



Full wwPDB EM Validation Report ⓘ

Apr 18, 2024 – 12:14 am BST

PDB ID : 8CDR
EMDB ID : EMD-16594
Title : Translocation intermediate 2 (TI-2) 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 : 2023-01-31
Resolution : 2.04 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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

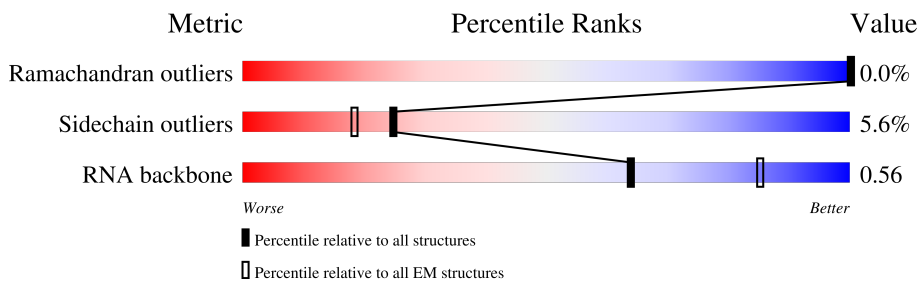
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.04 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




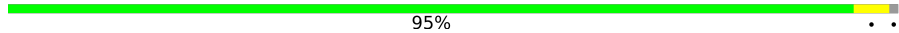














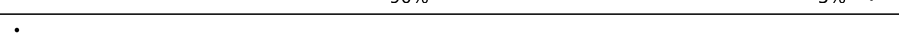
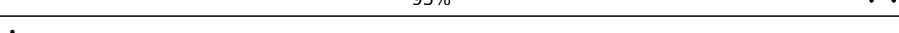
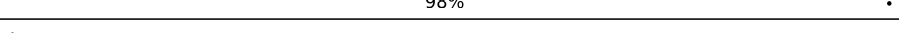

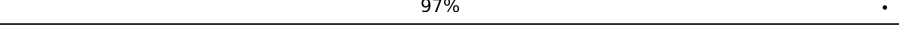
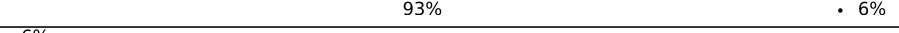
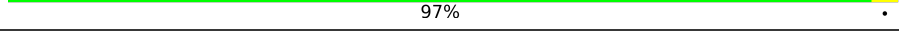


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	135	
2	1	108	
3	2	119	
4	3	82	
5	4	67	
6	5	56	
7	6	63	
8	7	319	

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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	

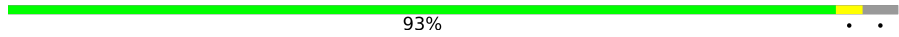
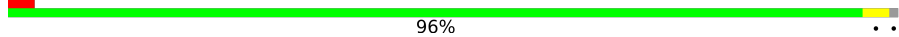








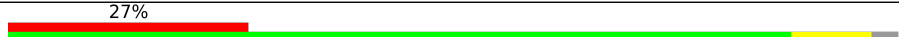


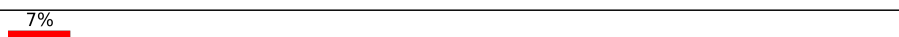
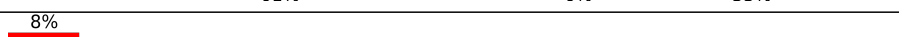
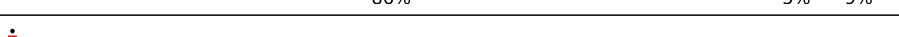
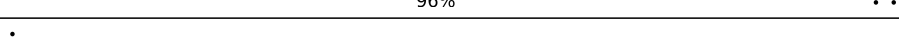


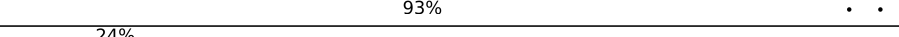

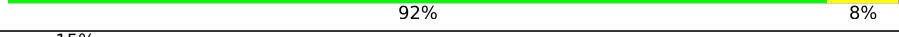
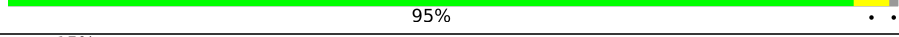

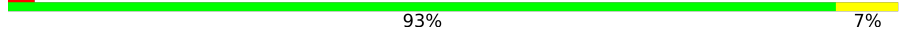
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Mol	Chain	Length	Quality of chain
34	JJ	244	89% 9%
35	K	127	94% 5%
36	KK	256	88% 9% 5%
37	L	136	96%
38	LL	191	95% 5%
39	M	149	95%
40	MM	221	94%
41	N	59	98%
42	NN	174	90% 7% 6%
43	O	105	90% 8%
44	OO	199	93%
45	P	113	95% 7%
46	PP	138	96%
47	Pp	2	100% 50% 50%
48	Q	130	95%
49	QQ	204	98%
50	R	107	97%
51	S	121	90% 10%
52	T	120	98%
53	U	100	93% 6% 5%
54	V	88	93% 5%
55	W	78	92% 6%
56	X	51	94%
57	Y	128	40% 59%
58	Z	25	92% 8%

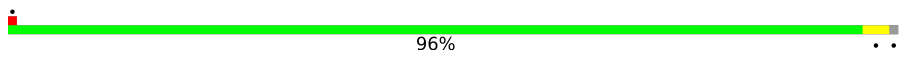
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Mol	Chain	Length	Quality of chain
59	a	106	 93%
60	b	92	 96%
61	c	1800	 72% 17% 11%
62	d	252	 79% 18%
63	e	255	 8% 78% 5% 17%
64	f	254	 83% 15%
65	g	240	 6% 75% 10% 15%
66	h	261	 93% 6%
67	i	225	 19% 82% 6% 12%
68	j	236	 15% 87% 6% 7%
69	k	190	 27% 88% 9%
70	l	200	 88% 8%
71	m	197	 5% 88% 6% 6%
72	n	105	 7% 61% 6% 33%
73	o	156	 8% 86% 5% 9%
74	p	151	 96%
75	q	137	 87% 6% 7%
76	r	142	 6% 61% 36%
77	s	143	 5% 93%
78	t	136	 24% 79% 9% 11%
79	u	146	 29% 92% 8%
80	v	144	 15% 95%
81	w	121	 15% 73% 10% 17%
82	x	87	 93% 7%
83	y	130	 94% 5%

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Mol	Chain	Length	Quality of chain
84	z	145	

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 207753 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
			Total	C	N	O		
1	0	134	1073	676	208	189	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	52	433	269	91	69	4	0	0

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

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

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

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

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

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

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

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

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

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

- Molecule 12 is a protein called Elongation factor 2.

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O		
19	D	176	1423	875	308	240	0	0

- 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	0	0
			770	499	126	145		

- 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	0	0
			2748	1729	522	494	3		

- 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	0	0
			963	607	180	169	7		

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

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

- 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	0	0
			521	336	102	82	1		

- 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	0	0
			1230	795	221	213	1		

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

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

- 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	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	0	0
			1092	710	202	180		

- Molecule 38 is a protein called 60S ribosomal protein L9-A.

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 dipeptide.

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
			Total	C	N	O	S		
48	Q	127	1020	647	205	167	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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-A.

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	205	Total	C	N	O	S	0	0
			1593	1008	293	286	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
			Total	C	N	O		
69	k	184	1481	951	265	265	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	n	70	596	388	96	110	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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).

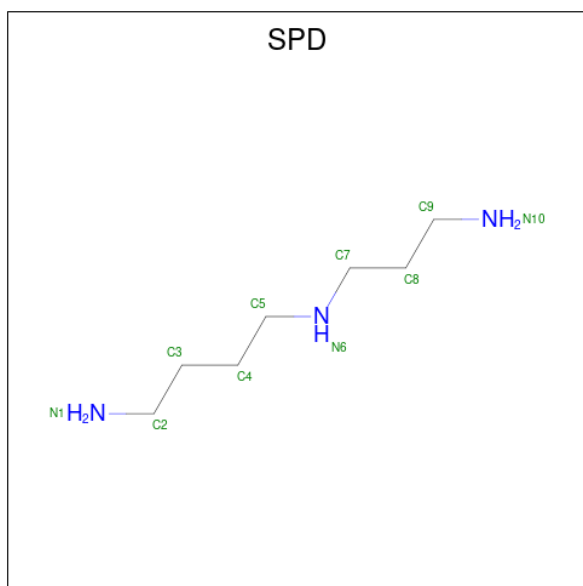
Mol	Chain	Residues	Atoms		AltConf
86	AA	200	Total	Mg	0
			200	200	
86	Aa	1	Total	Mg	0
			1	1	
86	B	1	Total	Mg	0
			1	1	
86	BB	5	Total	Mg	0
			5	5	
86	Bb	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
86	CC	4	Total	Mg	0
			4	4	
86	FF	1	Total	Mg	0
			1	1	
86	H	1	Total	Mg	0
			1	1	
86	MM	1	Total	Mg	0
			1	1	
86	QQ	1	Total	Mg	0
			1	1	
86	c	50	Total	Mg	0
			50	50	
86	q	1	Total	Mg	0
			1	1	

- Molecule 87 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

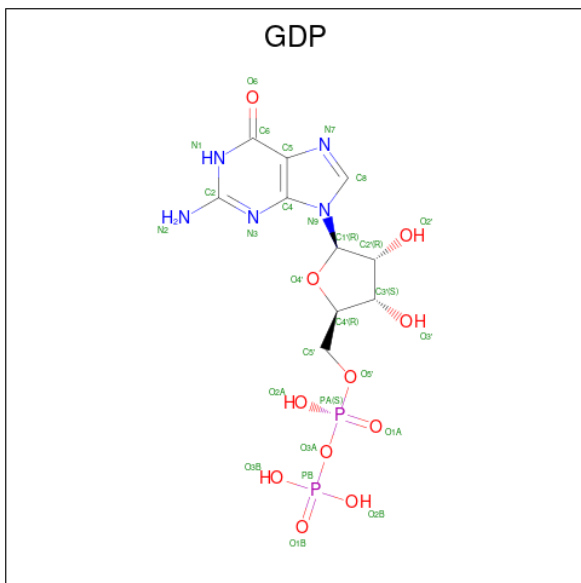


Mol	Chain	Residues	Atoms			AltConf
87	AA	1	Total	C	N	0
			10	7	3	
87	AA	1	Total	C	N	0
			10	7	3	
87	AA	1	Total	C	N	0
			10	7	3	
87	c	1	Total	C	N	0
			10	7	3	

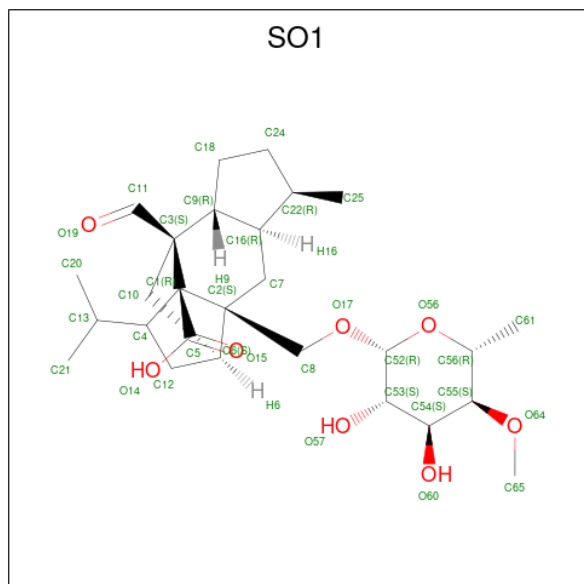
- Molecule 88 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
88	AA	13	Total K 13 13	0
88	CC	1	Total K 1 1	0
88	EE	1	Total K 1 1	0
88	MM	1	Total K 1 1	0
88	Q	1	Total K 1 1	0
88	a	1	Total K 1 1	0
88	c	2	Total K 2 2	0
88	q	1	Total K 1 1	0

- Molecule 89 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



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
			Total	C	O	
90	Aa	1	35	27	8	0

- Molecule 91 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
91	2	1	1	1	0
91	A	2	2	2	0
91	AA	851	851	851	0
91	B	2	2	2	0
91	BB	22	22	22	0
91	CC	20	20	20	0
91	Cc	1	1	1	0
91	D	3	3	3	0
91	EE	7	7	7	0

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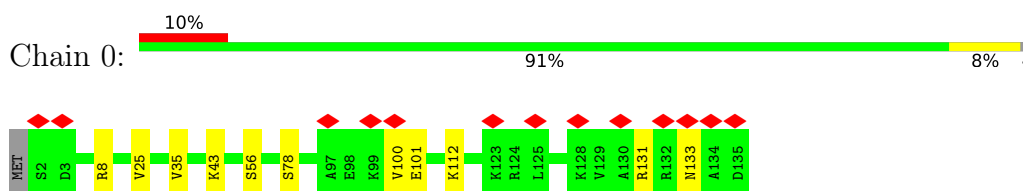
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Mol	Chain	Residues	Atoms		AltConf
91	F	3	Total 3	O 3	0
91	FF	4	Total 4	O 4	0
91	GG	4	Total 4	O 4	0
91	H	2	Total 2	O 2	0
91	HH	2	Total 2	O 2	0
91	J	2	Total 2	O 2	0
91	JJ	1	Total 1	O 1	0
91	M	3	Total 3	O 3	0
91	MM	1	Total 1	O 1	0
91	N	1	Total 1	O 1	0
91	Q	4	Total 4	O 4	0
91	QQ	7	Total 7	O 7	0
91	V	3	Total 3	O 3	0
91	a	2	Total 2	O 2	0
91	c	131	Total 131	O 131	0
91	h	1	Total 1	O 1	0
91	o	2	Total 2	O 2	0
91	p	3	Total 3	O 3	0
91	z	1	Total 1	O 1	0

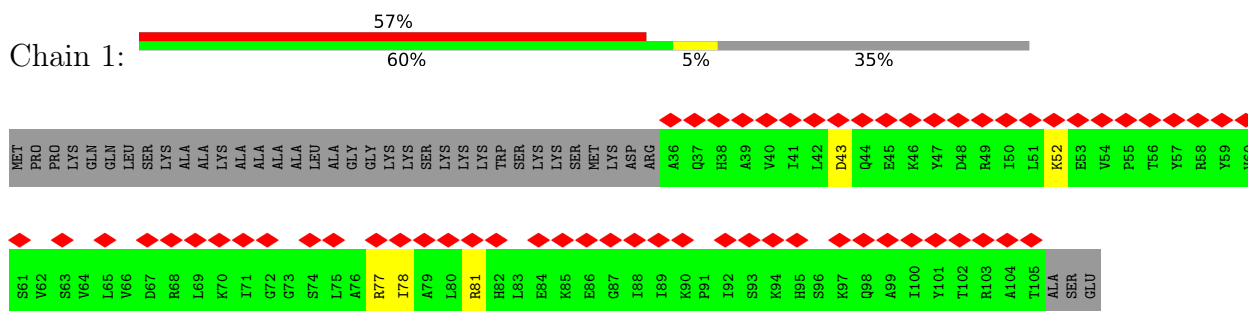
3 Residue-property plots [i](#)

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.

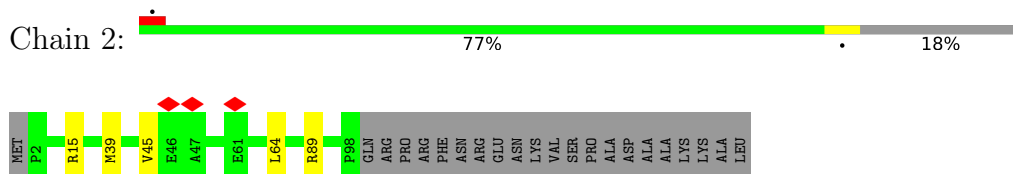
- Molecule 1: 40S ribosomal protein S24-A



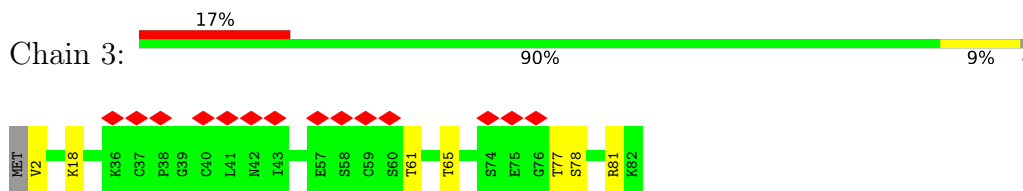
- Molecule 2: 40S ribosomal protein S25-A



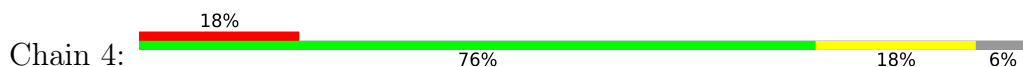
- Molecule 3: 40S ribosomal protein S26

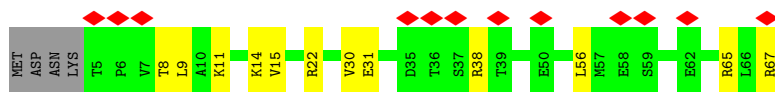


- Molecule 4: 40S ribosomal protein S27-A

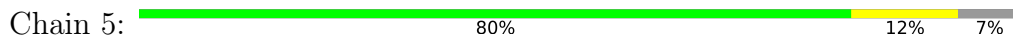


- Molecule 5: 40S ribosomal protein S28-A

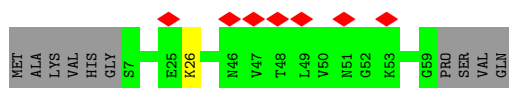
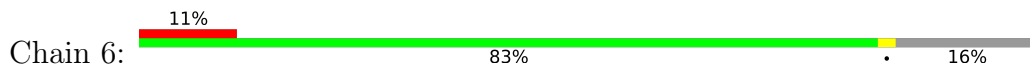




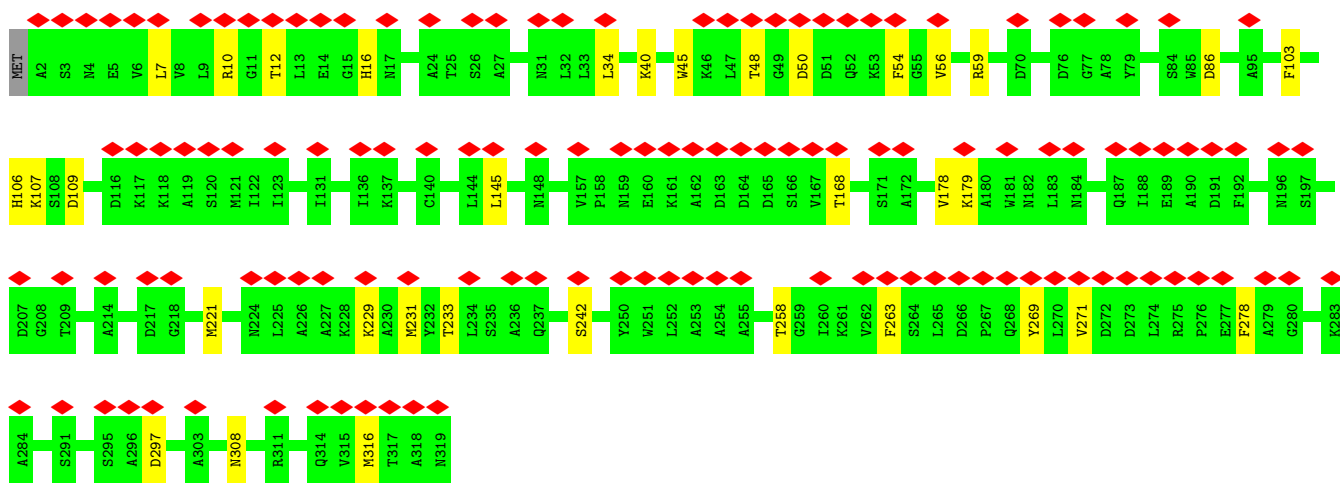
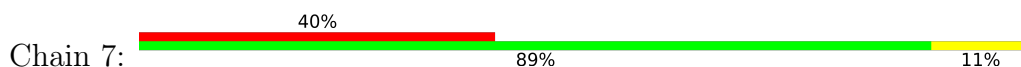
• Molecule 6: HLJ1_G0030400.mRNA.1.CDS.1



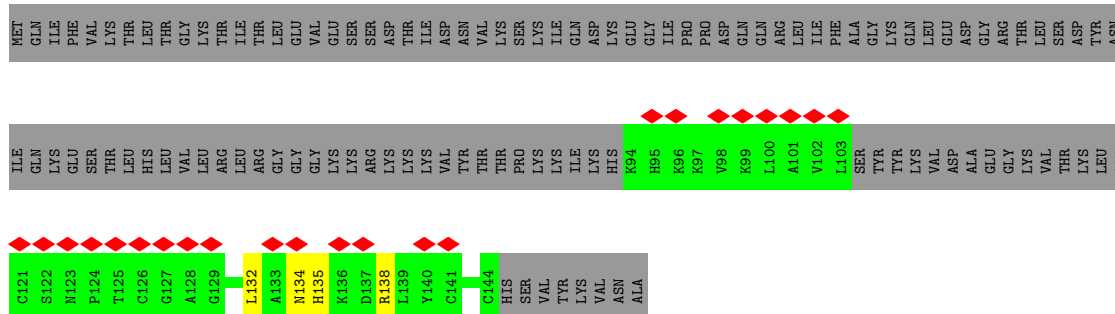
• Molecule 7: 40S ribosomal protein S30-A



• Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein



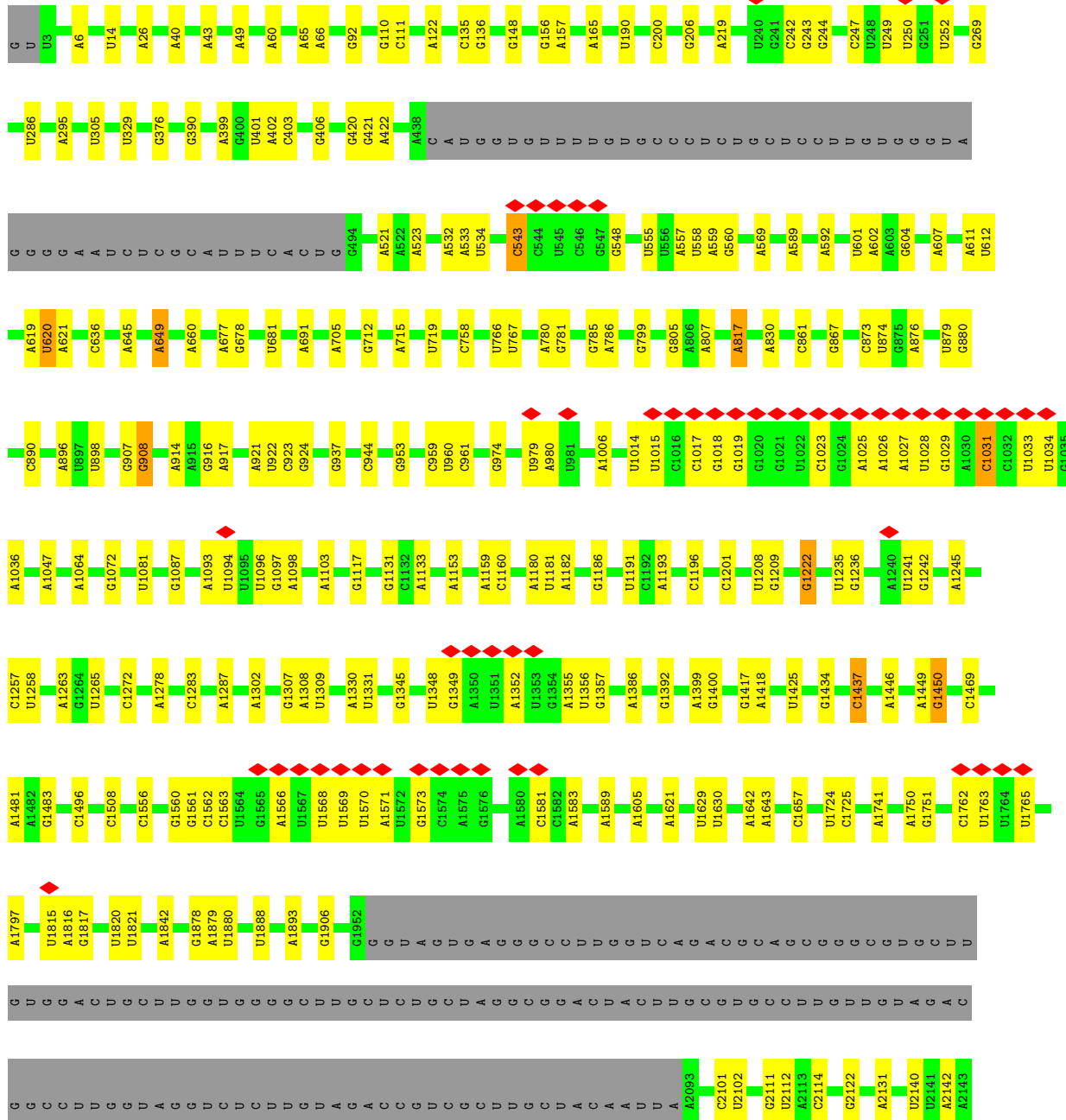
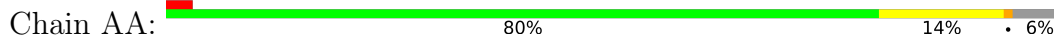
• Molecule 9: Ubiquitin-40S ribosomal protein S31

