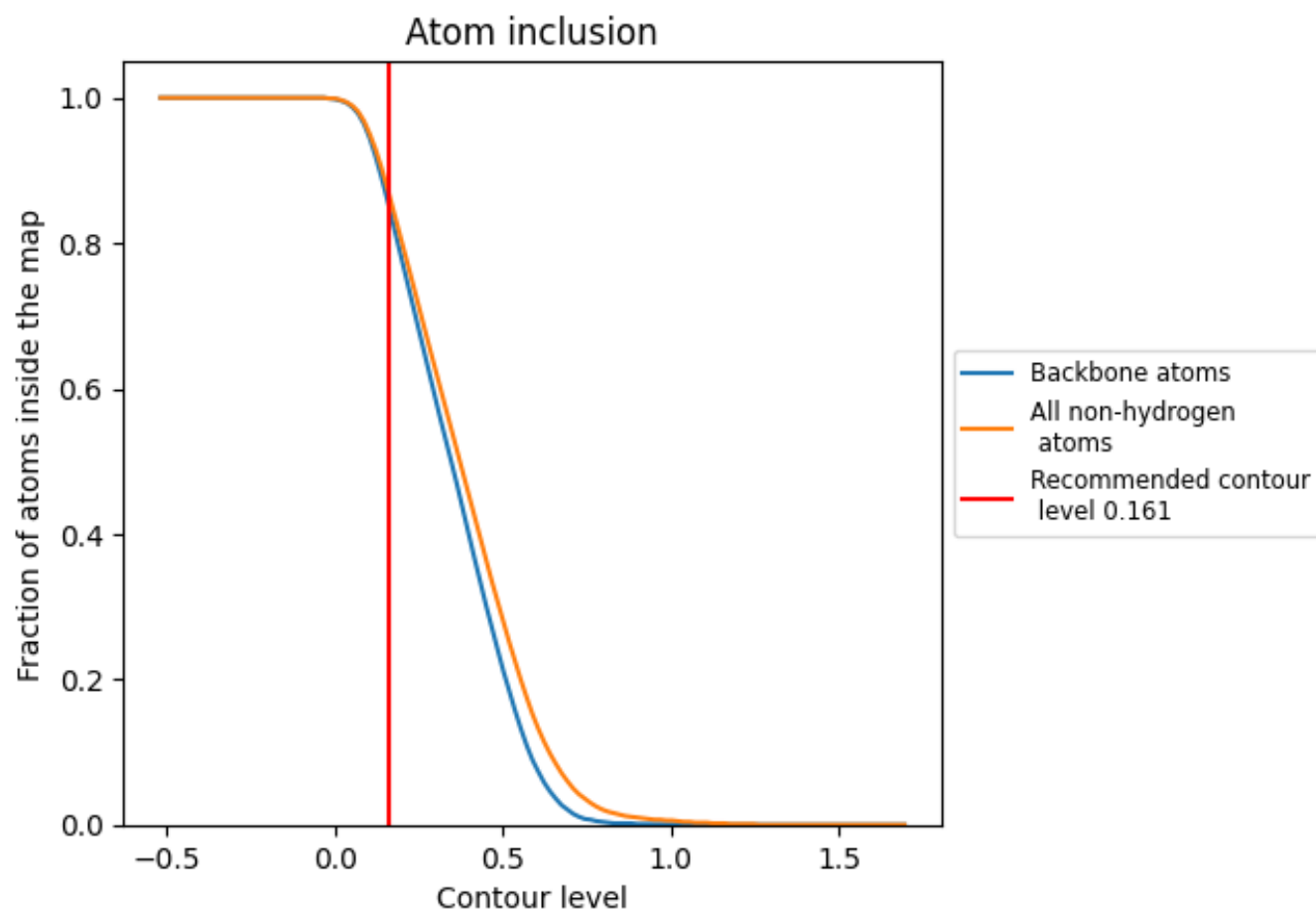
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.161).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 87% 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 (0.161) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.6170
0	 0.7540	 0.5610
1	 0.0770	 0.3350
2	 0.9190	 0.6460
3	 0.8290	 0.6120
4	 0.4760	 0.4890
5	 0.8400	 0.5540
6	 0.7660	 0.5470
7	 0.3680	 0.3870
8	 0.1620	 0.3330
A	 0.9720	 0.6990
AA	 0.9430	 0.6480
Aa	 0.5790	 0.5000
B	 0.9750	 0.7100
BB	 0.9880	 0.6610
Bb	 0.5280	 0.4710
C	 0.9750	 0.7010
CC	 0.9790	 0.6760
Cc	 0.6390	 0.4500
D	 0.9200	 0.6740
DD	 0.5460	 0.5050
Dd	 0.9440	 0.6290
E	 0.9630	 0.6920
EE	 0.9720	 0.7070
Ee	 0.2220	 0.3650
F	 0.9330	 0.6750
FF	 0.9630	 0.6930
G	 0.8690	 0.6200
GG	 0.9640	 0.6970
H	 0.9670	 0.7020
HH	 0.8640	 0.6280
I	 0.9510	 0.6930
II	 0.9290	 0.6700
J	 0.9460	 0.6840
JJ	 0.9570	 0.6890



















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Chain	Atom inclusion	Q-score
K	 0.9560	 0.6880
KK	 0.8840	 0.6480
L	 0.9320	 0.6650
LL	 0.9270	 0.6690
M	 0.9570	 0.6890
MM	 0.9280	 0.6760
N	 0.8920	 0.6320
NN	 0.7960	 0.5810
O	 0.9360	 0.6800
OO	 0.9190	 0.6680
P	 0.9030	 0.6550
PP	 0.9550	 0.6810
Pp	 0.4210	 0.5790
Q	 0.9680	 0.7080
QQ	 0.9920	 0.7100
R	 0.9930	 0.7180
S	 0.9540	 0.6890
T	 0.9460	 0.6700
U	 0.8980	 0.6410
V	 0.9890	 0.7080
W	 0.8350	 0.6320
X	 0.9690	 0.6830
Y	 0.9550	 0.6950
Z	 0.9430	 0.6750
a	 0.9300	 0.6730
b	 0.9400	 0.6970
c	 0.8830	 0.5730
d	 0.8700	 0.6060
e	 0.8680	 0.6250
f	 0.9160	 0.6460
g	 0.6420	 0.4980
h	 0.8810	 0.6060
i	 0.4930	 0.4690
j	 0.6650	 0.5120
k	 0.7110	 0.5520
l	 0.8730	 0.6200
m	 0.8680	 0.6050
n	 0.5600	 0.4460
o	 0.8940	 0.6490
p	 0.9300	 0.6640
q	 0.9360	 0.6420
r	 0.4970	 0.4680

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Chain	Atom inclusion	Q-score
s	 0.6440	 0.5120
t	 0.6260	 0.5000
u	 0.4110	 0.4570
v	 0.5780	 0.4670
w	 0.6060	 0.4890
x	 0.8890	 0.6340
y	 0.9730	 0.6910
z	 0.8740	 0.6230