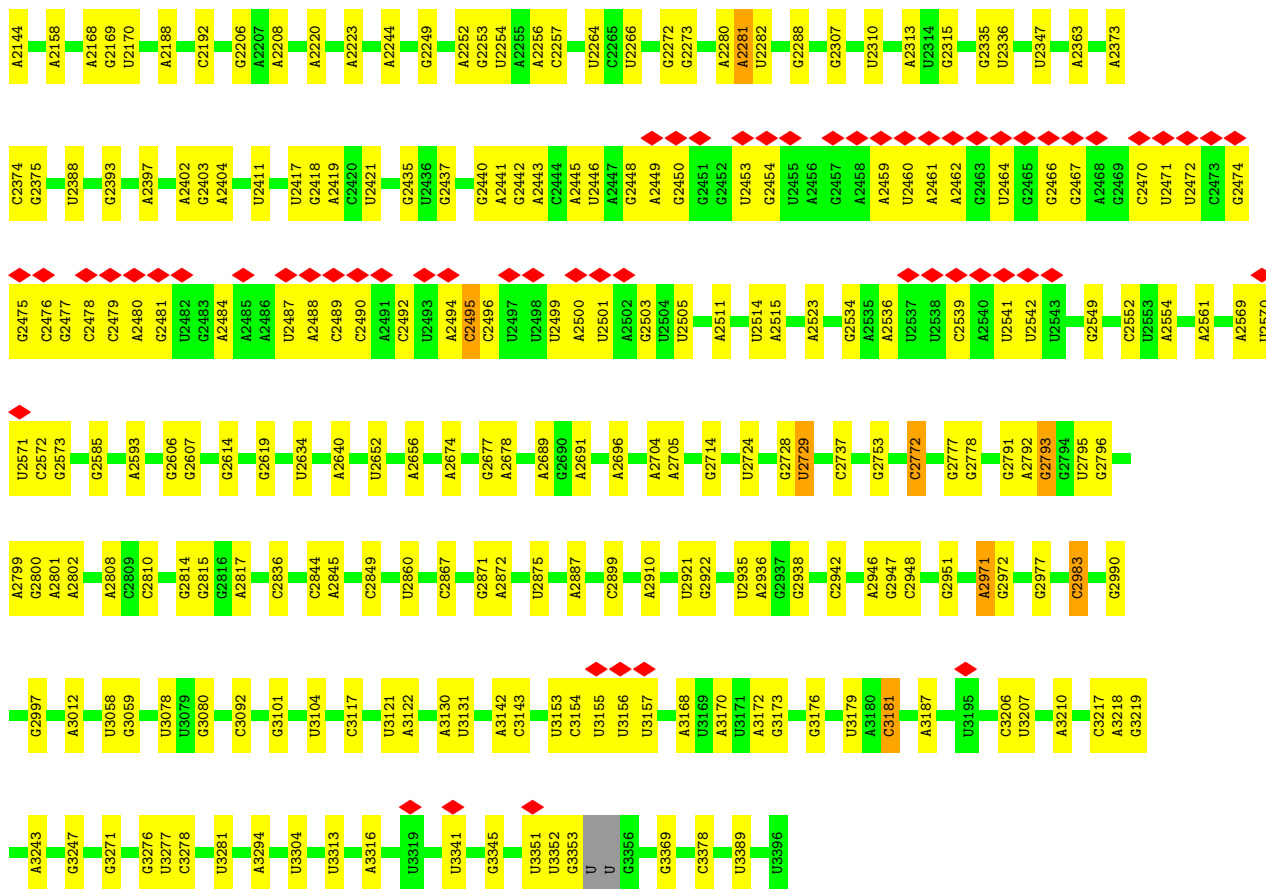


• Molecule 10: 60S ribosomal protein L16-A

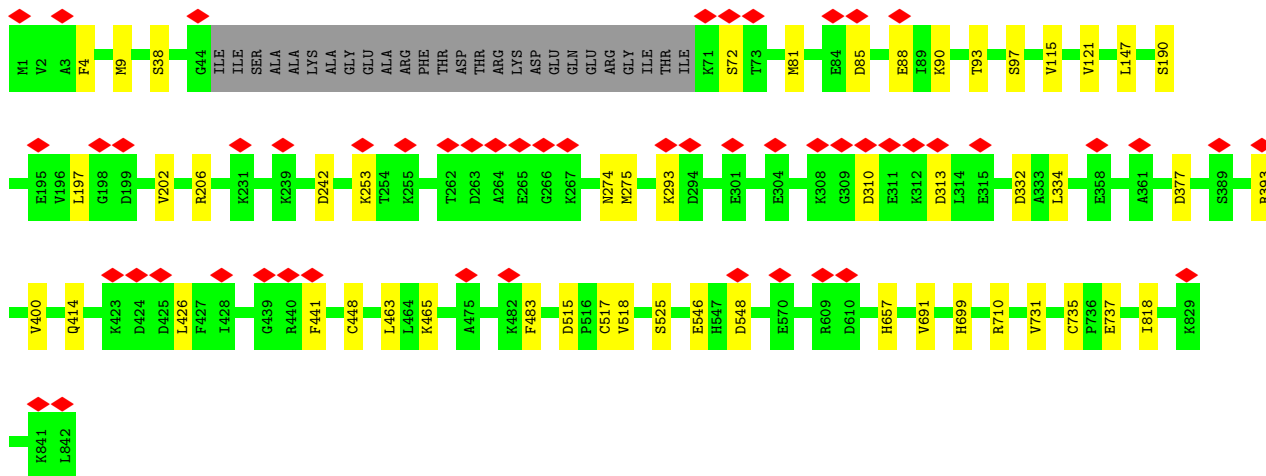


• Molecule 11: 25S ribosomal RNA

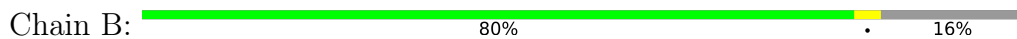


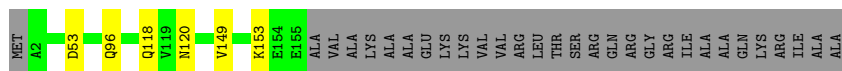


- Molecule 12: Elongation factor 2



- Molecule 13: 60S ribosomal protein L17-A

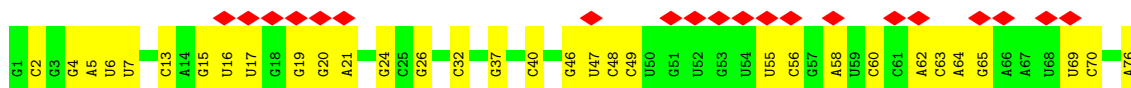




• Molecule 14: 5S ribosomal RNA



• Molecule 15: Transfer RNA Phe



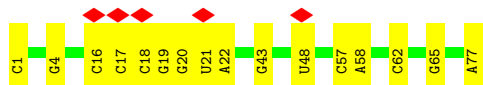
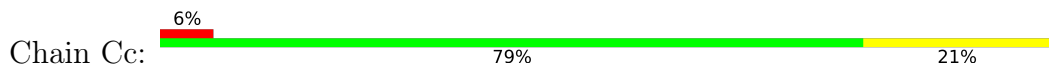
• Molecule 16: 60S ribosomal protein L18-A



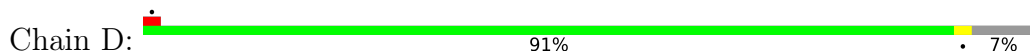
• Molecule 17: 5.8S ribosomal RNA



• Molecule 18: Transfer RNA fMet

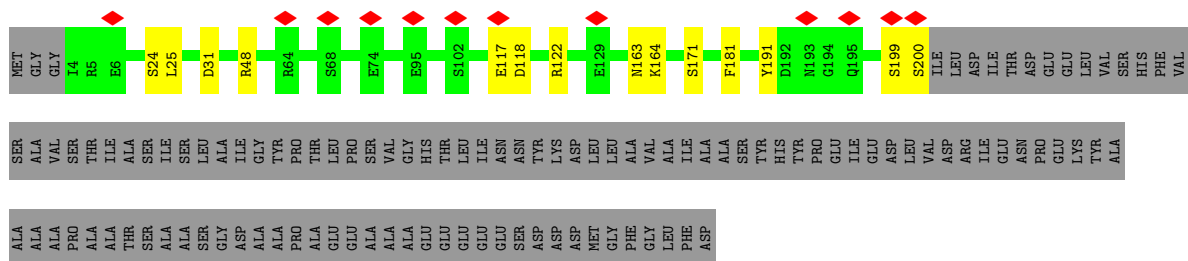


• Molecule 19: 60S ribosomal protein L19-A

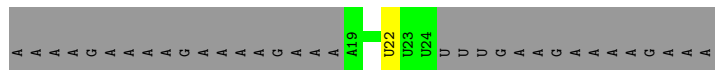


• Molecule 20: 60S acidic ribosomal protein P0

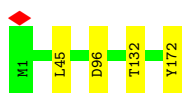




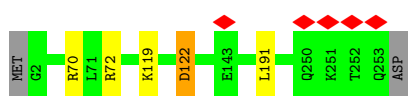
• Molecule 21: Messenger RNA



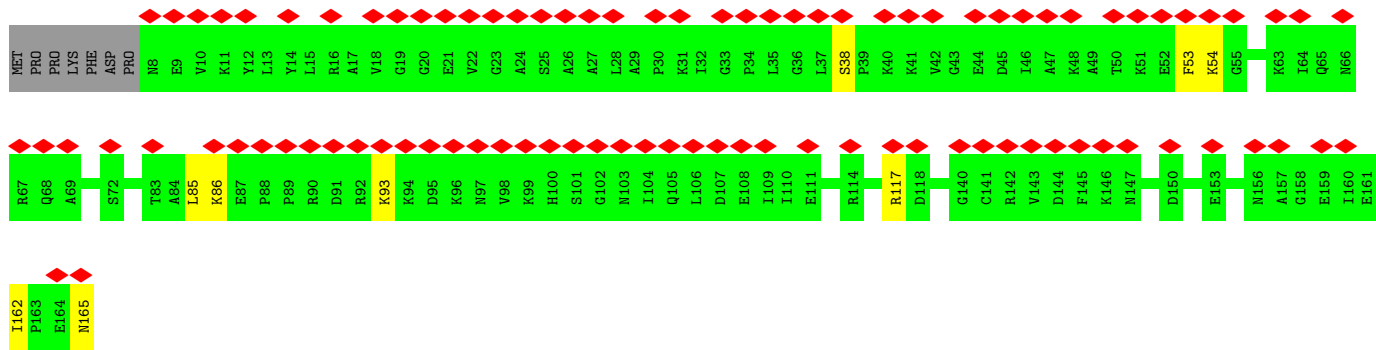
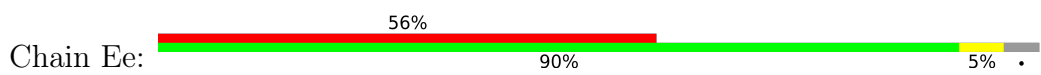
• Molecule 22: 60S ribosomal protein L20-A



• Molecule 23: 60S ribosomal protein L2-A




• Molecule 24: 60S ribosomal protein L12-A

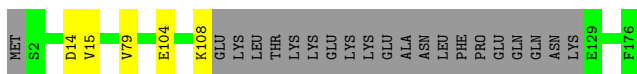


• Molecule 25: 60S ribosomal protein L21-A




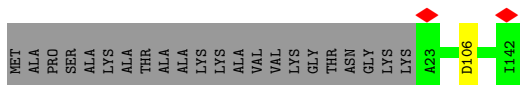
- Molecule 32: 60S ribosomal protein L6-A

Chain II:  85% 12%




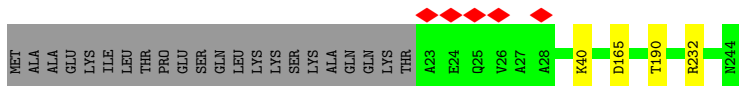
- Molecule 33: 60S ribosomal protein L25

Chain J:  84% 15%



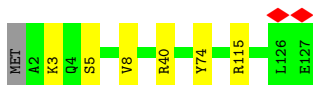
- Molecule 34: 60S ribosomal protein L7-A

Chain JJ:  89% 9%

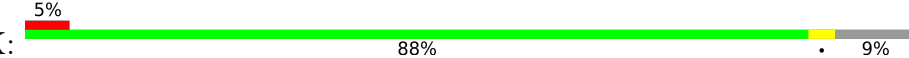


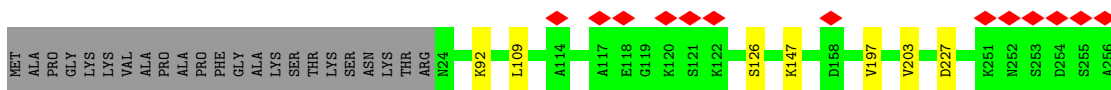
- Molecule 35: 60S ribosomal protein L26-A

Chain K:  94% 5%



- Molecule 36: 60S ribosomal protein L8-A

Chain KK:  88% 9% 5%



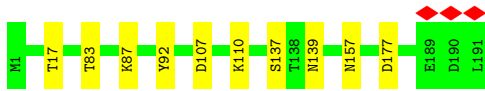
- Molecule 37: 60S ribosomal protein L27-A

Chain L:  96%



- Molecule 38: 60S ribosomal protein L9-A

Chain LL:  95% 5%



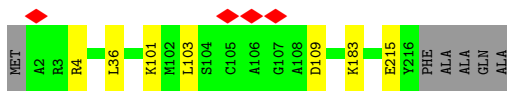
- Molecule 39: 60S ribosomal protein L28

Chain M: 95%



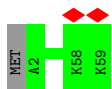
- Molecule 40: 60S ribosomal protein L10

Chain MM: 94%



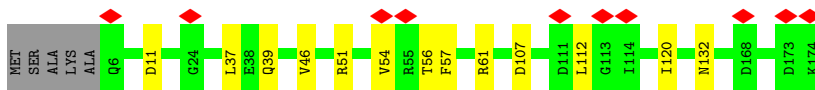
- Molecule 41: 60S ribosomal protein L29

Chain N: 98%



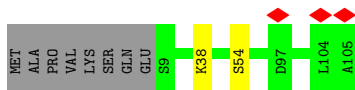
- Molecule 42: 60S ribosomal protein L11-A

Chain NN: 90% 6% 7%



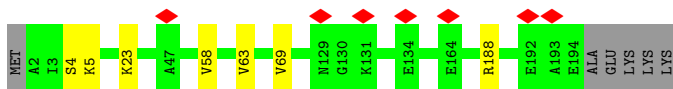
- Molecule 43: 60S ribosomal protein L30

Chain O: 90% 8%

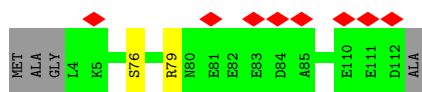
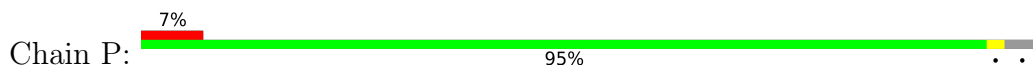


- Molecule 44: 60S ribosomal protein L13-A

Chain OO: 93%



- Molecule 45: 60S ribosomal protein L31-A



• Molecule 46: 60S ribosomal protein L14-A



• Molecule 47: dipeptide



• Molecule 48: 60S ribosomal protein L32



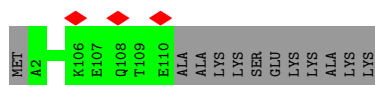
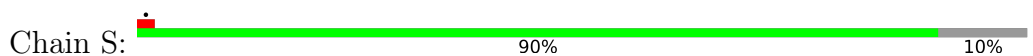
• Molecule 49: 60S ribosomal protein L15-A

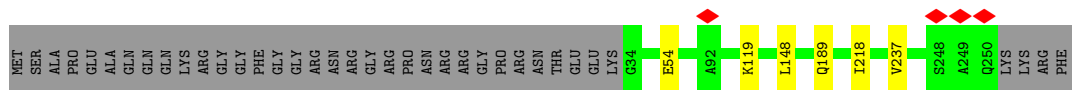


• Molecule 50: 60S ribosomal protein L33-A

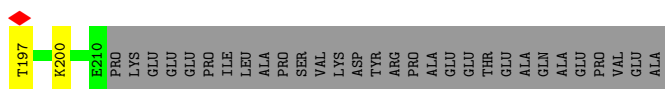
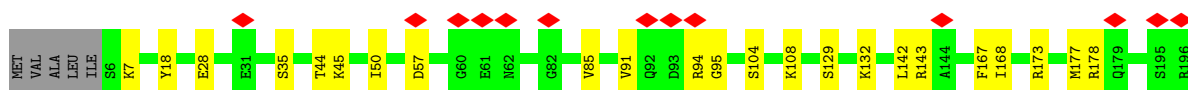
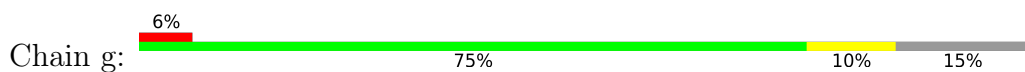


• Molecule 51: 60S ribosomal protein L34-A

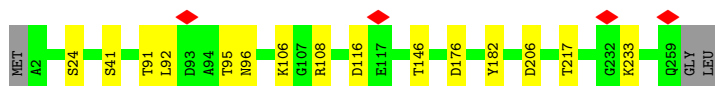




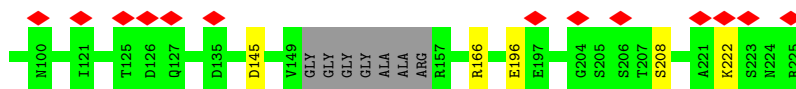
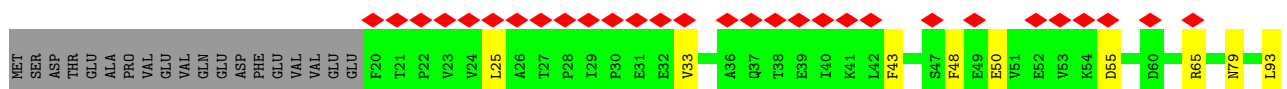
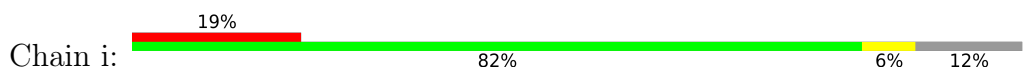
• Molecule 65: RPS3 isoform 1



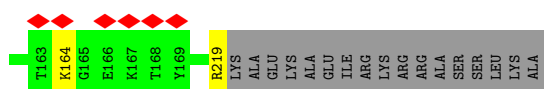
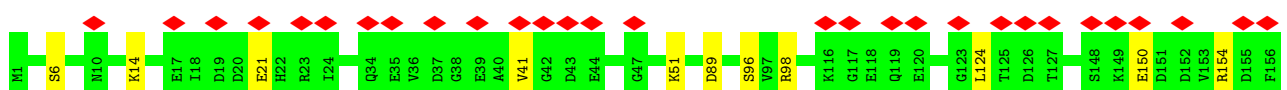
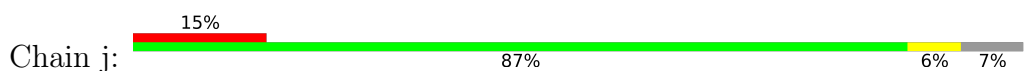
• Molecule 66: 40S ribosomal protein S4-A



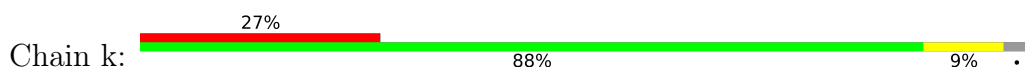
• Molecule 67: 40S ribosomal protein S5



• Molecule 68: 40S ribosomal protein S6-A

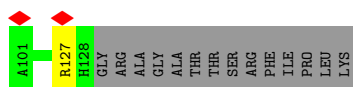
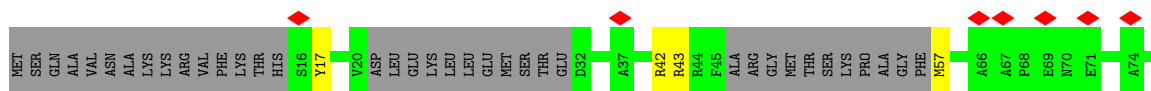


• Molecule 69: 40S ribosomal protein S7-A

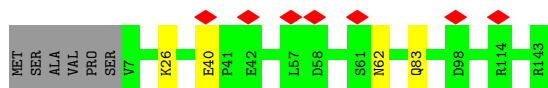
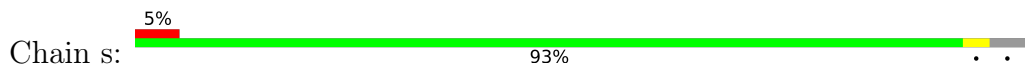




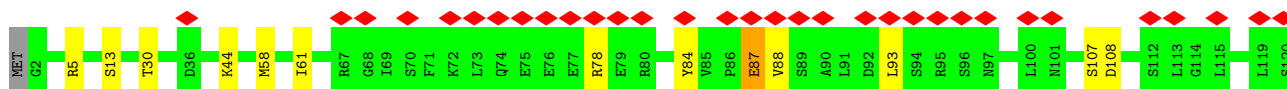
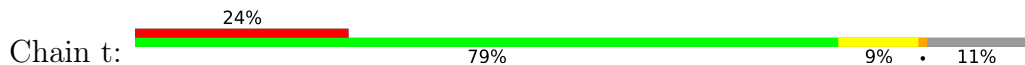
- Molecule 76: 40S ribosomal protein S15



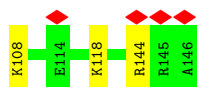
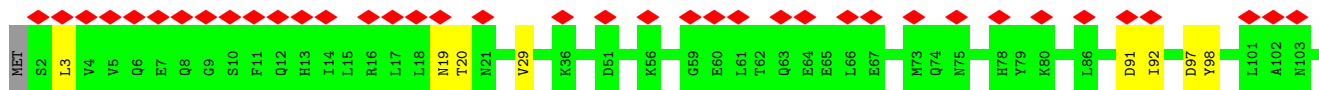
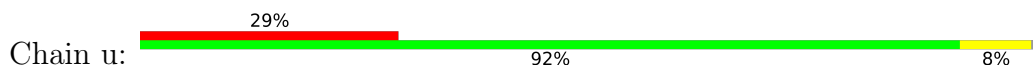
- Molecule 77: 40S ribosomal protein S16-A



- Molecule 78: 40S ribosomal protein S17-A

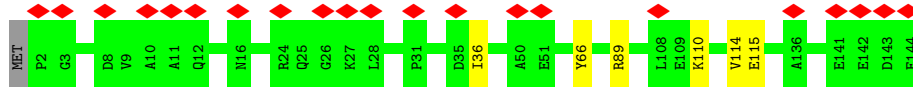


- Molecule 79: 40S ribosomal protein S18-A

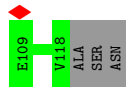
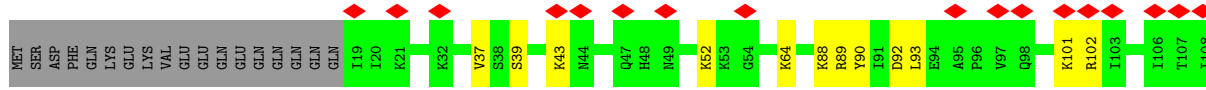
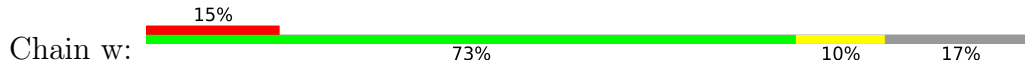


- Molecule 80: 40S ribosomal protein S19-A

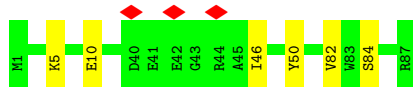
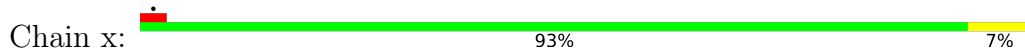




- Molecule 81: 40S ribosomal protein S20



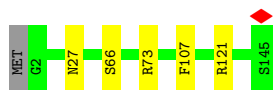
- Molecule 82: 40S ribosomal protein S21-A



- Molecule 83: 40S ribosomal protein S22-A



- Molecule 84: 40S ribosomal protein S23-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55762	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	1.666	Depositor
Minimum map value	-0.477	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.157	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 i

5.1 Standard geometry i

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

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	0.27	0/1087	0.55	0/1449
2	1	0.25	0/571	0.61	0/768
3	2	0.24	0/782	0.56	0/1047
4	3	0.24	0/620	0.54	0/838
5	4	0.25	0/499	0.64	1/670 (0.1%)
6	5	0.27	0/443	0.58	0/588
7	6	0.24	0/433	0.59	0/575
8	7	0.25	0/2489	0.57	1/3389 (0.0%)
9	8	0.23	0/279	0.48	0/369
10	A	0.26	0/1585	0.51	0/2128
11	AA	0.24	0/75545	0.78	28/117782 (0.0%)
12	Aa	0.26	0/6470	0.52	0/8759
13	B	0.25	0/1245	0.53	0/1676
14	BB	0.21	0/2883	0.73	0/4491
15	Bb	0.23	0/1788	0.84	0/2786
16	C	0.25	0/1465	0.55	0/1965
17	CC	0.23	0/3746	0.76	0/5832
18	Cc	0.30	1/1836 (0.1%)	0.75	0/2859
19	D	0.24	0/1440	0.55	0/1921
20	DD	0.26	0/1558	0.51	0/2107
21	Dd	0.23	0/138	0.91	0/212
22	E	0.26	0/1481	0.54	0/1990
23	EE	0.26	0/1948	0.56	1/2617 (0.0%)
24	Ee	0.25	0/1210	0.56	0/1627
25	F	0.25	0/1300	0.51	0/1743
26	FF	0.25	0/3146	0.53	0/4228
27	G	0.28	0/786	0.54	0/1065
28	GG	0.24	0/2800	0.50	0/3790
29	H	0.27	0/978	0.55	0/1316
30	HH	0.25	0/2425	0.50	0/3271
31	I	0.26	0/533	0.51	0/707

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	II	0.27	0/1251	0.52	0/1682
33	J	0.26	0/974	0.51	0/1314
34	JJ	0.26	0/1821	0.48	0/2451
35	K	0.25	0/1004	0.53	0/1341
36	KK	0.25	0/1836	0.47	0/2481
37	L	0.27	0/1118	0.50	0/1497
38	LL	0.26	0/1539	0.51	0/2073
39	M	0.25	0/1204	0.53	0/1612
40	MM	0.25	0/1779	0.53	0/2386
41	N	0.24	0/473	0.49	0/629
42	NN	0.25	0/1374	0.58	0/1842
43	O	0.25	0/750	0.44	0/1008
44	OO	0.25	0/1568	0.56	0/2106
45	P	0.25	0/897	0.55	0/1205
46	PP	0.25	0/1068	0.51	0/1438
47	Pp	0.29	0/19	0.45	0/23
48	Q	0.24	0/1041	0.50	0/1394
49	QQ	0.26	0/1757	0.59	1/2354 (0.0%)
50	R	0.27	0/868	0.54	0/1168
51	S	0.26	0/871	0.56	0/1164
52	T	0.25	0/978	0.50	0/1301
53	U	0.25	0/778	0.56	0/1034
54	V	0.25	0/680	0.58	0/901
55	W	0.26	0/618	0.52	0/826
56	X	0.24	0/443	0.63	0/588
57	Y	0.24	0/423	0.53	0/562
58	Z	0.23	0/234	0.69	0/300
59	a	0.26	0/831	0.56	0/1097
60	b	0.24	0/701	0.55	0/934
61	c	0.21	0/37760	0.78	22/58811 (0.0%)
62	d	0.25	0/1623	0.50	0/2222
63	e	0.24	0/1714	0.55	0/2308
64	f	0.25	0/1665	0.52	0/2263
65	g	0.27	0/1614	0.56	0/2169
66	h	0.25	0/2097	0.54	0/2823
67	i	0.24	0/1591	0.56	0/2151
68	j	0.25	0/1790	0.57	0/2393
69	k	0.26	0/1506	0.55	0/2028
70	l	0.25	0/1482	0.57	0/1980
71	m	0.24	0/1519	0.52	0/2035
72	n	0.29	0/610	0.51	0/821
73	o	0.25	0/1172	0.53	0/1580
74	p	0.25	0/1215	0.50	0/1638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	q	0.25	0/901	0.60	0/1217
76	r	0.26	0/747	0.58	0/1002
77	s	0.25	0/1099	0.52	0/1473
78	t	0.24	0/971	0.60	1/1303 (0.1%)
79	u	0.24	0/1211	0.56	0/1628
80	v	0.26	0/1130	0.53	0/1517
81	w	0.26	0/810	0.52	0/1095
82	x	0.26	0/693	0.54	0/935
83	y	0.25	0/1038	0.52	0/1395
84	z	0.24	0/1139	0.53	0/1518
All	All	0.24	1/219504 (0.0%)	0.69	55/321581 (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
24	Ee	0	1
34	JJ	0	1
37	L	0	1
59	a	0	1
63	e	0	1
67	i	0	1
69	k	0	1
77	s	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Cc	1	C	OP3-P	-10.61	1.48	1.61

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	c	94	U	C2-N3-C4	14.27	135.56	127.00
11	AA	3278	C	N1-C2-O2	7.71	123.53	118.90
11	AA	3278	C	C2-N1-C1'	7.46	127.01	118.80
61	c	94	U	N3-C4-C5	7.26	118.95	114.60
61	c	1473	U	C2-N1-C1'	7.13	126.25	117.70
61	c	1389	C	C2-N1-C1'	7.12	126.63	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	1283	C	N3-C2-O2	-7.03	116.98	121.90
11	AA	620	U	C2-N1-C1'	6.98	126.08	117.70
61	c	965	U	C2-N1-C1'	6.73	125.78	117.70
11	AA	2495	C	C2-N1-C1'	6.70	126.17	118.80
61	c	1596	C	C2-N1-C1'	6.64	126.10	118.80
11	AA	406	G	O4'-C1'-N9	6.63	113.50	108.20
61	c	1596	C	N1-C2-O2	6.58	122.85	118.90
11	AA	922	U	C2-N1-C1'	6.46	125.45	117.70
11	AA	620	U	N1-C2-O2	6.42	127.30	122.80
61	c	1096	C	N1-C2-O2	6.42	122.75	118.90
8	7	34	LEU	CA-CB-CG	6.37	129.94	115.30
11	AA	3278	C	N3-C2-O2	-6.33	117.47	121.90
61	c	1473	U	N1-C2-O2	6.23	127.16	122.80
11	AA	2983	C	C2-N1-C1'	6.20	125.62	118.80
61	c	1096	C	C2-N1-C1'	5.94	125.34	118.80
11	AA	620	U	N3-C2-O2	-5.92	118.06	122.20
49	QQ	145	ASP	CB-CG-OD1	5.77	123.49	118.30
11	AA	2772	C	N1-C2-O2	5.70	122.32	118.90
11	AA	3058	U	C2-N1-C1'	5.66	124.49	117.70
11	AA	1283	C	N1-C2-O2	5.62	122.27	118.90
61	c	1000	C	C2-N1-C1'	5.62	124.98	118.80
11	AA	1222	G	O4'-C1'-N9	5.59	112.67	108.20
11	AA	1031	C	C2-N1-C1'	5.58	124.94	118.80
61	c	94	U	N1-C2-N3	5.58	118.25	114.90
61	c	1473	U	N3-C2-O2	-5.49	118.35	122.20
61	c	794	U	OP2-P-O3'	5.48	117.26	105.20
61	c	1596	C	N3-C2-O2	-5.43	118.10	121.90
11	AA	543	C	N1-C2-O2	5.36	122.12	118.90
5	4	9	LEU	CA-CB-CG	5.35	127.61	115.30
11	AA	922	U	N1-C2-O2	5.34	126.54	122.80
61	c	1389	C	N1-C2-O2	5.33	122.10	118.90
61	c	139	C	C2-N1-C1'	5.33	124.66	118.80
11	AA	1496	C	C2-N1-C1'	5.32	124.65	118.80
11	AA	2836	C	C6-N1-C2	-5.30	118.18	120.30
61	c	139	C	N1-C2-O2	5.28	122.07	118.90
61	c	531	C	C2-N1-C1'	5.24	124.56	118.80
11	AA	3181	C	C2-N1-C1'	5.14	124.46	118.80
11	AA	2495	C	C6-N1-C1'	-5.14	114.64	120.80
11	AA	2772	C	C2-N1-C1'	5.14	124.45	118.80
11	AA	3181	C	N1-C2-O2	5.12	121.97	118.90
11	AA	2971	A	P-O3'-C3'	5.12	125.84	119.70
61	c	794	U	P-O3'-C3'	5.10	125.82	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	3278	C	C6-N1-C1'	-5.09	114.69	120.80
61	c	1000	C	N1-C2-O2	5.09	121.95	118.90
11	AA	2836	C	C2-N1-C1'	5.08	124.39	118.80
23	EE	122	ASP	CB-CG-OD1	5.07	122.87	118.30
78	t	87	GLU	CA-CB-CG	5.06	124.53	113.40
11	AA	3278	C	C6-N1-C2	-5.05	118.28	120.30
61	c	1096	C	N3-C2-O2	-5.04	118.38	121.90

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	Ee	86	LYS	Peptide
34	JJ	232	ARG	Peptide
37	L	102	GLU	Peptide
59	a	7	THR	Peptide
63	e	38	PHE	Peptide
67	i	65	ARG	Peptide
69	k	64	VAL	Peptide
77	s	40	GLU	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%)	90 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
5	4	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
6	5	50/56 (89%)	49 (98%)	1 (2%)	0	100	100
7	6	51/63 (81%)	50 (98%)	1 (2%)	0	100	100
8	7	316/319 (99%)	303 (96%)	13 (4%)	0	100	100
9	8	32/152 (21%)	25 (78%)	7 (22%)	0	100	100
10	A	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
12	Aa	811/842 (96%)	786 (97%)	25 (3%)	0	100	100
13	B	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
16	C	183/186 (98%)	182 (100%)	1 (0%)	0	100	100
19	D	174/189 (92%)	170 (98%)	4 (2%)	0	100	100
20	DD	195/312 (62%)	191 (98%)	4 (2%)	0	100	100
22	E	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
23	EE	250/254 (98%)	244 (98%)	6 (2%)	0	100	100
24	Ee	156/165 (94%)	150 (96%)	6 (4%)	0	100	100
25	F	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
26	FF	384/387 (99%)	375 (98%)	9 (2%)	0	100	100
27	G	95/121 (78%)	92 (97%)	3 (3%)	0	100	100
28	GG	359/362 (99%)	348 (97%)	11 (3%)	0	100	100
29	H	127/137 (93%)	126 (99%)	1 (1%)	0	100	100
30	HH	294/297 (99%)	286 (97%)	8 (3%)	0	100	100
31	I	61/155 (39%)	61 (100%)	0	0	100	100
32	II	151/176 (86%)	147 (97%)	4 (3%)	0	100	100
33	J	118/142 (83%)	115 (98%)	3 (2%)	0	100	100
34	JJ	220/244 (90%)	216 (98%)	4 (2%)	0	100	100
35	K	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
36	KK	231/256 (90%)	227 (98%)	4 (2%)	0	100	100
37	L	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
38	LL	189/191 (99%)	181 (96%)	8 (4%)	0	100	100
39	M	146/149 (98%)	142 (97%)	4 (3%)	0	100	100
40	MM	213/221 (96%)	210 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	N	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
42	NN	167/174 (96%)	161 (96%)	6 (4%)	0	100	100
43	O	95/105 (90%)	95 (100%)	0	0	100	100
44	OO	191/199 (96%)	177 (93%)	13 (7%)	1 (0%)	29	18
45	P	107/113 (95%)	103 (96%)	4 (4%)	0	100	100
46	PP	134/138 (97%)	133 (99%)	1 (1%)	0	100	100
48	Q	125/130 (96%)	125 (100%)	0	0	100	100
49	QQ	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
50	R	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
51	S	107/121 (88%)	107 (100%)	0	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%)	82 (100%)	0	0	100	100
55	W	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
56	X	48/51 (94%)	46 (96%)	2 (4%)	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%)	93 (93%)	7 (7%)	0	100	100
60	b	89/92 (97%)	89 (100%)	0	0	100	100
62	d	204/252 (81%)	196 (96%)	8 (4%)	0	100	100
63	e	210/255 (82%)	202 (96%)	8 (4%)	0	100	100
64	f	215/254 (85%)	204 (95%)	11 (5%)	0	100	100
65	g	203/240 (85%)	192 (95%)	10 (5%)	1 (0%)	29	18
66	h	256/261 (98%)	249 (97%)	7 (3%)	0	100	100
67	i	195/225 (87%)	188 (96%)	7 (4%)	0	100	100
68	j	217/236 (92%)	215 (99%)	2 (1%)	0	100	100
69	k	182/190 (96%)	174 (96%)	8 (4%)	0	100	100
70	l	180/200 (90%)	168 (93%)	12 (7%)	0	100	100
71	m	183/197 (93%)	179 (98%)	4 (2%)	0	100	100
72	n	68/105 (65%)	63 (93%)	5 (7%)	0	100	100
73	o	140/156 (90%)	133 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	p	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
75	q	125/137 (91%)	116 (93%)	9 (7%)	0	100	100
76	r	85/142 (60%)	82 (96%)	3 (4%)	0	100	100
77	s	135/143 (94%)	125 (93%)	10 (7%)	0	100	100
78	t	119/136 (88%)	115 (97%)	4 (3%)	0	100	100
79	u	143/146 (98%)	131 (92%)	12 (8%)	0	100	100
80	v	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
81	w	98/121 (81%)	98 (100%)	0	0	100	100
82	x	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
83	y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
84	z	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
All	All	11741/13056 (90%)	11362 (97%)	377 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	OO	63	VAL
65	g	95	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	112/113 (99%)	101 (90%)	11 (10%)	8	3
2	1	61/89 (68%)	56 (92%)	5 (8%)	11	5
3	2	83/101 (82%)	78 (94%)	5 (6%)	19	11
4	3	70/71 (99%)	63 (90%)	7 (10%)	7	2
5	4	56/60 (93%)	45 (80%)	11 (20%)	1	0
6	5	46/49 (94%)	39 (85%)	7 (15%)	3	0
7	6	46/54 (85%)	45 (98%)	1 (2%)	52	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	7	259/262 (99%)	226 (87%)	33 (13%)	4	1
9	8	30/135 (22%)	26 (87%)	4 (13%)	4	1
10	A	160/162 (99%)	152 (95%)	8 (5%)	24	16
12	Aa	694/714 (97%)	645 (93%)	49 (7%)	14	7
13	B	125/146 (86%)	119 (95%)	6 (5%)	25	18
16	C	150/151 (99%)	149 (99%)	1 (1%)	84	84
19	D	143/154 (93%)	139 (97%)	4 (3%)	43	37
20	DD	167/254 (66%)	153 (92%)	14 (8%)	11	4
22	E	156/156 (100%)	152 (97%)	4 (3%)	46	39
23	EE	193/196 (98%)	188 (97%)	5 (3%)	46	39
24	Ee	129/136 (95%)	121 (94%)	8 (6%)	18	10
25	F	136/137 (99%)	129 (95%)	7 (5%)	24	15
26	FF	320/323 (99%)	312 (98%)	8 (2%)	47	40
27	G	84/107 (78%)	80 (95%)	4 (5%)	25	18
28	GG	288/289 (100%)	278 (96%)	10 (4%)	36	29
29	H	101/105 (96%)	99 (98%)	2 (2%)	55	50
30	HH	244/245 (100%)	235 (96%)	9 (4%)	34	27
31	I	55/129 (43%)	54 (98%)	1 (2%)	59	55
32	II	133/153 (87%)	128 (96%)	5 (4%)	33	26
33	J	104/118 (88%)	103 (99%)	1 (1%)	76	75
34	JJ	186/205 (91%)	183 (98%)	3 (2%)	62	59
35	K	109/110 (99%)	103 (94%)	6 (6%)	21	13
36	KK	187/208 (90%)	180 (96%)	7 (4%)	34	27
37	L	115/116 (99%)	111 (96%)	4 (4%)	36	29
38	LL	171/171 (100%)	161 (94%)	10 (6%)	20	11
39	M	118/119 (99%)	112 (95%)	6 (5%)	24	15
40	MM	184/187 (98%)	177 (96%)	7 (4%)	33	26
41	N	46/47 (98%)	46 (100%)	0	100	100
42	NN	147/150 (98%)	134 (91%)	13 (9%)	10	4
43	O	81/88 (92%)	79 (98%)	2 (2%)	47	40
44	OO	154/159 (97%)	148 (96%)	6 (4%)	32	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	P	94/97 (97%)	92 (98%)	2 (2%)	53	48
46	PP	107/109 (98%)	104 (97%)	3 (3%)	43	37
47	Pp	2/2 (100%)	1 (50%)	1 (50%)	0	0
48	Q	109/111 (98%)	105 (96%)	4 (4%)	34	27
49	QQ	175/176 (99%)	173 (99%)	2 (1%)	73	73
50	R	90/91 (99%)	88 (98%)	2 (2%)	52	46
51	S	94/103 (91%)	94 (100%)	0	100	100
52	T	104/105 (99%)	102 (98%)	2 (2%)	57	53
53	U	81/82 (99%)	75 (93%)	6 (7%)	13	6
54	V	69/71 (97%)	67 (97%)	2 (3%)	42	35
55	W	68/69 (99%)	63 (93%)	5 (7%)	13	6
56	X	45/46 (98%)	43 (96%)	2 (4%)	28	21
57	Y	47/116 (40%)	46 (98%)	1 (2%)	53	48
58	Z	23/23 (100%)	21 (91%)	2 (9%)	10	4
59	a	87/91 (96%)	85 (98%)	2 (2%)	50	44
60	b	71/72 (99%)	68 (96%)	3 (4%)	30	22
62	d	165/210 (79%)	157 (95%)	8 (5%)	25	18
63	e	189/224 (84%)	176 (93%)	13 (7%)	15	8
64	f	176/205 (86%)	170 (97%)	6 (3%)	37	30
65	g	166/195 (85%)	142 (86%)	24 (14%)	3	1
66	h	220/222 (99%)	205 (93%)	15 (7%)	16	8
67	i	172/191 (90%)	159 (92%)	13 (8%)	13	6
68	j	188/201 (94%)	175 (93%)	13 (7%)	15	8
69	k	165/170 (97%)	149 (90%)	16 (10%)	8	3
70	l	146/161 (91%)	138 (94%)	8 (6%)	21	13
71	m	158/166 (95%)	146 (92%)	12 (8%)	13	6
72	n	65/98 (66%)	59 (91%)	6 (9%)	9	3
73	o	127/137 (93%)	119 (94%)	8 (6%)	18	9
74	p	127/128 (99%)	122 (96%)	5 (4%)	32	25
75	q	81/105 (77%)	73 (90%)	8 (10%)	8	3
76	r	77/118 (65%)	72 (94%)	5 (6%)	17	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	s	114/119 (96%)	111 (97%)	3 (3%)	46	39
78	t	105/124 (85%)	92 (88%)	13 (12%)	4	1
79	u	128/129 (99%)	117 (91%)	11 (9%)	10	4
80	v	115/116 (99%)	109 (95%)	6 (5%)	23	14
81	w	94/114 (82%)	82 (87%)	12 (13%)	4	1
82	x	74/74 (100%)	68 (92%)	6 (8%)	11	5
83	y	110/111 (99%)	103 (94%)	7 (6%)	17	9
84	z	119/120 (99%)	114 (96%)	5 (4%)	30	22
All	All	9990/10971 (91%)	9434 (94%)	556 (6%)	25	12

All (556) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	8	ARG
1	0	25	VAL
1	0	35	VAL
1	0	43	LYS
1	0	56	SER
1	0	78	SER
1	0	100	VAL
1	0	101	GLU
1	0	112	LYS
1	0	131	ARG
1	0	133	ASN
2	1	43	ASP
2	1	52	LYS
2	1	77	ARG
2	1	78	ILE
2	1	81	ARG
3	2	15	ARG
3	2	39	MET
3	2	45	VAL
3	2	64	LEU
3	2	89	ARG
4	3	2	VAL
4	3	18	LYS
4	3	61	THR
4	3	65	THR
4	3	77	THR

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Mol	Chain	Res	Type
4	3	78	SER
4	3	81	ARG
5	4	8	THR
5	4	11	LYS
5	4	14	LYS
5	4	15	VAL
5	4	22	ARG
5	4	30	VAL
5	4	31	GLU
5	4	38	ARG
5	4	56	LEU
5	4	65	ARG
5	4	67	ARG
6	5	8	PHE
6	5	9	SER
6	5	12	ARG
6	5	16	LYS
6	5	19	ARG
6	5	39	CYS
6	5	49	ASP
7	6	26	LYS
8	7	7	LEU
8	7	10	ARG
8	7	12	THR
8	7	16	HIS
8	7	40	LYS
8	7	45	TRP
8	7	48	THR
8	7	50	ASP
8	7	54	PHE
8	7	56	VAL
8	7	59	ARG
8	7	86	ASP
8	7	103	PHE
8	7	106	HIS
8	7	107	LYS
8	7	109	ASP
8	7	145	LEU
8	7	168	THR
8	7	178	VAL
8	7	179	LYS
8	7	221	MET

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Mol	Chain	Res	Type
8	7	229	LYS
8	7	231	MET
8	7	233	THR
8	7	242	SER
8	7	258	THR
8	7	263	PHE
8	7	269	TYR
8	7	271	VAL
8	7	278	PHE
8	7	297	ASP
8	7	308	ASN
8	7	316	MET
9	8	132	LEU
9	8	134	ASN
9	8	135	HIS
9	8	138	ARG
10	A	3	VAL
10	A	14	HIS
10	A	59	ARG
10	A	117	ARG
10	A	155	LYS
10	A	167	TYR
10	A	182	ASN
10	A	192	LYS
12	Aa	4	PHE
12	Aa	9	MET
12	Aa	38	SER
12	Aa	72	SER
12	Aa	81	MET
12	Aa	85	ASP
12	Aa	88	GLU
12	Aa	90	LYS
12	Aa	93	THR
12	Aa	97	SER
12	Aa	115	VAL
12	Aa	121	VAL
12	Aa	147	LEU
12	Aa	190	SER
12	Aa	197	LEU
12	Aa	202	VAL
12	Aa	206	ARG
12	Aa	242	ASP

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Mol	Chain	Res	Type
12	Aa	253	LYS
12	Aa	274	ASN
12	Aa	275	MET
12	Aa	293	LYS
12	Aa	310	ASP
12	Aa	313	ASP
12	Aa	332	ASP
12	Aa	334	LEU
12	Aa	377	ASP
12	Aa	393	ARG
12	Aa	400	VAL
12	Aa	414	GLN
12	Aa	426	LEU
12	Aa	441	PHE
12	Aa	448	CYS
12	Aa	463	LEU
12	Aa	465	LYS
12	Aa	483	PHE
12	Aa	515	ASP
12	Aa	517	CYS
12	Aa	518	VAL
12	Aa	525	SER
12	Aa	546	GLU
12	Aa	548	ASP
12	Aa	657	HIS
12	Aa	691	VAL
12	Aa	710	ARG
12	Aa	731	VAL
12	Aa	735	CYS
12	Aa	737	GLU
12	Aa	818	ILE
13	B	53	ASP
13	B	96	GLN
13	B	118	GLN
13	B	120	ASN
13	B	149	VAL
13	B	153	LYS
16	C	148	GLU
19	D	151	ARG
19	D	160	GLU
19	D	170	ARG
19	D	173	ARG

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Mol	Chain	Res	Type
20	DD	24	SER
20	DD	25	LEU
20	DD	31	ASP
20	DD	48	ARG
20	DD	117	GLU
20	DD	118	ASP
20	DD	122	ARG
20	DD	163	ASN
20	DD	164	LYS
20	DD	171	SER
20	DD	181	PHE
20	DD	191	TYR
20	DD	199	SER
20	DD	200	SER
22	E	45	LEU
22	E	96	ASP
22	E	132	THR
22	E	172	TYR
23	EE	70	ARG
23	EE	72	ARG
23	EE	119	LYS
23	EE	122	ASP
23	EE	191	LEU
24	Ee	38	SER
24	Ee	53	PHE
24	Ee	54	LYS
24	Ee	85	LEU
24	Ee	93	LYS
24	Ee	117	ARG
24	Ee	162	ILE
24	Ee	165	ASN
25	F	18	ASP
25	F	19	PHE
25	F	26	HIS
25	F	52	MET
25	F	83	ARG
25	F	97	LYS
25	F	139	ARG
26	FF	104	THR
26	FF	139	GLN
26	FF	206	ASP
26	FF	207	SER

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Mol	Chain	Res	Type
26	FF	261	MET
26	FF	332	ARG
26	FF	344	THR
26	FF	349	LYS
27	G	47	VAL
27	G	49	ASN
27	G	74	LYS
27	G	91	ASP
28	GG	6	VAL
28	GG	12	THR
28	GG	37	THR
28	GG	54	GLU
28	GG	60	THR
28	GG	82	THR
28	GG	120	TYR
28	GG	124	SER
28	GG	177	ASP
28	GG	343	LYS
29	H	9	THR
29	H	120	LYS
30	HH	107	ARG
30	HH	125	VAL
30	HH	137	ASP
30	HH	187	THR
30	HH	210	GLU
30	HH	218	ARG
30	HH	229	ASP
30	HH	261	THR
30	HH	264	GLN
31	I	1	MET
32	II	14	ASP
32	II	15	VAL
32	II	79	VAL
32	II	104	GLU
32	II	108	LYS
33	J	106	ASP
34	JJ	40	LYS
34	JJ	165	ASP
34	JJ	190	THR
35	K	3	LYS
35	K	5	SER
35	K	8	VAL

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Mol	Chain	Res	Type
35	K	40	ARG
35	K	74	TYR
35	K	115	ARG
36	KK	92	LYS
36	KK	109	LEU
36	KK	126	SER
36	KK	147	LYS
36	KK	197	VAL
36	KK	203	VAL
36	KK	227	ASP
37	L	31	GLU
37	L	52	LYS
37	L	60	LYS
37	L	95	VAL
38	LL	17	THR
38	LL	83	THR
38	LL	87	LYS
38	LL	92	TYR
38	LL	107	ASP
38	LL	110	LYS
38	LL	137	SER
38	LL	139	ASN
38	LL	157	ASN
38	LL	177	ASP
39	M	8	THR
39	M	60	TYR
39	M	86	LYS
39	M	92	LYS
39	M	93	SER
39	M	121	VAL
40	MM	4	ARG
40	MM	36	LEU
40	MM	101	LYS
40	MM	103	LEU
40	MM	109	ASP
40	MM	183	LYS
40	MM	215	GLU
42	NN	11	ASP
42	NN	37	LEU
42	NN	39	GLN
42	NN	46	VAL
42	NN	51	ARG

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Mol	Chain	Res	Type
42	NN	54	VAL
42	NN	56	THR
42	NN	57	PHE
42	NN	61	ARG
42	NN	107	ASP
42	NN	112	LEU
42	NN	120	ILE
42	NN	132	ASN
43	O	38	LYS
43	O	54	SER
44	OO	4	SER
44	OO	5	LYS
44	OO	23	LYS
44	OO	58	VAL
44	OO	69	VAL
44	OO	188	ARG
45	P	76	SER
45	P	79	ARG
46	PP	3	THR
46	PP	25	LYS
46	PP	82	SER
47	Pp	1	MET
48	Q	23	ASP
48	Q	31	ASN
48	Q	41	VAL
48	Q	51	SER
49	QQ	99	ARG
49	QQ	122	ASN
50	R	21	ARG
50	R	31	LYS
52	T	19	SER
52	T	37	SER
53	U	17	VAL
53	U	36	ARG
53	U	56	ARG
53	U	57	LEU
53	U	59	ASP
53	U	98	ARG
54	V	71	SER
54	V	84	SER
55	W	6	THR
55	W	21	LYS

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Mol	Chain	Res	Type
55	W	39	ARG
55	W	48	SER
55	W	78	LEU
56	X	30	ARG
56	X	49	MET
57	Y	81	SER
58	Z	1	MET
58	Z	24	SER
59	a	16	THR
59	a	80	ARG
60	b	60	CYS
60	b	63	THR
60	b	70	THR
62	d	8	ASP
62	d	13	ASP
62	d	101	ARG
62	d	114	SER
62	d	116	LYS
62	d	151	SER
62	d	153	SER
62	d	157	ASP
63	e	21	VAL
63	e	33	LYS
63	e	41	ARG
63	e	47	LEU
63	e	73	LEU
63	e	80	SER
63	e	82	ARG
63	e	107	THR
63	e	144	ARG
63	e	203	ASP
63	e	205	PHE
63	e	213	ARG
63	e	231	LEU
64	f	54	GLU
64	f	119	LYS
64	f	148	LEU
64	f	189	GLN
64	f	218	ILE
64	f	237	VAL
65	g	7	LYS
65	g	18	TYR

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Mol	Chain	Res	Type
65	g	28	GLU
65	g	35	SER
65	g	44	THR
65	g	45	LYS
65	g	50	ILE
65	g	57	ASP
65	g	85	VAL
65	g	91	VAL
65	g	94	ARG
65	g	104	SER
65	g	108	LYS
65	g	129	SER
65	g	132	LYS
65	g	142	LEU
65	g	143	ARG
65	g	167	PHE
65	g	168	ILE
65	g	173	ARG
65	g	177	MET
65	g	178	ARG
65	g	197	THR
65	g	200	LYS
66	h	24	SER
66	h	41	SER
66	h	91	THR
66	h	92	LEU
66	h	95	THR
66	h	96	ASN
66	h	106	LYS
66	h	108	ARG
66	h	116	ASP
66	h	146	THR
66	h	176	ASP
66	h	182	TYR
66	h	206	ASP
66	h	217	THR
66	h	233	LYS
67	i	25	LEU
67	i	33	VAL
67	i	43	PHE
67	i	48	PHE
67	i	50	GLU

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Mol	Chain	Res	Type
67	i	55	ASP
67	i	79	ASN
67	i	93	LEU
67	i	145	ASP
67	i	166	ARG
67	i	196	GLU
67	i	208	SER
67	i	222	LYS
68	j	6	SER
68	j	14	LYS
68	j	21	GLU
68	j	41	VAL
68	j	51	LYS
68	j	89	ASP
68	j	96	SER
68	j	98	ARG
68	j	124	LEU
68	j	150	GLU
68	j	154	ARG
68	j	164	LYS
68	j	219	ARG
69	k	7	LYS
69	k	16	LEU
69	k	24	PHE
69	k	25	VAL
69	k	35	LYS
69	k	39	ARG
69	k	42	GLN
69	k	47	ARG
69	k	77	LEU
69	k	85	PHE
69	k	86	GLN
69	k	99	LEU
69	k	108	GLN
69	k	159	VAL
69	k	163	ASP
69	k	168	SER
70	l	17	LYS
70	l	21	PHE
70	l	58	LEU
70	l	69	SER
70	l	97	THR

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Mol	Chain	Res	Type
70	l	141	ARG
70	l	149	SER
70	l	151	LYS
71	m	3	ARG
71	m	29	LYS
71	m	50	SER
71	m	65	LYS
71	m	66	ASP
71	m	79	ARG
71	m	87	SER
71	m	94	ASP
71	m	128	LEU
71	m	172	VAL
71	m	179	ARG
71	m	186	GLU
72	n	1	MET
72	n	3	MET
72	n	5	LYS
72	n	47	GLN
72	n	52	LYS
72	n	68	LEU
73	o	6	THR
73	o	7	VAL
73	o	21	ASN
73	o	31	THR
73	o	46	LYS
73	o	67	ARG
73	o	118	GLN
73	o	142	VAL
74	p	30	SER
74	p	60	VAL
74	p	64	ARG
74	p	97	SER
74	p	107	LYS
75	q	20	TYR
75	q	26	THR
75	q	30	VAL
75	q	38	THR
75	q	92	LYS
75	q	108	SER
75	q	110	LEU
75	q	114	ARG

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Mol	Chain	Res	Type
76	r	17	TYR
76	r	42	ARG
76	r	43	ARG
76	r	57	MET
76	r	127	ARG
77	s	26	LYS
77	s	62	ASN
77	s	83	GLN
78	t	5	ARG
78	t	13	SER
78	t	30	THR
78	t	44	LYS
78	t	58	MET
78	t	61	ILE
78	t	78	ARG
78	t	84	TYR
78	t	87	GLU
78	t	88	VAL
78	t	93	LEU
78	t	107	SER
78	t	108	ASP
79	u	3	LEU
79	u	19	ASN
79	u	20	THR
79	u	29	VAL
79	u	91	ASP
79	u	92	ILE
79	u	97	ASP
79	u	98	TYR
79	u	108	LYS
79	u	118	LYS
79	u	144	ARG
80	v	36	ILE
80	v	66	TYR
80	v	89	ARG
80	v	110	LYS
80	v	114	VAL
80	v	115	GLU
81	w	37	VAL
81	w	39	SER
81	w	43	LYS
81	w	52	LYS

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Mol	Chain	Res	Type
81	w	64	LYS
81	w	88	LYS
81	w	89	ARG
81	w	90	TYR
81	w	92	ASP
81	w	93	LEU
81	w	101	LYS
81	w	102	ARG
82	x	5	LYS
82	x	10	GLU
82	x	46	ILE
82	x	50	TYR
82	x	82	VAL
82	x	84	SER
83	y	3	ARG
83	y	30	SER
83	y	31	SER
83	y	51	GLU
83	y	55	ASP
83	y	88	LYS
83	y	117	ARG
84	z	27	ASN
84	z	66	SER
84	z	73	ARG
84	z	107	PHE
84	z	121	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	98	GLN
5	4	43	ASN
8	7	64	HIS
24	Ee	105	GLN
29	H	98	ASN
38	LL	139	ASN
63	e	149	GLN
63	e	199	ASN
72	n	29	GLN
72	n	47	GLN
75	q	99	GLN
78	t	29	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	3193/3396 (94%)	452 (14%)	16 (0%)
14	BB	121/121 (100%)	7 (5%)	2 (1%)
15	Bb	75/76 (98%)	31 (41%)	0
17	CC	157/158 (99%)	22 (14%)	0
18	Cc	76/77 (98%)	15 (19%)	0
21	Dd	5/39 (12%)	1 (20%)	0
61	c	1593/1800 (88%)	290 (18%)	0
All	All	5220/5667 (92%)	818 (15%)	18 (0%)

All (818) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
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	60	A
11	AA	65	A
11	AA	66	A
11	AA	92	G
11	AA	110	G
11	AA	111	C
11	AA	122	A
11	AA	135	C
11	AA	136	G
11	AA	148	G
11	AA	156	G
11	AA	157	A
11	AA	165	A
11	AA	190	U
11	AA	200	C
11	AA	206	G
11	AA	219	A
11	AA	242	C
11	AA	243	G
11	AA	244	G
11	AA	247	C
11	AA	249	U
11	AA	250	U

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Mol	Chain	Res	Type
11	AA	252	U
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	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	521	A
11	AA	523	A
11	AA	532	A
11	AA	533	A
11	AA	534	U
11	AA	543	C
11	AA	548	G
11	AA	555	U
11	AA	557	A
11	AA	558	U
11	AA	559	A
11	AA	560	G
11	AA	569	A
11	AA	589	A
11	AA	592	A
11	AA	601	U
11	AA	602	A
11	AA	604	G
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	677	A

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Mol	Chain	Res	Type
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	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	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
11	AA	924	G
11	AA	937	G
11	AA	944	C
11	AA	953	G
11	AA	959	C
11	AA	960	U
11	AA	961	C
11	AA	974	G
11	AA	979	U
11	AA	980	A
11	AA	1006	A
11	AA	1014	U

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Mol	Chain	Res	Type
11	AA	1015	U
11	AA	1017	C
11	AA	1018	G
11	AA	1019	G
11	AA	1023	C
11	AA	1025	A
11	AA	1026	A
11	AA	1027	A
11	AA	1028	U
11	AA	1029	G
11	AA	1031	C
11	AA	1034	U
11	AA	1036	A
11	AA	1047	A
11	AA	1064	A
11	AA	1072	G
11	AA	1081	U
11	AA	1087	G
11	AA	1093	A
11	AA	1094	U
11	AA	1096	U
11	AA	1097	G
11	AA	1098	A
11	AA	1103	A
11	AA	1117	G
11	AA	1131	G
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	1186	G
11	AA	1191	U
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

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Mol	Chain	Res	Type
11	AA	1241	U
11	AA	1242	G
11	AA	1245	A
11	AA	1257	C
11	AA	1258	U
11	AA	1263	A
11	AA	1265	U
11	AA	1272	C
11	AA	1278	A
11	AA	1287	A
11	AA	1302	A
11	AA	1307	G
11	AA	1308	A
11	AA	1309	U
11	AA	1330	A
11	AA	1331	U
11	AA	1345	G
11	AA	1348	U
11	AA	1349	G
11	AA	1352	A
11	AA	1355	A
11	AA	1356	U
11	AA	1357	G
11	AA	1386	A
11	AA	1392	G
11	AA	1399	A
11	AA	1400	G
11	AA	1417	G
11	AA	1418	A
11	AA	1425	U
11	AA	1434	G
11	AA	1437	OMC
11	AA	1446	A
11	AA	1450	OMG
11	AA	1469	C
11	AA	1481	A
11	AA	1483	G
11	AA	1508	C
11	AA	1556	C
11	AA	1560	G
11	AA	1561	G
11	AA	1562	C

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Mol	Chain	Res	Type
11	AA	1563	C
11	AA	1566	A
11	AA	1568	U
11	AA	1569	U
11	AA	1570	U
11	AA	1571	A
11	AA	1573	G
11	AA	1581	C
11	AA	1583	A
11	AA	1589	A
11	AA	1605	A
11	AA	1621	A
11	AA	1629	U
11	AA	1630	U
11	AA	1642	A
11	AA	1643	A
11	AA	1657	C
11	AA	1724	U
11	AA	1725	C
11	AA	1741	A
11	AA	1750	A
11	AA	1751	G
11	AA	1762	C
11	AA	1763	U
11	AA	1765	U
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	1878	G
11	AA	1879	A
11	AA	1880	U
11	AA	1893	A
11	AA	1906	G
11	AA	2102	U
11	AA	2111	G
11	AA	2112	U
11	AA	2114	C
11	AA	2122	G

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Mol	Chain	Res	Type
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	2188	A
11	AA	2192	C
11	AA	2206	G
11	AA	2208	A
11	AA	2223	A
11	AA	2244	A
11	AA	2249	G
11	AA	2252	A
11	AA	2253	G
11	AA	2254	U
11	AA	2257	C
11	AA	2264	U
11	AA	2266	U
11	AA	2272	G
11	AA	2273	G
11	AA	2281	A2M
11	AA	2282	U
11	AA	2307	G
11	AA	2310	U
11	AA	2313	A
11	AA	2315	G
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

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Mol	Chain	Res	Type
11	AA	2419	A
11	AA	2435	G
11	AA	2437	G
11	AA	2440	G
11	AA	2441	A
11	AA	2442	G
11	AA	2443	A
11	AA	2445	A
11	AA	2446	U
11	AA	2448	G
11	AA	2449	A
11	AA	2450	G
11	AA	2453	U
11	AA	2454	G
11	AA	2459	A
11	AA	2460	U
11	AA	2461	A
11	AA	2462	A
11	AA	2464	U
11	AA	2466	G
11	AA	2467	G
11	AA	2470	C
11	AA	2471	U
11	AA	2472	U
11	AA	2474	G
11	AA	2475	G
11	AA	2476	C
11	AA	2477	G
11	AA	2478	C
11	AA	2479	C
11	AA	2480	A
11	AA	2481	G
11	AA	2484	A
11	AA	2487	U
11	AA	2488	A
11	AA	2489	C
11	AA	2490	C
11	AA	2492	C
11	AA	2494	A
11	AA	2495	C
11	AA	2496	C
11	AA	2499	U

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Mol	Chain	Res	Type
11	AA	2500	A
11	AA	2501	U
11	AA	2503	G
11	AA	2505	U
11	AA	2511	A
11	AA	2514	U
11	AA	2515	A
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	2561	A
11	AA	2569	A
11	AA	2570	U
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	2674	A
11	AA	2677	G
11	AA	2678	A
11	AA	2689	A
11	AA	2691	A
11	AA	2696	A
11	AA	2704	A
11	AA	2705	A
11	AA	2714	G
11	AA	2728	G
11	AA	2729	OMU
11	AA	2737	C
11	AA	2753	G

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Mol	Chain	Res	Type
11	AA	2772	C
11	AA	2777	G
11	AA	2778	G
11	AA	2793	OMG
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	2849	C
11	AA	2860	U
11	AA	2867	C
11	AA	2871	G
11	AA	2872	A
11	AA	2875	U
11	AA	2887	A
11	AA	2899	C
11	AA	2910	A
11	AA	2935	U
11	AA	2936	A
11	AA	2938	G
11	AA	2942	C
11	AA	2947	G
11	AA	2951	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	3059	G
11	AA	3078	U
11	AA	3080	G
11	AA	3092	C

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Mol	Chain	Res	Type
11	AA	3101	G
11	AA	3104	U
11	AA	3117	C
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
11	AA	3179	U
11	AA	3181	C
11	AA	3187	A
11	AA	3206	C
11	AA	3207	U
11	AA	3210	A
11	AA	3217	C
11	AA	3218	A
11	AA	3219	G
11	AA	3243	A
11	AA	3247	G
11	AA	3271	G
11	AA	3276	G
11	AA	3277	U
11	AA	3281	U
11	AA	3294	A
11	AA	3304	U
11	AA	3313	U
11	AA	3316	A
11	AA	3341	U
11	AA	3345	G
11	AA	3351	U
11	AA	3352	U
11	AA	3353	G

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Mol	Chain	Res	Type
11	AA	3369	G
11	AA	3378	C
11	AA	3389	U
14	BB	7	G
14	BB	11	A
14	BB	54	U
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	7	U
15	Bb	13	C
15	Bb	15	G
15	Bb	16	U
15	Bb	17	U
15	Bb	19	G
15	Bb	20	G
15	Bb	21	A
15	Bb	24	G
15	Bb	26	G
15	Bb	32	C
15	Bb	40	C
15	Bb	46	G
15	Bb	47	U
15	Bb	48	C
15	Bb	49	C
15	Bb	55	U
15	Bb	56	C
15	Bb	58	A
15	Bb	60	C
15	Bb	62	A
15	Bb	63	C
15	Bb	64	A
15	Bb	65	G
15	Bb	69	U
15	Bb	70	C
15	Bb	76	A
17	CC	23	U

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Mol	Chain	Res	Type
17	CC	34	U
17	CC	35	C
17	CC	39	G
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
17	CC	90	U
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	57	C
18	Cc	58	A
18	Cc	62	C
18	Cc	65	G
18	Cc	77	A
21	Dd	22	U
61	c	2	A
61	c	4	C
61	c	26	A
61	c	27	U
61	c	28	A2M

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Mol	Chain	Res	Type
61	c	34	G
61	c	43	A
61	c	47	A
61	c	61	A
61	c	67	A
61	c	68	A
61	c	69	G
61	c	71	A
61	c	72	A
61	c	78	A
61	c	81	G
61	c	114	C
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	153	G
61	c	161	U
61	c	168	A
61	c	176	C
61	c	183	U
61	c	184	C
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	321	C
61	c	322	G

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Mol	Chain	Res	Type
61	c	333	A
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	416	A
61	c	423	G
61	c	424	C
61	c	426	G
61	c	428	A
61	c	434	G
61	c	439	U
61	c	444	C
61	c	445	A
61	c	448	C
61	c	455	C
61	c	468	A
61	c	475	A
61	c	477	A
61	c	514	G
61	c	515	A
61	c	519	C
61	c	526	A
61	c	534	A
61	c	537	G
61	c	538	A
61	c	540	G
61	c	542	A
61	c	555	A
61	c	557	G
61	c	558	U
61	c	559	C
61	c	565	C
61	c	578	OMU
61	c	579	A
61	c	582	U
61	c	583	C
61	c	594	A

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Mol	Chain	Res	Type
61	c	611	U
61	c	619	A2M
61	c	620	A
61	c	623	A
61	c	624	G
61	c	639	U
61	c	642	G
61	c	643	G
61	c	644	C
61	c	648	G
61	c	650	U
61	c	651	G
61	c	691	C
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	766	U
61	c	767	U
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	793	A
61	c	794	U
61	c	795	U
61	c	812	A
61	c	814	A
61	c	818	C
61	c	820	U
61	c	822	U
61	c	852	C
61	c	853	G
61	c	859	A
61	c	860	U

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Mol	Chain	Res	Type
61	c	863	A
61	c	895	G
61	c	898	A
61	c	906	A
61	c	913	G
61	c	914	G
61	c	933	A
61	c	935	U
61	c	951	A
61	c	960	U
61	c	966	A
61	c	987	G
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	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	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	1097	U
61	c	1100	G
61	c	1138	A
61	c	1150	G
61	c	1158	C
61	c	1159	C
61	c	1162	C
61	c	1185	U

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Mol	Chain	Res	Type
61	c	1194	A
61	c	1196	A
61	c	1199	G
61	c	1200	G
61	c	1202	A
61	c	1207	C
61	c	1212	G
61	c	1217	A
61	c	1218	G
61	c	1220	C
61	c	1221	A
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	1230	A
61	c	1237	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	1259	U
61	c	1261	G
61	c	1262	U
61	c	1263	G
61	c	1270	G
61	c	1274	C
61	c	1286	U
61	c	1297	G
61	c	1314	U
61	c	1315	U
61	c	1316	G
61	c	1320	U
61	c	1321	A
61	c	1336	A
61	c	1338	C

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Mol	Chain	Res	Type
61	c	1339	C
61	c	1340	U
61	c	1346	A
61	c	1347	U
61	c	1354	G
61	c	1356	U
61	c	1357	A
61	c	1361	U
61	c	1363	U
61	c	1368	G
61	c	1372	U
61	c	1373	C
61	c	1388	A
61	c	1390	U
61	c	1398	U
61	c	1411	A
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	1459	C
61	c	1460	A
61	c	1469	A
61	c	1471	A
61	c	1472	C
61	c	1478	G
61	c	1490	C
61	c	1492	A
61	c	1496	U
61	c	1506	G
61	c	1510	U
61	c	1516	A
61	c	1521	G
61	c	1524	A
61	c	1535	U

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Mol	Chain	Res	Type
61	c	1536	G
61	c	1537	C
61	c	1542	G
61	c	1557	U
61	c	1559	A
61	c	1575	G7M
61	c	1590	G
61	c	1601	G
61	c	1616	G
61	c	1619	C
61	c	1631	A
61	c	1633	A
61	c	1634	C
61	c	1657	U
61	c	1658	G
61	c	1678	A
61	c	1681	A
61	c	1683	C
61	c	1716	C
61	c	1717	G
61	c	1755	A
61	c	1756	A
61	c	1757	G
61	c	1762	A
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 (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	AA	601	U
11	AA	619	A
11	AA	873	C
11	AA	916	G
11	AA	1033	U

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Mol	Chain	Res	Type
11	AA	1235	U
11	AA	1562	C
11	AA	2101	C
11	AA	2253	G
11	AA	2418	G
11	AA	2487	U
11	AA	2500	A
11	AA	2792	A
11	AA	2971	A
11	AA	3121	U
11	AA	3206	C
14	BB	1	G
14	BB	72	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	OMU	AA	2921	11,86	19,22,23	3.05	8 (42%)	26,31,34	1.71	5 (19%)
61	OMG	c	1428	86,61	18,26,27	1.12	2 (11%)	19,38,41	0.83	1 (5%)
11	1MA	AA	2142	11,86	16,25,26	0.93	2 (12%)	18,37,40	1.09	2 (11%)
11	OMC	AA	2959	11,86	19,22,23	0.54	0	26,31,34	0.67	0
61	A2M	c	420	61	18,25,26	3.58	8 (44%)	18,36,39	3.34	3 (16%)
11	OMC	AA	650	11	19,22,23	0.53	0	26,31,34	0.66	0
11	A2M	AA	2281	11	18,25,26	3.64	8 (44%)	18,36,39	3.40	4 (22%)
11	OMG	AA	805	11	18,26,27	1.11	2 (11%)	19,38,41	0.87	1 (5%)
11	A2M	AA	2280	11	18,25,26	3.59	8 (44%)	18,36,39	3.36	3 (16%)
11	A2M	AA	876	11	18,25,26	3.59	8 (44%)	18,36,39	3.36	4 (22%)
61	A2M	c	541	61	18,25,26	3.58	8 (44%)	18,36,39	3.33	4 (22%)
11	OMG	AA	2791	11	18,26,27	1.11	2 (11%)	19,38,41	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	A2M	c	619	86,61	18,25,26	3.61	8 (44%)	18,36,39	3.43	3 (16%)
11	OMC	AA	663	11	19,22,23	0.53	0	26,31,34	0.75	0
11	A2M	AA	1133	11,86	18,25,26	3.59	8 (44%)	18,36,39	3.39	3 (16%)
11	5MC	AA	2870	11,88	18,22,23	0.66	0	26,32,35	0.62	0
61	OMU	c	1269	61	19,22,23	3.10	8 (42%)	26,31,34	1.68	5 (19%)
11	OMC	AA	2337	11	19,22,23	0.51	0	26,31,34	0.62	0
61	OMU	c	578	61	19,22,23	3.08	8 (42%)	26,31,34	1.68	4 (15%)
11	A2M	AA	2220	11	18,25,26	3.57	8 (44%)	18,36,39	3.36	4 (22%)
11	OMU	AA	898	11	19,22,23	3.06	8 (42%)	26,31,34	1.67	5 (19%)
15	YYG	Bb	37	15	31,42,43	2.20	8 (25%)	33,62,65	1.81	9 (27%)
11	UR3	AA	2634	11	19,22,23	2.88	6 (31%)	26,32,35	1.30	1 (3%)
61	A2M	c	28	61	18,25,26	3.60	8 (44%)	18,36,39	3.38	4 (22%)
61	4AC	c	1280	61	21,24,25	3.56	10 (47%)	29,34,37	1.60	5 (17%)
11	A2M	AA	2256	11	18,25,26	3.58	8 (44%)	18,36,39	3.48	4 (22%)
11	OMG	AA	2815	11	18,26,27	1.11	2 (11%)	19,38,41	0.84	1 (5%)
11	A2M	AA	817	11,86	18,25,26	3.58	8 (44%)	18,36,39	3.43	3 (16%)
61	OMC	c	1007	61	19,22,23	0.52	0	26,31,34	0.65	0
11	OMU	AA	1888	11	19,22,23	3.06	8 (42%)	26,31,34	1.75	5 (19%)
12	DDE	Aa	699	12	14,20,21	0.87	0	14,28,30	1.00	1 (7%)
11	OMG	AA	1450	11	18,26,27	1.10	2 (11%)	19,38,41	0.81	1 (5%)
11	A2M	AA	807	11	18,25,26	3.59	8 (44%)	18,36,39	3.41	4 (22%)
61	A2M	c	100	86,61	18,25,26	3.59	8 (44%)	18,36,39	3.32	4 (22%)
61	OMG	c	1271	61	18,26,27	1.11	2 (11%)	19,38,41	0.84	1 (5%)
11	A2M	AA	649	11	18,25,26	3.58	8 (44%)	18,36,39	3.34	4 (22%)
61	OMG	c	562	61	18,26,27	1.12	2 (11%)	19,38,41	0.86	1 (5%)
11	OMG	AA	2793	11	18,26,27	1.15	2 (11%)	19,38,41	0.88	1 (5%)
61	A2M	c	436	61	18,25,26	3.60	8 (44%)	18,36,39	3.35	3 (16%)
11	A2M	AA	1449	11,86	18,25,26	3.60	8 (44%)	18,36,39	3.35	4 (22%)
61	B8N	c	1191	61	24,29,30	3.06	6 (25%)	29,42,45	1.74	6 (20%)
61	OMG	c	1572	61	18,26,27	1.12	2 (11%)	19,38,41	0.88	1 (5%)
61	G7M	c	1575	18,61	20,26,27	2.46	7 (35%)	17,39,42	1.16	1 (5%)
11	OMG	AA	2288	11	18,26,27	1.13	2 (11%)	19,38,41	0.84	1 (5%)
11	A2M	AA	2640	11	18,25,26	3.59	8 (44%)	18,36,39	3.33	4 (22%)
61	A2M	c	796	61	18,25,26	3.62	8 (44%)	18,36,39	3.35	3 (16%)
11	OMG	AA	867	11,88	18,26,27	1.14	2 (11%)	19,38,41	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	OMC	AA	2948	11	19,22,23	0.54	0	26,31,34	0.82	1 (3%)
11	OMG	AA	908	11	18,26,27	1.14	2 (11%)	19,38,41	0.83	1 (5%)
11	OMU	AA	2417	11	19,22,23	3.05	8 (42%)	26,31,34	1.68	5 (19%)
61	MA6	c	1781	61	18,26,27	1.01	2 (11%)	19,38,41	3.42	2 (10%)
61	A2M	c	974	61	18,25,26	3.58	8 (44%)	18,36,39	3.37	3 (16%)
61	OMC	c	1639	86,61	19,22,23	0.52	0	26,31,34	0.60	0
61	MA6	c	1782	61	18,26,27	1.03	2 (11%)	19,38,41	3.47	2 (10%)
11	OMG	AA	2922	11	18,26,27	1.12	2 (11%)	19,38,41	0.87	1 (5%)
61	OMG	c	1126	61	18,26,27	1.15	2 (11%)	19,38,41	0.87	1 (5%)
11	OMC	AA	1437	11,86	19,22,23	0.54	0	26,31,34	0.83	1 (3%)
11	OMG	AA	2619	11,15	18,26,27	1.13	2 (11%)	19,38,41	0.85	1 (5%)
61	OMC	c	414	61	19,22,23	0.51	0	26,31,34	0.64	0
61	4AC	c	1773	61	21,24,25	3.52	10 (47%)	29,34,37	1.57	5 (17%)
11	1MA	AA	645	11,86	16,25,26	0.92	2 (12%)	18,37,40	1.07	2 (11%)
11	A2M	AA	2946	11,86	18,25,26	3.58	8 (44%)	18,36,39	3.30	3 (16%)
11	OMU	AA	2421	11	19,22,23	3.07	8 (42%)	26,31,34	1.71	4 (15%)
11	5MC	AA	2278	11,86	18,22,23	0.55	0	26,32,35	0.64	0
11	OMU	AA	2724	11	19,22,23	3.05	8 (42%)	26,31,34	1.68	5 (19%)
11	OMC	AA	2197	11,88	19,22,23	0.50	0	26,31,34	0.59	0
11	OMU	AA	2729	11	19,22,23	3.04	8 (42%)	26,31,34	1.67	5 (19%)
11	OMU	AA	2347	11	19,22,23	3.07	8 (42%)	26,31,34	1.67	4 (15%)

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. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMU	AA	2921	11,86	-	0/9/27/28	0/2/2/2
61	OMG	c	1428	86,61	-	2/5/27/28	0/3/3/3
11	1MA	AA	2142	11,86	-	0/3/25/26	0/3/3/3
11	OMC	AA	2959	11,86	-	0/9/27/28	0/2/2/2
61	A2M	c	420	61	-	1/5/27/28	0/3/3/3
11	OMC	AA	650	11	-	0/9/27/28	0/2/2/2
11	A2M	AA	2281	11	-	2/5/27/28	0/3/3/3
11	OMG	AA	805	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	2280	11	-	1/5/27/28	0/3/3/3
11	A2M	AA	876	11	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	A2M	c	541	61	-	0/5/27/28	0/3/3/3
11	OMG	AA	2791	11	-	0/5/27/28	0/3/3/3
61	A2M	c	619	86,61	-	2/5/27/28	0/3/3/3
11	OMC	AA	663	11	-	1/9/27/28	0/2/2/2
11	A2M	AA	1133	11,86	-	0/5/27/28	0/3/3/3
11	5MC	AA	2870	11,88	-	4/7/25/26	0/2/2/2
61	OMU	c	1269	61	-	4/9/27/28	0/2/2/2
11	OMC	AA	2337	11	-	0/9/27/28	0/2/2/2
61	OMU	c	578	61	-	3/9/27/28	0/2/2/2
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
15	YYG	Bb	37	15	-	4/20/42/43	0/3/4/4
11	UR3	AA	2634	11	-	0/7/25/26	0/2/2/2
61	A2M	c	28	61	-	2/5/27/28	0/3/3/3
61	4AC	c	1280	61	-	2/11/29/30	0/2/2/2
11	A2M	AA	2256	11	-	3/5/27/28	0/3/3/3
11	OMG	AA	2815	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	817	11,86	-	2/5/27/28	0/3/3/3
61	OMC	c	1007	61	-	0/9/27/28	0/2/2/2
11	OMU	AA	1888	11	-	0/9/27/28	0/2/2/2
12	DDE	Aa	699	12	-	8/20/21/23	0/1/1/1
11	OMG	AA	1450	11	-	2/5/27/28	0/3/3/3
11	A2M	AA	807	11	-	1/5/27/28	0/3/3/3
61	A2M	c	100	86,61	-	1/5/27/28	0/3/3/3
61	OMG	c	1271	61	-	1/5/27/28	0/3/3/3
11	A2M	AA	649	11	-	1/5/27/28	0/3/3/3
61	OMG	c	562	61	-	0/5/27/28	0/3/3/3
11	OMG	AA	2793	11	-	1/5/27/28	0/3/3/3
61	A2M	c	436	61	-	0/5/27/28	0/3/3/3
11	A2M	AA	1449	11,86	-	0/5/27/28	0/3/3/3
61	B8N	c	1191	61	-	7/16/34/35	0/2/2/2
61	OMG	c	1572	61	-	2/5/27/28	0/3/3/3
61	G7M	c	1575	18,61	-	3/3/25/26	0/3/3/3
11	OMG	AA	2288	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	2640	11	-	0/5/27/28	0/3/3/3
61	A2M	c	796	61	-	0/5/27/28	0/3/3/3
11	OMG	AA	867	11,88	-	1/5/27/28	0/3/3/3
11	OMC	AA	2948	11	-	0/9/27/28	0/2/2/2
11	OMG	AA	908	11	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMU	AA	2417	11	-	1/9/27/28	0/2/2/2
61	MA6	c	1781	61	-	0/7/29/30	0/3/3/3
61	A2M	c	974	61	-	0/5/27/28	0/3/3/3
61	OMC	c	1639	86,61	-	0/9/27/28	0/2/2/2
61	MA6	c	1782	61	-	1/7/29/30	0/3/3/3
11	OMG	AA	2922	11	-	0/5/27/28	0/3/3/3
61	OMG	c	1126	61	-	0/5/27/28	0/3/3/3
11	OMC	AA	1437	11,86	-	2/9/27/28	0/2/2/2
11	OMG	AA	2619	11,15	-	1/5/27/28	0/3/3/3
61	OMC	c	414	61	-	0/9/27/28	0/2/2/2
61	4AC	c	1773	61	-	2/11/29/30	0/2/2/2
11	1MA	AA	645	11,86	-	0/3/25/26	0/3/3/3
11	A2M	AA	2946	11,86	-	0/5/27/28	0/3/3/3
11	OMU	AA	2421	11	-	1/9/27/28	0/2/2/2
11	5MC	AA	2278	11,86	-	0/7/25/26	0/2/2/2
11	OMU	AA	2724	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2197	11,88	-	4/9/27/28	0/2/2/2
11	OMU	AA	2729	11	-	0/9/27/28	0/2/2/2
11	OMU	AA	2347	11	-	0/9/27/28	0/2/2/2

All (325) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	807	A2M	C3'-C4'	-8.87	1.30	1.53
11	AA	2280	A2M	C3'-C4'	-8.84	1.30	1.53
61	c	796	A2M	C3'-C4'	-8.84	1.30	1.53
11	AA	1133	A2M	C3'-C4'	-8.84	1.30	1.53
61	c	541	A2M	C3'-C4'	-8.79	1.30	1.53
11	AA	817	A2M	C3'-C4'	-8.77	1.30	1.53
61	c	100	A2M	C3'-C4'	-8.77	1.30	1.53
61	c	619	A2M	C3'-C4'	-8.77	1.30	1.53
11	AA	2946	A2M	C3'-C4'	-8.76	1.30	1.53
11	AA	2640	A2M	C3'-C4'	-8.75	1.30	1.53
11	AA	876	A2M	C3'-C4'	-8.74	1.30	1.53
61	c	420	A2M	C3'-C4'	-8.72	1.30	1.53
11	AA	2220	A2M	C3'-C4'	-8.72	1.30	1.53
61	c	974	A2M	C3'-C4'	-8.71	1.30	1.53
61	c	436	A2M	C3'-C4'	-8.69	1.30	1.53
11	AA	1449	A2M	C3'-C4'	-8.66	1.30	1.53
11	AA	649	A2M	C3'-C4'	-8.63	1.30	1.53
61	c	28	A2M	C3'-C4'	-8.63	1.30	1.53
11	AA	2256	A2M	C3'-C4'	-8.49	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2281	A2M	C3'-C4'	-8.42	1.31	1.53
61	c	1191	B8N	C6-N1	7.94	1.56	1.36
11	AA	2256	A2M	O4'-C4'	7.84	1.62	1.45
11	AA	2281	A2M	O4'-C1'	-7.81	1.30	1.41
61	c	28	A2M	O4'-C4'	7.80	1.62	1.45
61	c	796	A2M	O4'-C4'	7.79	1.62	1.45
11	AA	1133	A2M	O4'-C4'	7.77	1.62	1.45
61	c	436	A2M	O4'-C4'	7.73	1.62	1.45
61	c	974	A2M	O4'-C4'	7.73	1.62	1.45
61	c	420	A2M	O4'-C4'	7.72	1.62	1.45
11	AA	2946	A2M	O4'-C4'	7.71	1.62	1.45
11	AA	2220	A2M	O4'-C4'	7.70	1.62	1.45
11	AA	2281	A2M	O4'-C4'	7.70	1.62	1.45
61	c	100	A2M	O4'-C4'	7.70	1.62	1.45
11	AA	1449	A2M	O4'-C4'	7.69	1.62	1.45
11	AA	2640	A2M	O4'-C4'	7.68	1.62	1.45
11	AA	649	A2M	O4'-C4'	7.67	1.62	1.45
11	AA	876	A2M	O4'-C4'	7.62	1.62	1.45
11	AA	817	A2M	O4'-C4'	7.56	1.61	1.45
61	c	541	A2M	O4'-C4'	7.54	1.61	1.45
61	c	1280	4AC	C4-N3	7.51	1.45	1.32
61	c	1191	B8N	C4-N3	-7.47	1.26	1.40
11	AA	2280	A2M	O4'-C4'	7.47	1.61	1.45
61	c	1269	OMU	C2-N1	7.46	1.50	1.38
11	AA	807	A2M	O4'-C4'	7.40	1.61	1.45
61	c	619	A2M	O4'-C1'	-7.40	1.30	1.41
61	c	619	A2M	O4'-C4'	7.39	1.61	1.45
61	c	1773	4AC	C4-N3	7.31	1.45	1.32
11	AA	2421	OMU	C2-N1	7.27	1.50	1.38
61	c	578	OMU	C2-N1	7.26	1.50	1.38
11	AA	2347	OMU	C2-N1	7.26	1.50	1.38
11	AA	2256	A2M	O4'-C1'	-7.25	1.31	1.41
11	AA	807	A2M	O4'-C1'	-7.23	1.31	1.41
15	Bb	37	YYG	C21-N20	7.20	1.52	1.34
11	AA	2724	OMU	C2-N1	7.17	1.50	1.38
11	AA	876	A2M	O4'-C1'	-7.16	1.31	1.41
11	AA	649	A2M	O4'-C1'	-7.15	1.31	1.41
11	AA	2921	OMU	C2-N1	7.14	1.49	1.38
11	AA	898	OMU	C2-N1	7.14	1.49	1.38
11	AA	1449	A2M	O4'-C1'	-7.14	1.31	1.41
11	AA	2280	A2M	O4'-C1'	-7.13	1.31	1.41
61	c	436	A2M	O4'-C1'	-7.13	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2417	OMU	C2-N1	7.12	1.49	1.38
11	AA	1888	OMU	C2-N1	7.11	1.49	1.38
11	AA	2729	OMU	C2-N1	7.08	1.49	1.38
61	c	28	A2M	O4'-C1'	-7.08	1.31	1.41
61	c	541	A2M	O4'-C1'	-7.07	1.31	1.41
11	AA	817	A2M	O4'-C1'	-7.06	1.31	1.41
11	AA	2640	A2M	O4'-C1'	-7.04	1.31	1.41
61	c	796	A2M	O4'-C1'	-6.98	1.31	1.41
61	c	974	A2M	O4'-C1'	-6.98	1.31	1.41
61	c	420	A2M	O4'-C1'	-6.97	1.31	1.41
11	AA	2946	A2M	O4'-C1'	-6.96	1.31	1.41
61	c	100	A2M	O4'-C1'	-6.96	1.31	1.41
61	c	1773	4AC	C6-C5	6.93	1.51	1.35
11	AA	2220	A2M	O4'-C1'	-6.90	1.31	1.41
61	c	578	OMU	C2-N3	6.87	1.50	1.38
11	AA	1133	A2M	O4'-C1'	-6.86	1.31	1.41
11	AA	2634	UR3	C2-N1	6.85	1.48	1.38
61	c	1269	OMU	C2-N3	6.82	1.50	1.38
11	AA	2347	OMU	C2-N3	6.81	1.50	1.38
11	AA	898	OMU	C2-N3	6.79	1.50	1.38
11	AA	2417	OMU	C2-N3	6.79	1.50	1.38
61	c	1280	4AC	C6-C5	6.79	1.50	1.35
11	AA	2724	OMU	C2-N3	6.78	1.50	1.38
11	AA	2634	UR3	C6-C5	6.77	1.50	1.35
11	AA	2921	OMU	C2-N3	6.76	1.50	1.38
11	AA	1888	OMU	C2-N3	6.76	1.50	1.38
11	AA	2729	OMU	C2-N3	6.75	1.50	1.38
11	AA	2421	OMU	C2-N3	6.73	1.50	1.38
61	c	1191	B8N	C2-N1	5.89	1.56	1.39
11	AA	2634	UR3	C2-N3	5.77	1.50	1.39
61	c	1280	4AC	C7-N4	5.74	1.47	1.37
11	AA	1888	OMU	C6-C5	5.73	1.48	1.35
61	c	578	OMU	C6-C5	5.73	1.48	1.35
11	AA	2421	OMU	C6-C5	5.73	1.48	1.35
61	c	1269	OMU	C6-C5	5.72	1.48	1.35
11	AA	2921	OMU	C6-C5	5.70	1.48	1.35
11	AA	898	OMU	C6-C5	5.70	1.48	1.35
11	AA	2417	OMU	C6-C5	5.69	1.48	1.35
11	AA	2729	OMU	C6-C5	5.69	1.48	1.35
11	AA	2347	OMU	C6-C5	5.69	1.48	1.35
11	AA	2724	OMU	C6-C5	5.65	1.48	1.35
61	c	1773	4AC	C7-N4	5.62	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	1191	B8N	C6-C5	5.56	1.42	1.34
15	Bb	37	YYG	O23-C21	5.46	1.43	1.34
61	c	1575	G7M	C2-N3	5.45	1.46	1.33
61	c	1280	4AC	C2-N3	5.23	1.47	1.36
61	c	1773	4AC	C4-N4	5.19	1.47	1.39
61	c	1280	4AC	C4-N4	5.18	1.47	1.39
61	c	1280	4AC	C2-N1	5.17	1.51	1.40
61	c	1773	4AC	C2-N1	5.12	1.51	1.40
61	c	1773	4AC	C2-N3	5.07	1.46	1.36
61	c	1575	G7M	C4-N3	5.02	1.49	1.37
61	c	1575	G7M	C2-N2	4.76	1.45	1.34
61	c	578	OMU	C4-N3	4.31	1.46	1.38
11	AA	2724	OMU	C4-N3	4.29	1.46	1.38
61	c	1280	4AC	CM7-C7	4.26	1.59	1.50
11	AA	2421	OMU	C4-N3	4.25	1.46	1.38
11	AA	2921	OMU	C4-N3	4.24	1.46	1.38
11	AA	898	OMU	C4-N3	4.22	1.46	1.38
11	AA	2417	OMU	C4-N3	4.21	1.46	1.38
11	AA	1888	OMU	C4-N3	4.19	1.46	1.38
11	AA	2347	OMU	C4-N3	4.19	1.46	1.38
61	c	1269	OMU	C4-N3	4.19	1.46	1.38
61	c	1280	4AC	C5-C4	4.15	1.49	1.40
11	AA	2729	OMU	C4-N3	4.13	1.46	1.38
61	c	1773	4AC	C5-C4	4.10	1.49	1.40
61	c	1773	4AC	CM7-C7	4.02	1.58	1.50
15	Bb	37	YYG	O18-C16	4.02	1.43	1.33
61	c	1191	B8N	C1'-C5	3.92	1.59	1.50
61	c	1575	G7M	C6-N1	3.77	1.43	1.37
11	AA	2634	UR3	C6-N1	3.41	1.46	1.38
61	c	1575	G7M	C5-C6	3.29	1.53	1.45
15	Bb	37	YYG	O6-C6	-3.26	1.18	1.22
61	c	436	A2M	C6-N6	3.17	1.45	1.34
61	c	796	A2M	C6-N6	3.17	1.45	1.34
61	c	541	A2M	C6-N6	3.16	1.45	1.34
61	c	420	A2M	C6-N6	3.16	1.45	1.34
61	c	28	A2M	C6-N6	3.16	1.45	1.34
11	AA	649	A2M	C6-N6	3.15	1.45	1.34
11	AA	2280	A2M	C6-N6	3.14	1.45	1.34
11	AA	876	A2M	C6-N6	3.14	1.45	1.34
11	AA	2640	A2M	C6-N6	3.14	1.45	1.34
11	AA	817	A2M	C6-N6	3.14	1.45	1.34
11	AA	2256	A2M	C6-N6	3.14	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	1449	A2M	C6-N6	3.14	1.45	1.34
61	c	619	A2M	C6-N6	3.13	1.45	1.34
11	AA	2220	A2M	C6-N6	3.13	1.45	1.34
61	c	974	A2M	C6-N6	3.13	1.45	1.34
11	AA	807	A2M	C6-N6	3.13	1.45	1.34
11	AA	2946	A2M	C6-N6	3.12	1.45	1.34
11	AA	1133	A2M	C6-N6	3.11	1.45	1.34
61	c	100	A2M	C6-N6	3.09	1.45	1.34
11	AA	2281	A2M	C6-N6	3.00	1.45	1.34
61	c	619	A2M	O3'-C3'	3.00	1.50	1.43
61	c	436	A2M	O3'-C3'	2.98	1.50	1.43
11	AA	2417	OMU	O4-C4	-2.97	1.18	1.24
11	AA	898	OMU	O4-C4	-2.97	1.18	1.24
11	AA	1888	OMU	O4-C4	-2.97	1.18	1.24
11	AA	1449	A2M	O3'-C3'	2.97	1.50	1.43
11	AA	2921	OMU	O4-C4	-2.97	1.18	1.24
61	c	578	OMU	C6-N1	2.95	1.45	1.38
11	AA	2281	A2M	O3'-C3'	2.95	1.49	1.43
11	AA	2421	OMU	O4-C4	-2.94	1.18	1.24
11	AA	2729	OMU	O4-C4	-2.94	1.18	1.24
11	AA	2347	OMU	O4-C4	-2.94	1.18	1.24
11	AA	2724	OMU	O4-C4	-2.93	1.18	1.24
61	c	1269	OMU	C6-N1	2.93	1.45	1.38
11	AA	2347	OMU	C6-N1	2.91	1.45	1.38
61	c	100	A2M	O3'-C3'	2.91	1.49	1.43
61	c	796	A2M	O3'-C3'	2.91	1.49	1.43
61	c	28	A2M	O3'-C3'	2.91	1.49	1.43
11	AA	2729	OMU	C6-N1	2.91	1.45	1.38
61	c	541	A2M	O3'-C3'	2.90	1.49	1.43
11	AA	898	OMU	C6-N1	2.90	1.45	1.38
11	AA	1888	OMU	C6-N1	2.90	1.45	1.38
11	AA	2921	OMU	C6-N1	2.90	1.45	1.38
61	c	1269	OMU	O4-C4	-2.89	1.18	1.24
11	AA	2640	A2M	O3'-C3'	2.89	1.49	1.43
61	c	420	A2M	O3'-C3'	2.89	1.49	1.43
11	AA	2421	OMU	C6-N1	2.89	1.45	1.38
11	AA	2417	OMU	C6-N1	2.89	1.45	1.38
11	AA	817	A2M	O3'-C3'	2.88	1.49	1.43
11	AA	908	OMG	C8-N7	-2.88	1.30	1.35
11	AA	649	A2M	O3'-C3'	2.88	1.49	1.43
61	c	578	OMU	O4-C4	-2.86	1.18	1.24
11	AA	2256	A2M	O3'-C3'	2.86	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	974	A2M	O3'-C3'	2.85	1.49	1.43
11	AA	867	OMG	C8-N7	-2.84	1.30	1.35
11	AA	2946	A2M	O3'-C3'	2.84	1.49	1.43
11	AA	1133	A2M	O3'-C3'	2.84	1.49	1.43
11	AA	807	A2M	O3'-C3'	2.83	1.49	1.43
11	AA	2220	A2M	O3'-C3'	2.83	1.49	1.43
61	c	1428	OMG	C8-N7	-2.82	1.30	1.35
11	AA	2280	A2M	O3'-C3'	2.82	1.49	1.43
11	AA	2288	OMG	C8-N7	-2.82	1.30	1.35
11	AA	2724	OMU	C6-N1	2.81	1.44	1.38
61	c	562	OMG	C8-N7	-2.80	1.30	1.35
11	AA	2619	OMG	C8-N7	-2.80	1.30	1.35
11	AA	876	A2M	O3'-C3'	2.79	1.49	1.43
61	c	1126	OMG	C8-N7	-2.79	1.30	1.35
11	AA	2281	A2M	C5-C4	-2.78	1.33	1.40
15	Bb	37	YYG	C13-C12	2.76	1.58	1.50
11	AA	2791	OMG	C8-N7	-2.74	1.30	1.35
61	c	1575	G7M	C2-N1	2.72	1.44	1.37
11	AA	2815	OMG	C8-N7	-2.72	1.30	1.35
61	c	1271	OMG	C8-N7	-2.72	1.30	1.35
11	AA	2793	OMG	C8-N7	-2.72	1.30	1.35
11	AA	817	A2M	C5-C4	-2.71	1.33	1.40
11	AA	2922	OMG	C8-N7	-2.70	1.30	1.35
11	AA	805	OMG	C8-N7	-2.69	1.30	1.35
61	c	619	A2M	C5-C4	-2.69	1.33	1.40
11	AA	1133	A2M	C5-C4	-2.68	1.33	1.40
11	AA	2946	A2M	C5-C4	-2.67	1.33	1.40
61	c	796	A2M	O2'-C2'	-2.67	1.35	1.42
61	c	974	A2M	C5-C4	-2.66	1.33	1.40
11	AA	2280	A2M	C5-C4	-2.66	1.33	1.40
11	AA	649	A2M	C5-C4	-2.66	1.33	1.40
15	Bb	37	YYG	C10-C11	2.65	1.54	1.50
61	c	100	A2M	C5-C4	-2.65	1.33	1.40
11	AA	2640	A2M	C5-C4	-2.65	1.33	1.40
61	c	28	A2M	C5-C4	-2.65	1.33	1.40
61	c	420	A2M	C5-C4	-2.64	1.33	1.40
11	AA	1450	OMG	C8-N7	-2.64	1.30	1.35
11	AA	2220	A2M	C5-C4	-2.64	1.33	1.40
15	Bb	37	YYG	C2-N1	-2.64	1.32	1.37
11	AA	807	A2M	C5-C4	-2.64	1.34	1.40
61	c	796	A2M	C5-C4	-2.63	1.34	1.40
61	c	28	A2M	O2'-C2'	-2.63	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	1449	A2M	C5-C4	-2.62	1.34	1.40
11	AA	2256	A2M	C5-C4	-2.62	1.34	1.40
11	AA	876	A2M	C5-C4	-2.62	1.34	1.40
61	c	436	A2M	C5-C4	-2.61	1.34	1.40
11	AA	876	A2M	O2'-C2'	-2.61	1.35	1.42
11	AA	2946	A2M	O2'-C2'	-2.60	1.36	1.42
61	c	1782	MA6	C5-C4	-2.59	1.34	1.40
61	c	1773	4AC	C6-N1	2.59	1.44	1.38
11	AA	1449	A2M	O2'-C2'	-2.59	1.36	1.42
11	AA	1133	A2M	O2'-C2'	-2.58	1.36	1.42
61	c	1781	MA6	C5-C4	-2.58	1.34	1.40
15	Bb	37	YYG	C4-N3	-2.58	1.35	1.40
11	AA	807	A2M	O2'-C2'	-2.58	1.36	1.42
61	c	100	A2M	O2'-C2'	-2.58	1.36	1.42
11	AA	2281	A2M	O2'-C2'	-2.57	1.36	1.42
61	c	541	A2M	C5-C4	-2.57	1.34	1.40
11	AA	2280	A2M	O2'-C2'	-2.57	1.36	1.42
61	c	1572	OMG	C8-N7	-2.57	1.30	1.35
61	c	541	A2M	O2'-C2'	-2.56	1.36	1.42
11	AA	817	A2M	O2'-C2'	-2.56	1.36	1.42
61	c	619	A2M	O2'-C2'	-2.54	1.36	1.42
61	c	1782	MA6	C2-N3	2.54	1.36	1.32
61	c	420	A2M	O2'-C2'	-2.53	1.36	1.42
61	c	436	A2M	O2'-C2'	-2.52	1.36	1.42
11	AA	2142	1MA	C8-N7	-2.51	1.30	1.35
11	AA	2640	A2M	O2'-C2'	-2.51	1.36	1.42
11	AA	2220	A2M	O2'-C2'	-2.49	1.36	1.42
61	c	974	A2M	O2'-C2'	-2.49	1.36	1.42
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	2421	OMU	C5-C4	2.48	1.49	1.43
61	c	578	OMU	C5-C4	2.48	1.49	1.43
61	c	1280	4AC	C6-N1	2.47	1.44	1.38
11	AA	2729	OMU	C5-C4	2.46	1.49	1.43
11	AA	645	1MA	C8-N7	-2.44	1.30	1.35
11	AA	2347	OMU	C5-C4	2.43	1.49	1.43
11	AA	649	A2M	O2'-C2'	-2.43	1.36	1.42
11	AA	2619	OMG	C5-C6	-2.42	1.42	1.47
11	AA	2793	OMG	C5-C6	-2.41	1.42	1.47
11	AA	2417	OMU	C5-C4	2.41	1.49	1.43
11	AA	898	OMU	C5-C4	2.41	1.49	1.43
61	c	1781	MA6	C2-N3	2.40	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2921	OMU	C5-C4	2.38	1.48	1.43
11	AA	2724	OMU	O2-C2	-2.37	1.18	1.23
61	c	1269	OMU	O2-C2	-2.36	1.18	1.23
11	AA	2921	OMU	O2-C2	-2.36	1.18	1.23
11	AA	898	OMU	O2-C2	-2.35	1.18	1.23
11	AA	2347	OMU	O2-C2	-2.35	1.18	1.23
11	AA	2421	OMU	O2-C2	-2.35	1.18	1.23
11	AA	2417	OMU	O2-C2	-2.34	1.18	1.23
11	AA	1888	OMU	O2-C2	-2.34	1.18	1.23
11	AA	867	OMG	C5-C6	-2.34	1.42	1.47
11	AA	2729	OMU	O2-C2	-2.33	1.18	1.23
11	AA	2288	OMG	C5-C6	-2.33	1.42	1.47
61	c	1126	OMG	C5-C6	-2.32	1.42	1.47
61	c	1428	OMG	C5-C6	-2.32	1.42	1.47
11	AA	2724	OMU	C5-C4	2.31	1.48	1.43
11	AA	805	OMG	C5-C6	-2.31	1.42	1.47
11	AA	2634	UR3	C4-N3	2.31	1.45	1.40
11	AA	2634	UR3	C5-C4	2.30	1.49	1.43
61	c	1271	OMG	C5-C6	-2.30	1.42	1.47
11	AA	908	OMG	C5-C6	-2.30	1.42	1.47
11	AA	2791	OMG	C5-C6	-2.29	1.42	1.47
61	c	1572	OMG	C5-C6	-2.29	1.42	1.47
61	c	1773	4AC	O7-C7	-2.28	1.18	1.23
11	AA	2815	OMG	C5-C6	-2.27	1.42	1.47
11	AA	2922	OMG	C5-C6	-2.27	1.42	1.47
11	AA	1450	OMG	C5-C6	-2.26	1.42	1.47
61	c	1280	4AC	O7-C7	-2.26	1.18	1.23
61	c	100	A2M	C2-N3	2.25	1.35	1.32
11	AA	2640	A2M	C2-N3	2.25	1.35	1.32
61	c	562	OMG	C5-C6	-2.24	1.42	1.47
61	c	541	A2M	C2-N3	2.23	1.35	1.32
61	c	578	OMU	O2-C2	-2.23	1.19	1.23
11	AA	645	1MA	C5-C4	-2.23	1.37	1.43
11	AA	2280	A2M	C2-N3	2.23	1.35	1.32
61	c	436	A2M	C2-N3	2.22	1.35	1.32
61	c	796	A2M	C2-N3	2.20	1.35	1.32
11	AA	1449	A2M	C2-N3	2.19	1.35	1.32
11	AA	2256	A2M	C2-N3	2.18	1.35	1.32
61	c	1575	G7M	O6-C6	-2.18	1.18	1.23
11	AA	2142	1MA	C5-C4	-2.18	1.37	1.43
61	c	420	A2M	C2-N3	2.17	1.35	1.32
11	AA	2256	A2M	O2'-C2'	-2.16	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	974	A2M	C2-N3	2.16	1.35	1.32
11	AA	2220	A2M	C2-N3	2.16	1.35	1.32
61	c	28	A2M	C2-N3	2.15	1.35	1.32
11	AA	807	A2M	C2-N3	2.14	1.35	1.32
11	AA	649	A2M	C2-N3	2.13	1.35	1.32
11	AA	876	A2M	C2-N3	2.12	1.35	1.32
11	AA	817	A2M	C2-N3	2.12	1.35	1.32
61	c	619	A2M	C2-N3	2.11	1.35	1.32
11	AA	2946	A2M	C2-N3	2.10	1.35	1.32
11	AA	2281	A2M	C2-N3	2.06	1.35	1.32
11	AA	1133	A2M	C2-N3	2.06	1.35	1.32
61	c	1191	B8N	O4-C4	-2.02	1.18	1.23

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	c	1782	MA6	N1-C6-N6	-13.86	102.47	117.06
61	c	1781	MA6	N1-C6-N6	-13.68	102.66	117.06
11	AA	817	A2M	C5-C6-N6	10.78	136.73	120.35
61	c	619	A2M	C5-C6-N6	10.72	136.64	120.35
11	AA	807	A2M	C5-C6-N6	10.71	136.63	120.35
61	c	974	A2M	C5-C6-N6	10.65	136.53	120.35
11	AA	1133	A2M	C5-C6-N6	10.63	136.50	120.35
11	AA	2220	A2M	C5-C6-N6	10.60	136.46	120.35
61	c	420	A2M	C5-C6-N6	10.55	136.39	120.35
11	AA	876	A2M	C5-C6-N6	10.53	136.36	120.35
11	AA	1449	A2M	C5-C6-N6	10.53	136.35	120.35
11	AA	2280	A2M	C5-C6-N6	10.51	136.33	120.35
61	c	436	A2M	C5-C6-N6	10.50	136.31	120.35
61	c	796	A2M	C5-C6-N6	10.50	136.30	120.35
11	AA	2256	A2M	C5-C6-N6	10.49	136.29	120.35
11	AA	2640	A2M	C5-C6-N6	10.45	136.23	120.35
61	c	28	A2M	C5-C6-N6	10.43	136.21	120.35
11	AA	649	A2M	C5-C6-N6	10.42	136.18	120.35
61	c	100	A2M	C5-C6-N6	10.42	136.18	120.35
61	c	541	A2M	C5-C6-N6	10.41	136.16	120.35
11	AA	2281	A2M	C5-C6-N6	10.35	136.09	120.35
11	AA	2946	A2M	C5-C6-N6	10.34	136.06	120.35
11	AA	817	A2M	N6-C6-N1	-7.39	103.24	118.57
61	c	619	A2M	N6-C6-N1	-7.32	103.39	118.57
11	AA	807	A2M	N6-C6-N1	-7.30	103.42	118.57
61	c	974	A2M	N6-C6-N1	-7.21	103.61	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	c	420	A2M	N6-C6-N1	-7.18	103.67	118.57
61	c	796	A2M	N6-C6-N1	-7.18	103.68	118.57
11	AA	2280	A2M	N6-C6-N1	-7.17	103.69	118.57
11	AA	2220	A2M	N6-C6-N1	-7.17	103.69	118.57
11	AA	2281	A2M	N6-C6-N1	-7.15	103.73	118.57
61	c	436	A2M	N6-C6-N1	-7.15	103.73	118.57
11	AA	1449	A2M	N6-C6-N1	-7.14	103.75	118.57
61	c	100	A2M	N6-C6-N1	-7.14	103.76	118.57
11	AA	2256	A2M	N6-C6-N1	-7.13	103.76	118.57
11	AA	1133	A2M	N6-C6-N1	-7.13	103.78	118.57
11	AA	649	A2M	N6-C6-N1	-7.11	103.82	118.57
11	AA	876	A2M	N6-C6-N1	-7.10	103.83	118.57
11	AA	2640	A2M	N6-C6-N1	-7.10	103.83	118.57
61	c	541	A2M	N6-C6-N1	-7.06	103.92	118.57
61	c	28	A2M	N6-C6-N1	-7.04	103.95	118.57
11	AA	2946	A2M	N6-C6-N1	-7.01	104.02	118.57
11	AA	1133	A2M	N3-C2-N1	-5.77	119.66	128.68
11	AA	817	A2M	N3-C2-N1	-5.67	119.82	128.68
61	c	619	A2M	N3-C2-N1	-5.65	119.85	128.68
61	c	1280	4AC	CM7-C7-N4	5.64	125.05	115.29
11	AA	2281	A2M	N3-C2-N1	-5.63	119.88	128.68
11	AA	649	A2M	N3-C2-N1	-5.61	119.91	128.68
61	c	1773	4AC	CM7-C7-N4	5.60	124.97	115.29
61	c	796	A2M	N3-C2-N1	-5.59	119.93	128.68
61	c	974	A2M	N3-C2-N1	-5.59	119.94	128.68
11	AA	2946	A2M	N3-C2-N1	-5.57	119.97	128.68
61	c	28	A2M	N3-C2-N1	-5.57	119.98	128.68
11	AA	876	A2M	N3-C2-N1	-5.55	120.00	128.68
11	AA	1449	A2M	N3-C2-N1	-5.55	120.01	128.68
11	AA	2256	A2M	N3-C2-N1	-5.55	120.01	128.68
61	c	100	A2M	N3-C2-N1	-5.52	120.06	128.68
11	AA	2220	A2M	N3-C2-N1	-5.51	120.06	128.68
61	c	436	A2M	N3-C2-N1	-5.50	120.07	128.68
61	c	420	A2M	N3-C2-N1	-5.50	120.09	128.68
11	AA	2280	A2M	N3-C2-N1	-5.49	120.10	128.68
61	c	541	A2M	N3-C2-N1	-5.49	120.10	128.68
61	c	1782	MA6	N3-C2-N1	-5.49	120.10	128.68
11	AA	2640	A2M	N3-C2-N1	-5.44	120.17	128.68
11	AA	807	A2M	N3-C2-N1	-5.39	120.25	128.68
61	c	1781	MA6	N3-C2-N1	-5.35	120.32	128.68
11	AA	1888	OMU	C4-N3-C2	-5.33	119.55	126.58
11	AA	2421	OMU	C4-N3-C2	-5.31	119.58	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	2921	OMU	C4-N3-C2	-5.26	119.64	126.58
11	AA	2417	OMU	C4-N3-C2	-5.18	119.75	126.58
15	Bb	37	YYG	O23-C21-N20	5.18	119.90	110.80
11	AA	2729	OMU	C4-N3-C2	-5.13	119.81	126.58
61	c	578	OMU	C4-N3-C2	-5.12	119.83	126.58
11	AA	2347	OMU	C4-N3-C2	-5.11	119.85	126.58
11	AA	898	OMU	C4-N3-C2	-5.08	119.88	126.58
61	c	1191	B8N	C5-C4-N3	5.06	125.55	116.17
61	c	1269	OMU	C4-N3-C2	-5.06	119.91	126.58
11	AA	2724	OMU	C4-N3-C2	-5.05	119.92	126.58
11	AA	2634	UR3	C4-N3-C2	-4.93	119.92	124.56
61	c	1191	B8N	C4-N3-C2	-4.35	119.95	125.46
11	AA	1888	OMU	N3-C2-N1	3.93	120.10	114.89
61	c	1269	OMU	N3-C2-N1	3.84	119.98	114.89
11	AA	2421	OMU	N3-C2-N1	3.83	119.97	114.89
11	AA	2921	OMU	N3-C2-N1	3.81	119.95	114.89
11	AA	2417	OMU	N3-C2-N1	3.76	119.89	114.89
11	AA	2347	OMU	N3-C2-N1	3.75	119.87	114.89
11	AA	898	OMU	N3-C2-N1	3.73	119.84	114.89
61	c	578	OMU	N3-C2-N1	3.64	119.72	114.89
11	AA	2724	OMU	N3-C2-N1	3.63	119.71	114.89
11	AA	2729	OMU	N3-C2-N1	3.62	119.70	114.89
11	AA	2921	OMU	C5-C4-N3	3.35	119.85	114.84
11	AA	2421	OMU	C5-C4-N3	3.34	119.84	114.84
11	AA	2729	OMU	C5-C4-N3	3.34	119.84	114.84
15	Bb	37	YYG	O18-C16-C15	3.33	120.04	111.52
11	AA	2417	OMU	C5-C4-N3	3.31	119.79	114.84
11	AA	1888	OMU	C5-C4-N3	3.30	119.77	114.84
61	c	578	OMU	C5-C4-N3	3.28	119.75	114.84
11	AA	2347	OMU	C5-C4-N3	3.28	119.74	114.84
11	AA	2724	OMU	C5-C4-N3	3.25	119.70	114.84
11	AA	898	OMU	C5-C4-N3	3.25	119.70	114.84
61	c	1269	OMU	C5-C4-N3	3.19	119.61	114.84
15	Bb	37	YYG	O23-C21-O22	-3.09	120.04	124.58
61	c	1280	4AC	C6-C5-C4	3.06	120.71	116.96
61	c	1191	B8N	N3-C2-N1	3.03	121.04	116.76
61	c	1575	G7M	C2-N1-C6	-3.02	119.54	125.10
15	Bb	37	YYG	C5-C6-N1	3.02	118.46	113.96
11	AA	2724	OMU	O4-C4-C5	-2.93	120.01	125.16
15	Bb	37	YYG	O22-C21-N20	-2.92	120.06	124.85
15	Bb	37	YYG	C8-N7-C5	2.90	108.51	102.99
11	AA	2921	OMU	O4-C4-C5	-2.90	120.07	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	c	578	OMU	O4-C4-C5	-2.89	120.07	125.16
11	AA	2256	A2M	O2'-C2'-C1'	2.87	114.79	109.09
11	AA	898	OMU	O4-C4-C5	-2.87	120.12	125.16
11	AA	2421	OMU	O4-C4-C5	-2.85	120.15	125.16
11	AA	2729	OMU	O4-C4-C5	-2.84	120.17	125.16
61	c	1280	4AC	O7-C7-N4	-2.82	117.25	121.82
11	AA	2417	OMU	O4-C4-C5	-2.81	120.22	125.16
11	AA	2347	OMU	O4-C4-C5	-2.78	120.27	125.16
11	AA	1888	OMU	O4-C4-C5	-2.75	120.33	125.16
15	Bb	37	YYG	C3-N3-C2	-2.74	117.57	120.13
61	c	1269	OMU	O4-C4-C5	-2.70	120.42	125.16
61	c	541	A2M	C1'-N9-C4	2.66	131.32	126.64
61	c	1773	4AC	O7-C7-N4	-2.63	117.56	121.82
61	c	1773	4AC	C6-C5-C4	2.62	120.16	116.96
61	c	1773	4AC	C5-C4-N3	-2.61	118.40	122.59
15	Bb	37	YYG	C3-N3-C4	2.59	121.31	116.71
11	AA	2281	A2M	O4'-C1'-C2'	-2.53	102.20	106.59
61	c	1191	B8N	O4-C4-N3	-2.50	115.74	119.98
61	c	1280	4AC	C5-C4-N3	-2.48	118.60	122.59
11	AA	2948	OMC	C1'-N1-C2	2.48	123.96	118.42
61	c	1773	4AC	O7-C7-CM7	-2.47	117.47	122.06
11	AA	2142	1MA	N1-C6-N6	2.43	125.96	119.77
11	AA	1437	OMC	C1'-N1-C2	2.41	123.80	118.42
11	AA	876	A2M	C1'-N9-C4	2.39	130.85	126.64
11	AA	2619	OMG	O6-C6-C5	2.36	128.99	124.37
11	AA	2815	OMG	O6-C6-C5	2.36	128.99	124.37
11	AA	2791	OMG	O6-C6-C5	2.35	128.97	124.37
11	AA	2922	OMG	O6-C6-C5	2.35	128.96	124.37
61	c	1280	4AC	O7-C7-CM7	-2.35	117.70	122.06
61	c	1271	OMG	O6-C6-C5	2.34	128.94	124.37
11	AA	2288	OMG	O6-C6-C5	2.34	128.94	124.37
11	AA	2640	A2M	C1'-N9-C4	2.34	130.74	126.64
11	AA	805	OMG	O6-C6-C5	2.33	128.92	124.37
61	c	1572	OMG	O6-C6-C5	2.33	128.92	124.37
61	c	562	OMG	O6-C6-C5	2.32	128.91	124.37
61	c	1191	B8N	C31-N3-C4	2.31	120.72	117.31
12	Aa	699	DDE	CBW-CBI-NAD	2.31	118.23	115.28
11	AA	645	1MA	N1-C6-N6	2.30	125.62	119.77
11	AA	2793	OMG	O6-C6-C5	2.29	128.85	124.37
11	AA	1450	OMG	O6-C6-C5	2.28	128.83	124.37
61	c	1428	OMG	O6-C6-C5	2.28	128.83	124.37
11	AA	867	OMG	O6-C6-C5	2.28	128.82	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	c	1126	OMG	O6-C6-C5	2.26	128.79	124.37
11	AA	908	OMG	O6-C6-C5	2.24	128.75	124.37
11	AA	1449	A2M	C1'-N9-C4	2.22	130.54	126.64
11	AA	2142	1MA	C5-C6-N1	-2.22	110.59	113.90
11	AA	1888	OMU	O2-C2-N1	-2.17	119.90	122.79
11	AA	807	A2M	C1'-N9-C4	2.16	130.44	126.64
61	c	1269	OMU	C1'-N1-C2	2.16	121.47	117.57
11	AA	2417	OMU	O2-C2-N1	-2.14	119.94	122.79
11	AA	649	A2M	C1'-N9-C4	2.14	130.40	126.64
15	Bb	37	YYG	O6-C6-C5	-2.12	120.42	124.17
61	c	100	A2M	C1'-N9-C4	2.11	130.36	126.64
11	AA	2724	OMU	C1'-N1-C2	2.11	121.39	117.57
11	AA	2729	OMU	O2-C2-N1	-2.09	120.00	122.79
11	AA	645	1MA	C5-C6-N1	-2.07	110.80	113.90
11	AA	2220	A2M	C1'-N9-C4	2.05	130.25	126.64
61	c	1191	B8N	O4'-C1'-C2'	2.05	108.03	105.14
11	AA	898	OMU	O2-C2-N1	-2.05	120.07	122.79
61	c	28	A2M	C2'-C3'-C4'	2.04	106.43	101.99
11	AA	2921	OMU	O2-C2-N1	-2.02	120.10	122.79

There are no chirality outliers.

All (78) 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	908	OMG	O4'-C4'-C5'-O5'
11	AA	1437	OMC	C1'-C2'-O2'-CM2
11	AA	1450	OMG	O4'-C4'-C5'-O5'
11	AA	2197	OMC	C2'-C1'-N1-C2
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	CBI-CBW-NCB-CAB
12	Aa	699	DDE	CBI-CBW-NCB-CAC
12	Aa	699	DDE	CBI-CBW-NCB-CAA
12	Aa	699	DDE	CAU-CBW-NCB-CAB
12	Aa	699	DDE	CAU-CBW-NCB-CAC

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Mol	Chain	Res	Type	Atoms
12	Aa	699	DDE	CAU-CBW-NCB-CAA
15	Bb	37	YYG	O22-C21-N20-C15
15	Bb	37	YYG	O23-C21-N20-C15
61	c	28	A2M	C3'-C4'-C5'-O5'
61	c	420	A2M	C1'-C2'-O2'-CM'
61	c	578	OMU	C1'-C2'-O2'-CM2
61	c	619	A2M	O4'-C4'-C5'-O5'
61	c	1191	B8N	N3-C31-C32-C33
61	c	1575	G7M	O4'-C4'-C5'-O5'
15	Bb	37	YYG	O17-C16-O18-C19
15	Bb	37	YYG	C15-C16-O18-C19
11	AA	908	OMG	C3'-C4'-C5'-O5'
11	AA	1450	OMG	C3'-C4'-C5'-O5'
61	c	619	A2M	C3'-C4'-C5'-O5'
61	c	1575	G7M	C3'-C4'-C5'-O5'
61	c	28	A2M	O4'-C4'-C5'-O5'
61	c	578	OMU	C3'-C4'-C5'-O5'
11	AA	2870	5MC	C2'-C1'-N1-C6
61	c	578	OMU	O4'-C4'-C5'-O5'
11	AA	2281	A2M	O4'-C4'-C5'-O5'
11	AA	2870	5MC	C2'-C1'-N1-C2
11	AA	807	A2M	C3'-C2'-O2'-CM'
11	AA	2280	A2M	O4'-C4'-C5'-O5'
61	c	1572	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
61	c	100	A2M	O4'-C4'-C5'-O5'
61	c	1271	OMG	C1'-C2'-O2'-CM2
11	AA	2870	5MC	O4'-C1'-N1-C6
61	c	1782	MA6	C4'-C5'-O5'-P
11	AA	908	OMG	C3'-C2'-O2'-CM2
11	AA	2793	OMG	C3'-C2'-O2'-CM2
61	c	1575	G7M	C4'-C5'-O5'-P
11	AA	2870	5MC	O4'-C1'-N1-C2
11	AA	817	A2M	C4'-C5'-O5'-P
11	AA	2197	OMC	O4'-C1'-N1-C2
11	AA	2281	A2M	C3'-C4'-C5'-O5'
11	AA	2197	OMC	O4'-C1'-N1-C6
61	c	1269	OMU	O4'-C1'-N1-C6
11	AA	867	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
61	c	1428	OMG	C4'-C5'-O5'-P
61	c	1269	OMU	C2'-C1'-N1-C6
61	c	1191	B8N	O4'-C1'-C5-C4
61	c	1269	OMU	C2'-C1'-N1-C2
61	c	1191	B8N	N34-C33-C34-O35
11	AA	2256	A2M	C4'-C5'-O5'-P
61	c	1428	OMG	O4'-C4'-C5'-O5'
12	Aa	699	DDE	CAU-CAT-CE1-NE2
61	c	1191	B8N	O4'-C4'-C5'-O5'
61	c	1191	B8N	C3'-C4'-C5'-O5'
61	c	1191	B8N	O4'-C1'-C5-C6
61	c	1269	OMU	O4'-C1'-N1-C2
61	c	1191	B8N	N34-C33-C34-O36
11	AA	1437	OMC	O4'-C4'-C5'-O5'
61	c	1572	OMG	C3'-C4'-C5'-O5'
11	AA	817	A2M	O4'-C4'-C5'-O5'
11	AA	2256	A2M	O4'-C4'-C5'-O5'
12	Aa	699	DDE	NAD-CBI-CBW-NCB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 302 ligands modelled in this entry, 296 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	$\# Z > 2$
87	SPD	AA	3449	-	9,9,9	0.32	0	8,8,8	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	GDP	Aa	1001	86	24,30,30	0.94	1 (4%)	30,47,47	1.25	4 (13%)
87	SPD	c	1904	-	9,9,9	0.32	0	8,8,8	0.87	0
87	SPD	AA	3448	-	9,9,9	0.33	0	8,8,8	0.87	0
87	SPD	AA	3450	-	9,9,9	0.32	0	8,8,8	0.76	0
90	SO1	Aa	1002	-	35,39,39	1.10	2 (5%)	39,64,64	0.98	1 (2%)

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
87	SPD	AA	3449	-	-	0/7/7/7	-
89	GDP	Aa	1001	86	-	6/12/32/32	0/3/3/3
87	SPD	c	1904	-	-	2/7/7/7	-
87	SPD	AA	3448	-	-	1/7/7/7	-
87	SPD	AA	3450	-	-	2/7/7/7	-
90	SO1	Aa	1002	-	-	11/21/104/104	0/7/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	Aa	1002	SO1	C2-C6	-3.70	1.49	1.55
89	Aa	1001	GDP	C6-N1	-2.46	1.34	1.37
90	Aa	1002	SO1	C16-C22	-2.25	1.51	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	Aa	1001	GDP	PA-O3A-PB	-3.33	121.39	132.83
90	Aa	1002	SO1	C12-C6-C10	-3.07	105.47	107.91
89	Aa	1001	GDP	C3'-C2'-C1'	2.91	105.37	100.98
89	Aa	1001	GDP	C8-N7-C5	2.33	107.44	102.99
89	Aa	1001	GDP	C5-C6-N1	2.31	118.03	113.95

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	Aa	1001	GDP	C5'-O5'-PA-O1A

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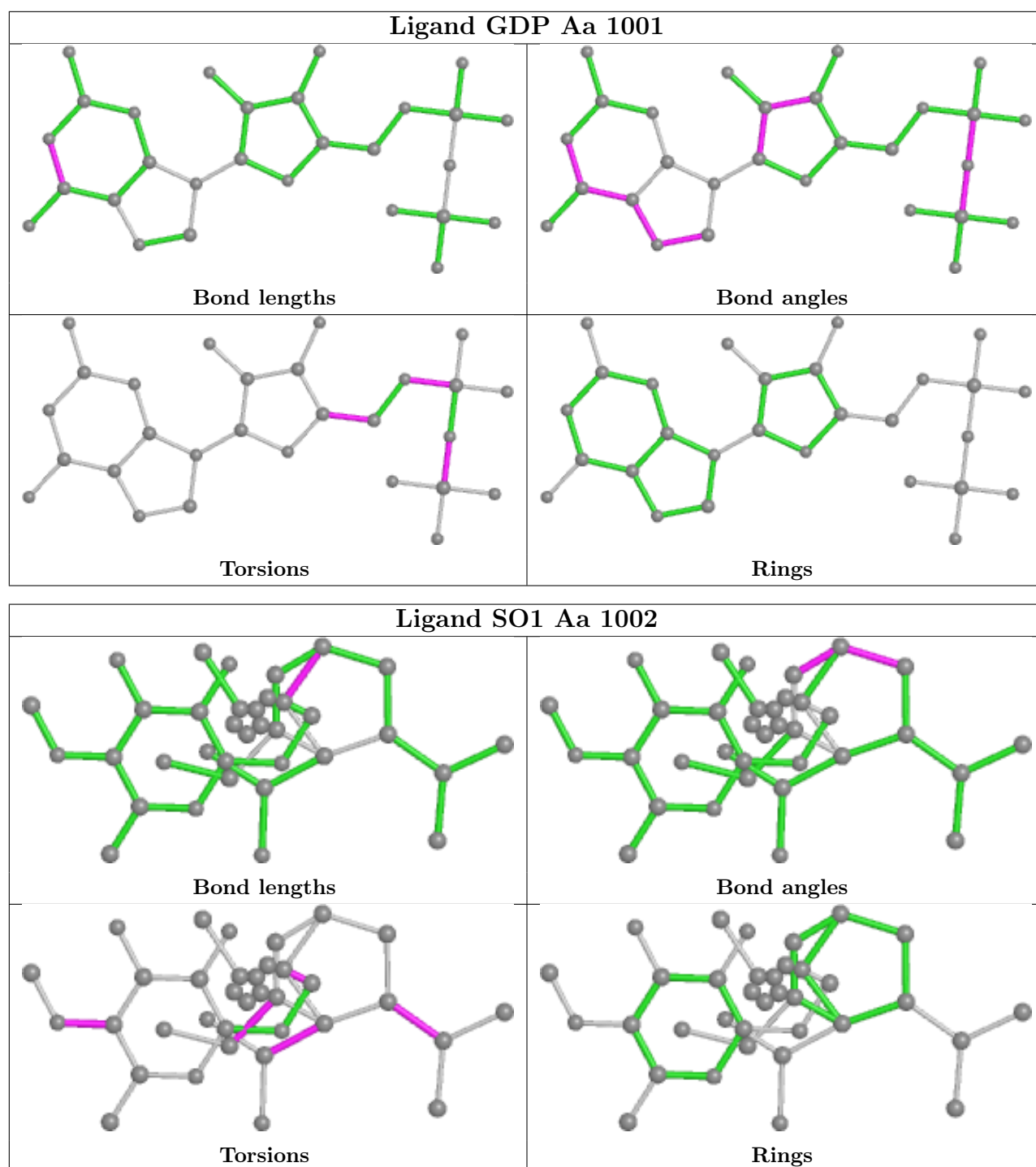
Continued from previous page...

Mol	Chain	Res	Type	Atoms
89	Aa	1001	GDP	C5'-O5'-PA-O2A
89	Aa	1001	GDP	O4'-C4'-C5'-O5'
90	Aa	1002	SO1	C2-C1-C5-O14
90	Aa	1002	SO1	C2-C1-C5-O15
90	Aa	1002	SO1	C20-C13-C4-C1
90	Aa	1002	SO1	C21-C13-C4-C1
90	Aa	1002	SO1	C20-C13-C4-C12
90	Aa	1002	SO1	C21-C13-C4-C12
90	Aa	1002	SO1	O19-C11-C3-C1
90	Aa	1002	SO1	O19-C11-C3-C10
89	Aa	1001	GDP	C3'-C4'-C5'-O5'
87	AA	3450	SPD	C2-C3-C4-C5
90	Aa	1002	SO1	C54-C55-O64-C65
89	Aa	1001	GDP	C5'-O5'-PA-O3A
87	c	1904	SPD	C4-C5-N6-C7
87	AA	3450	SPD	C4-C5-N6-C7
89	Aa	1001	GDP	PA-O3A-PB-O2B
87	AA	3448	SPD	C7-C8-C9-N10
90	Aa	1002	SO1	C4-C1-C5-O15
87	c	1904	SPD	N1-C2-C3-C4
90	Aa	1002	SO1	C1-C2-C8-O17

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.

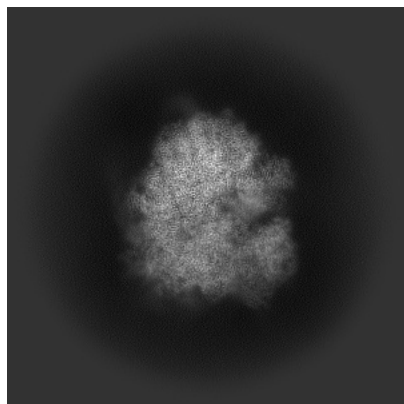
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16594. These allow visual inspection of the internal detail of the map and identification of artifacts.

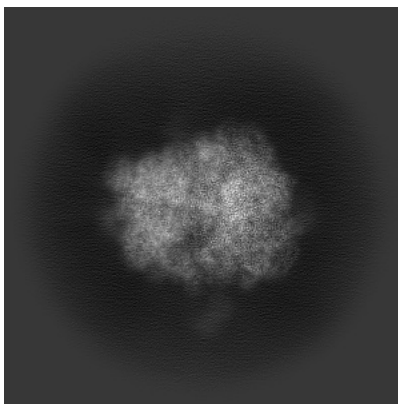
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

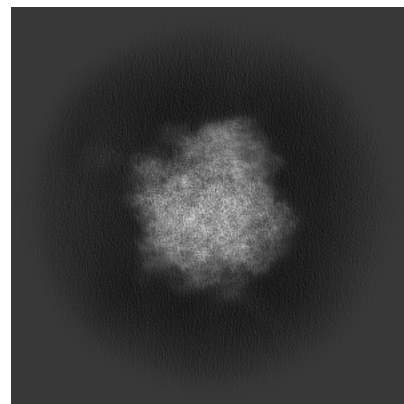
6.1.1 Primary map



X

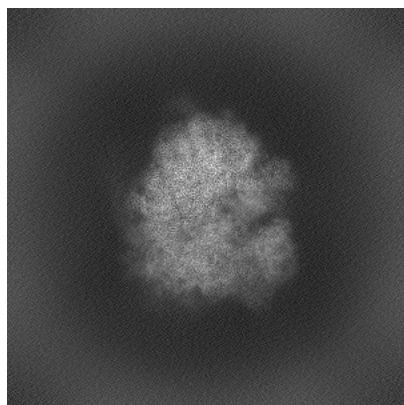


Y

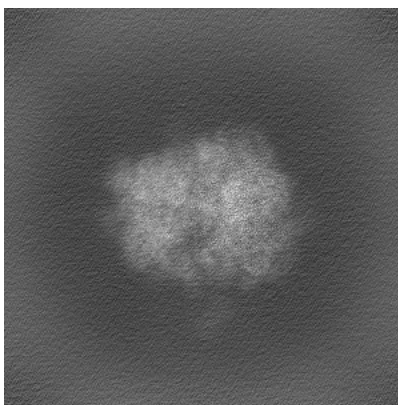


Z

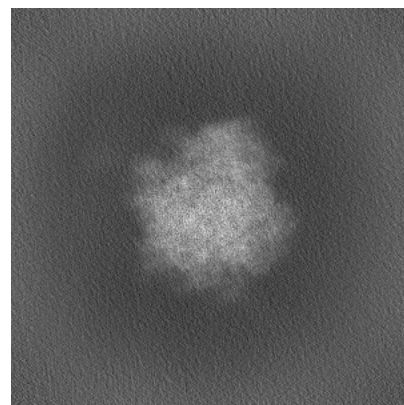
6.1.2 Raw map



X



Y

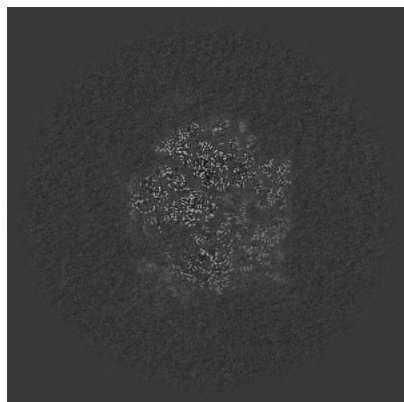


Z

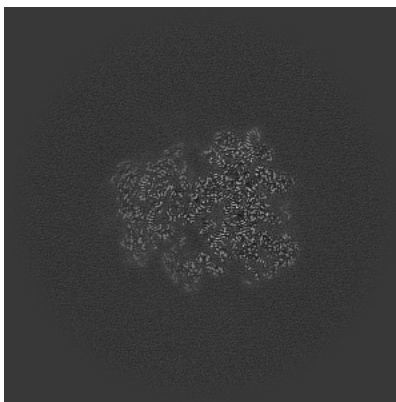
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

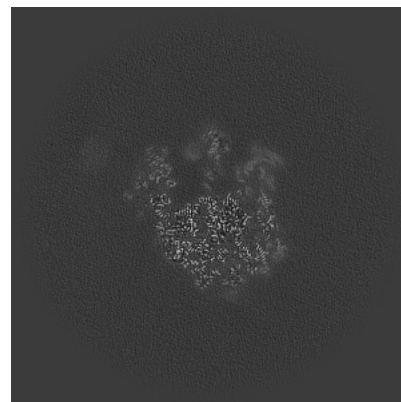
6.2.1 Primary map



X Index: 300

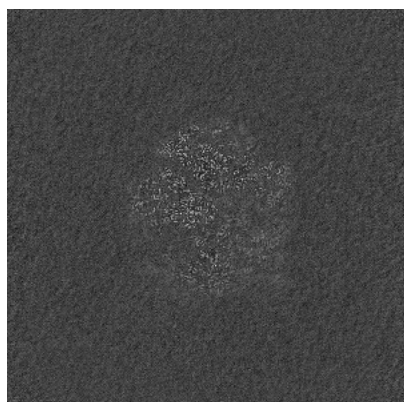


Y Index: 300

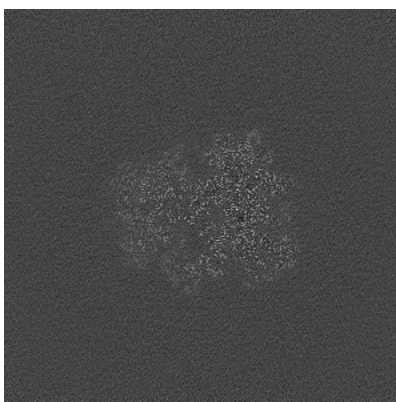


Z Index: 300

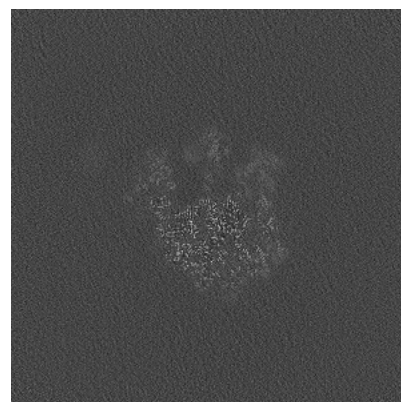
6.2.2 Raw map



X Index: 300



Y Index: 300

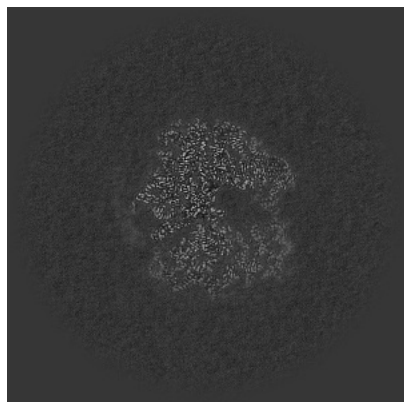


Z Index: 300

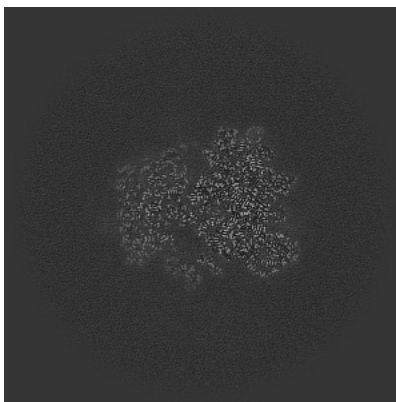
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

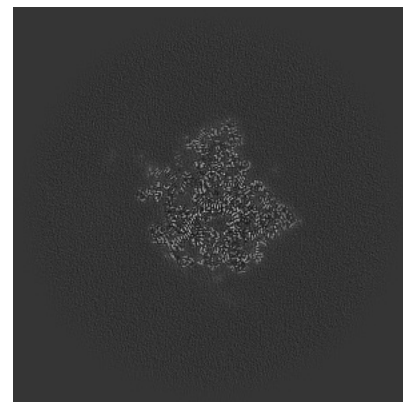
6.3.1 Primary map



X Index: 321

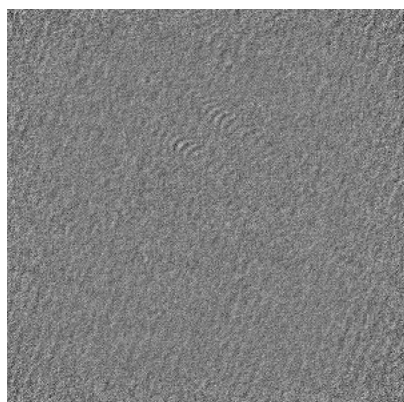


Y Index: 295

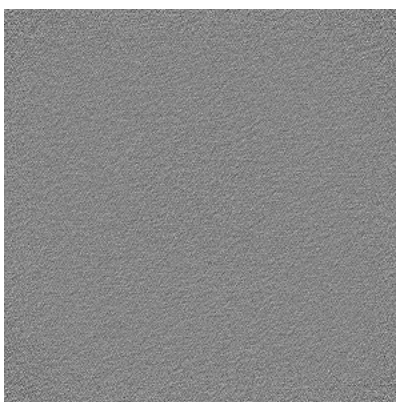


Z Index: 343

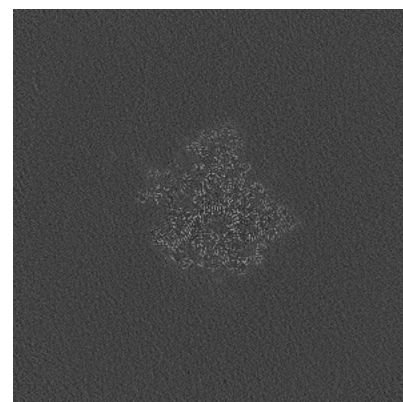
6.3.2 Raw map



X Index: 0



Y Index: 0

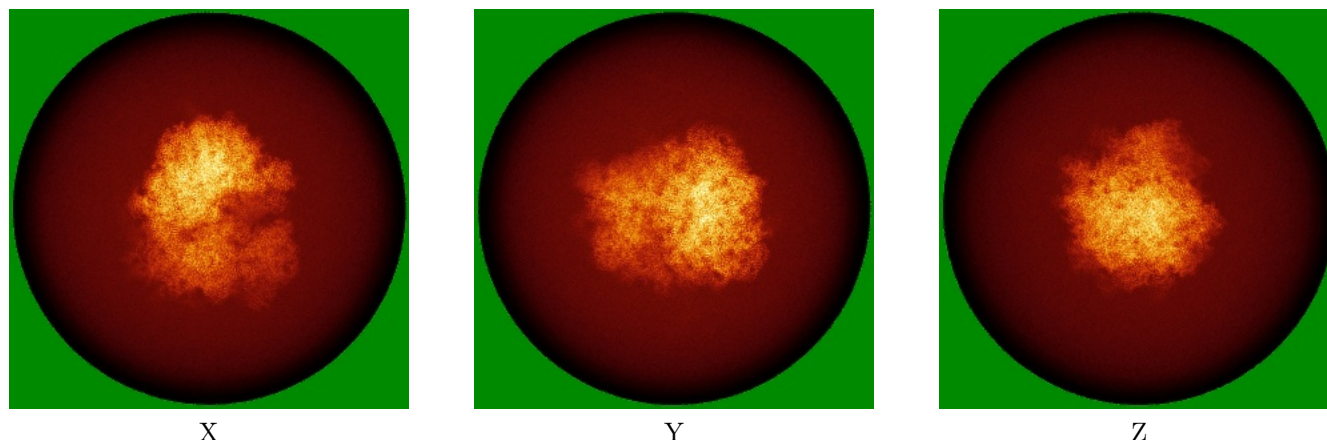


Z Index: 343

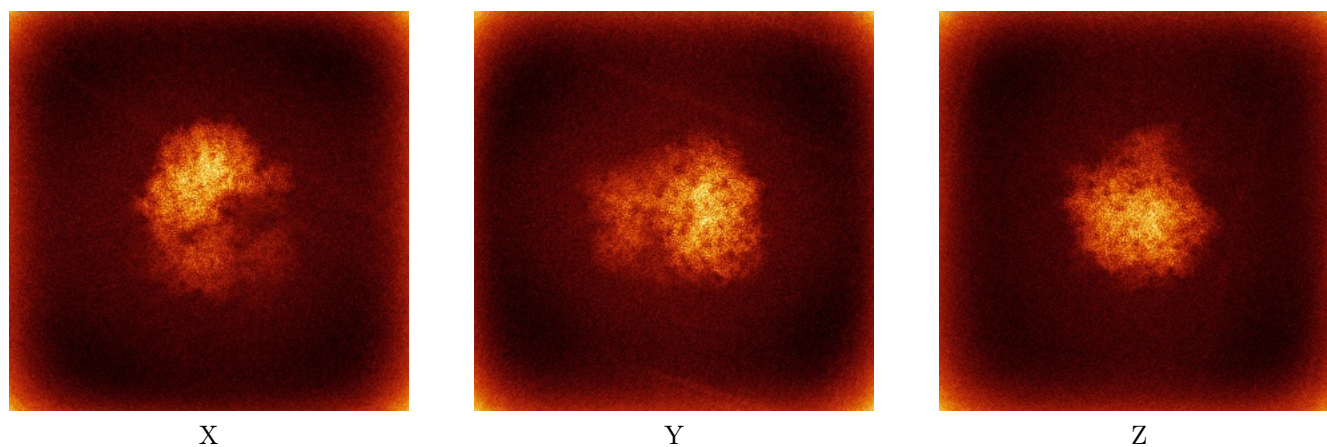
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



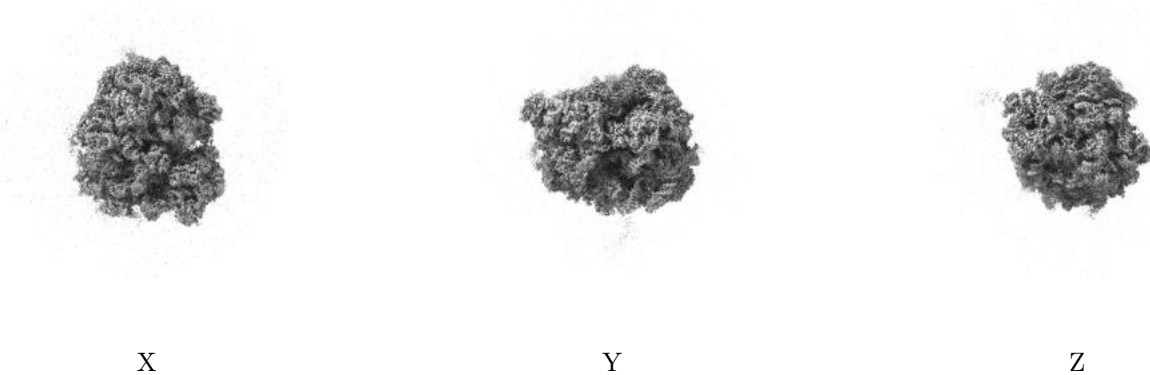
6.4.2 Raw map



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

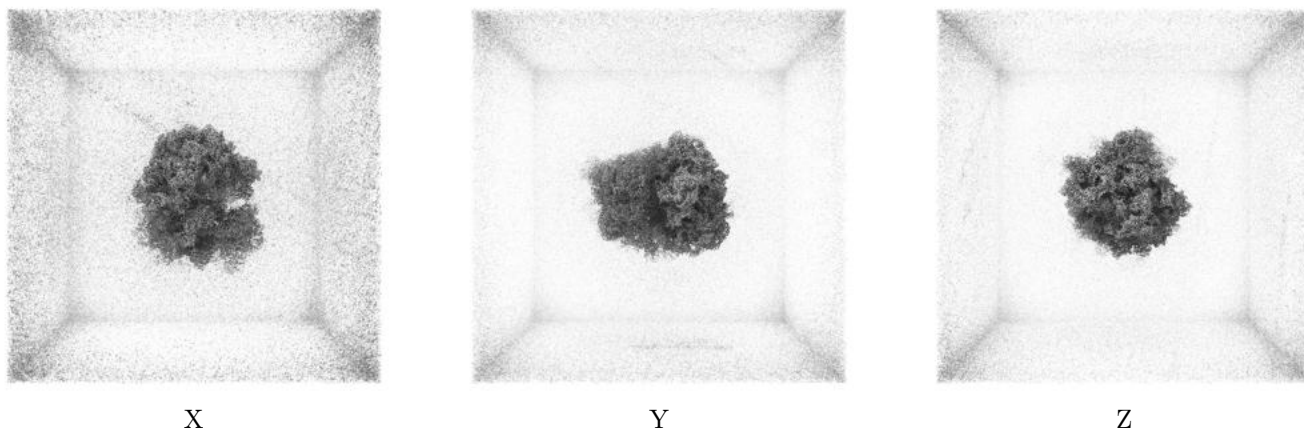
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.157. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

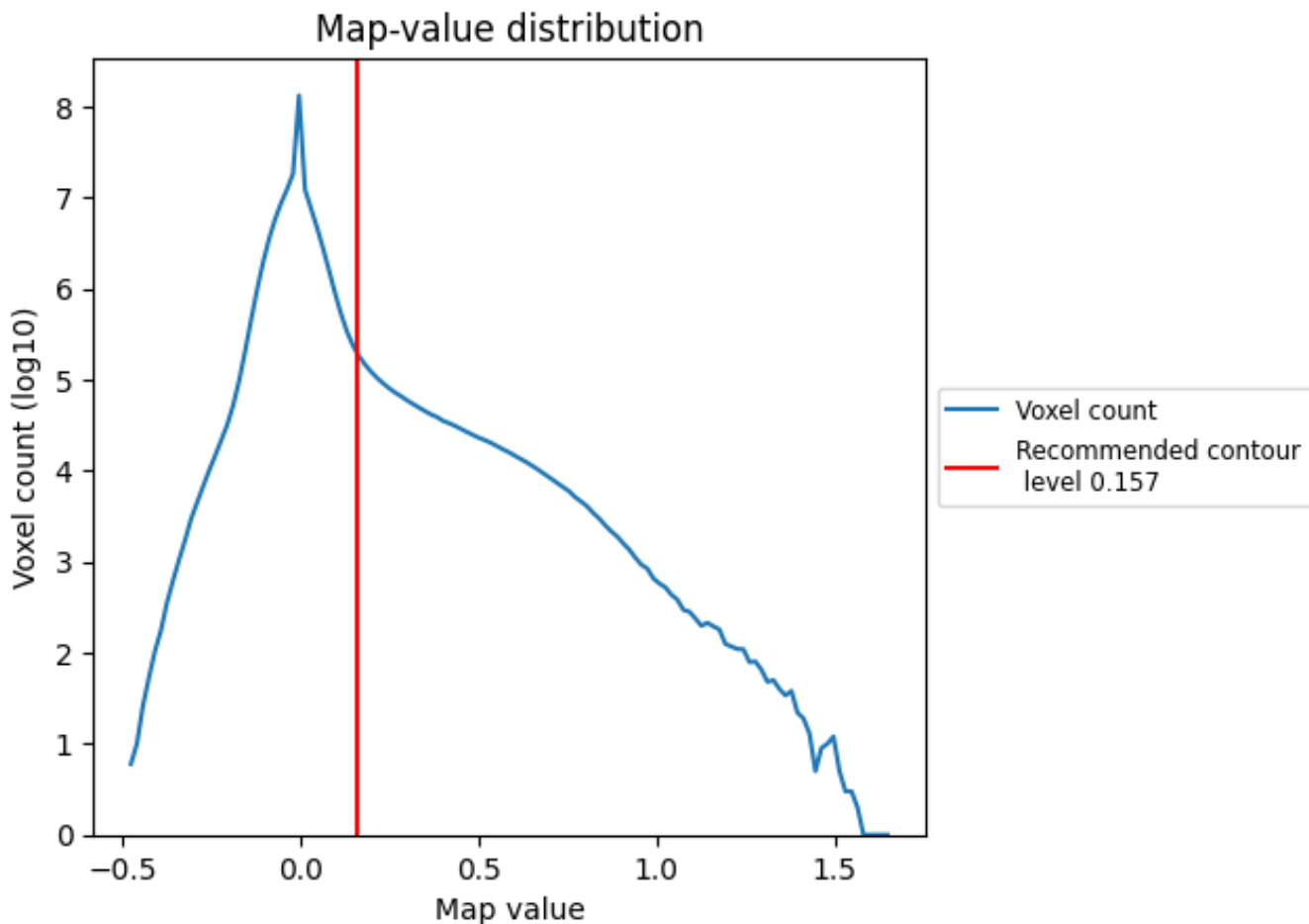
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

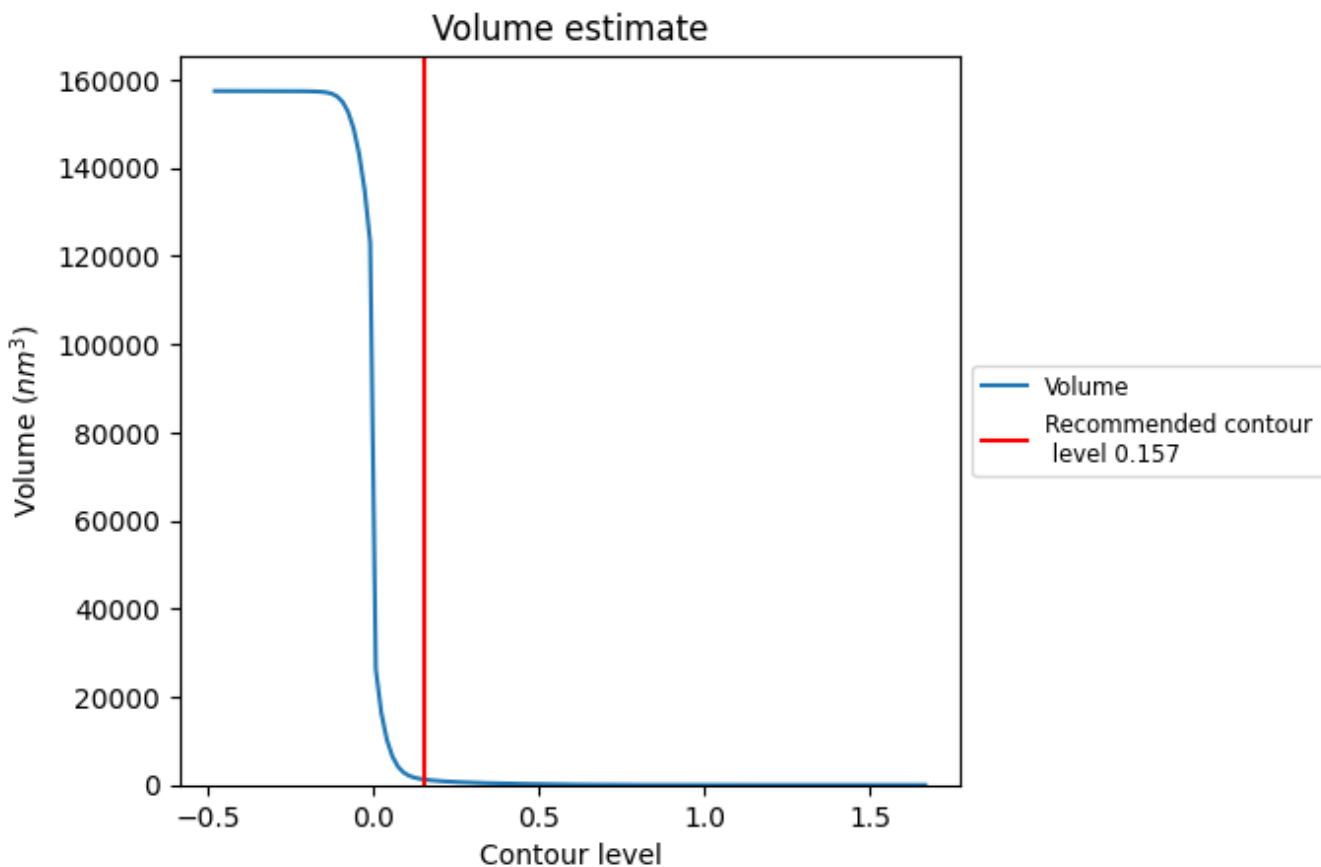
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

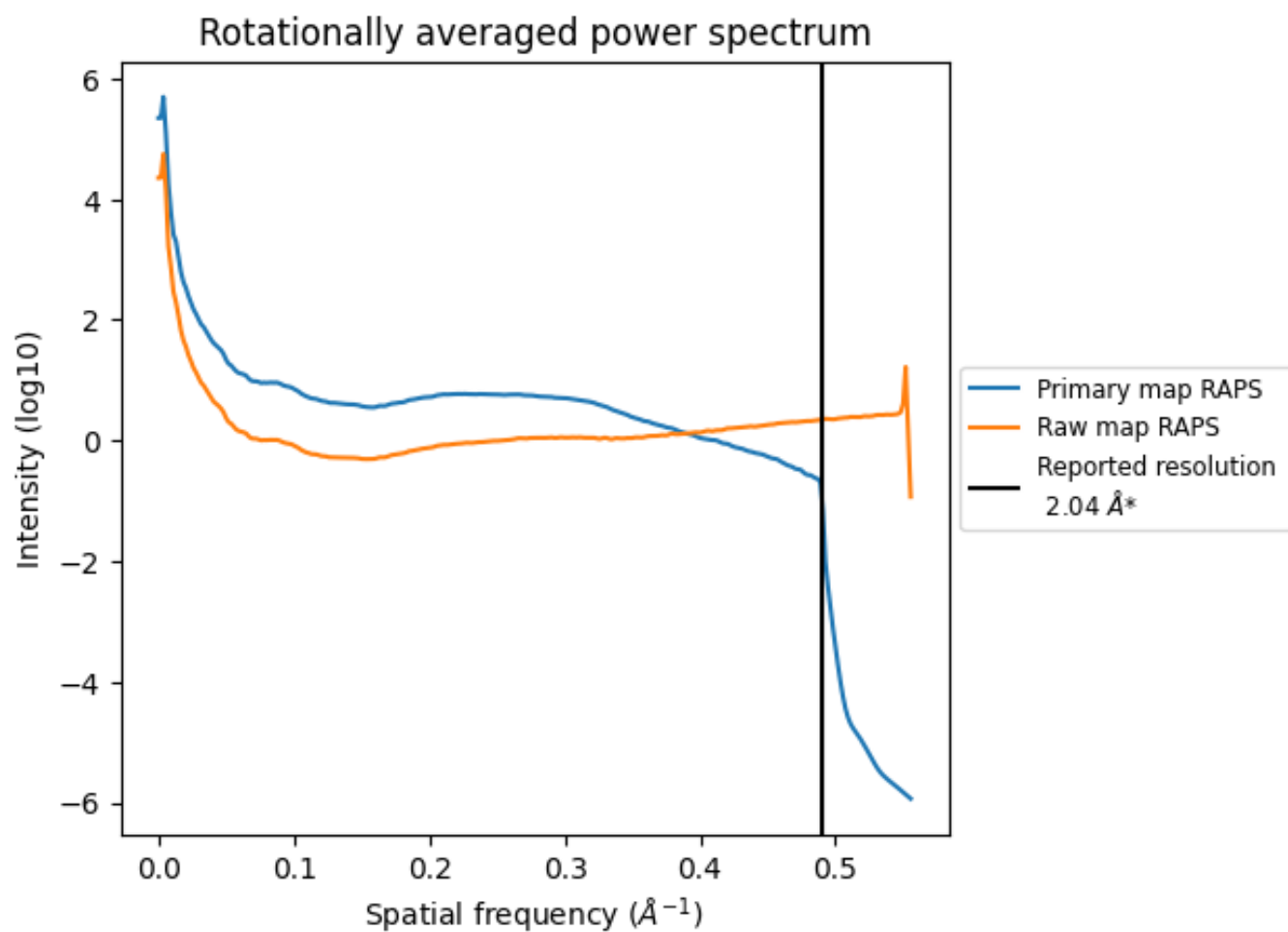
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1219 nm³; this corresponds to an approximate mass of 1101 kDa.

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

7.3 Rotationally averaged power spectrum i

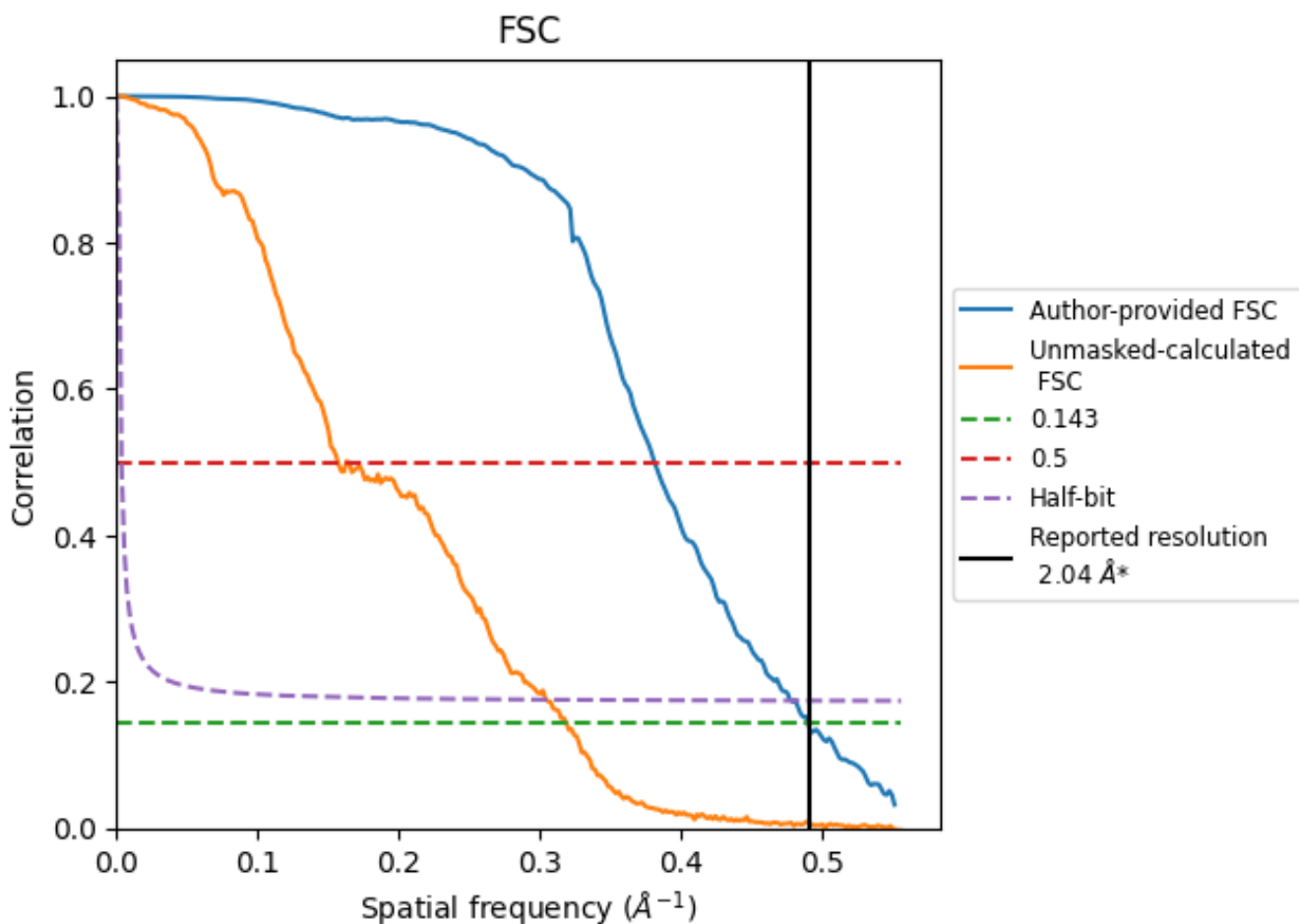


*Reported resolution corresponds to spatial frequency of 0.490 Å⁻¹

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 0.490 Å⁻¹

8.2 Resolution estimates [i](#)

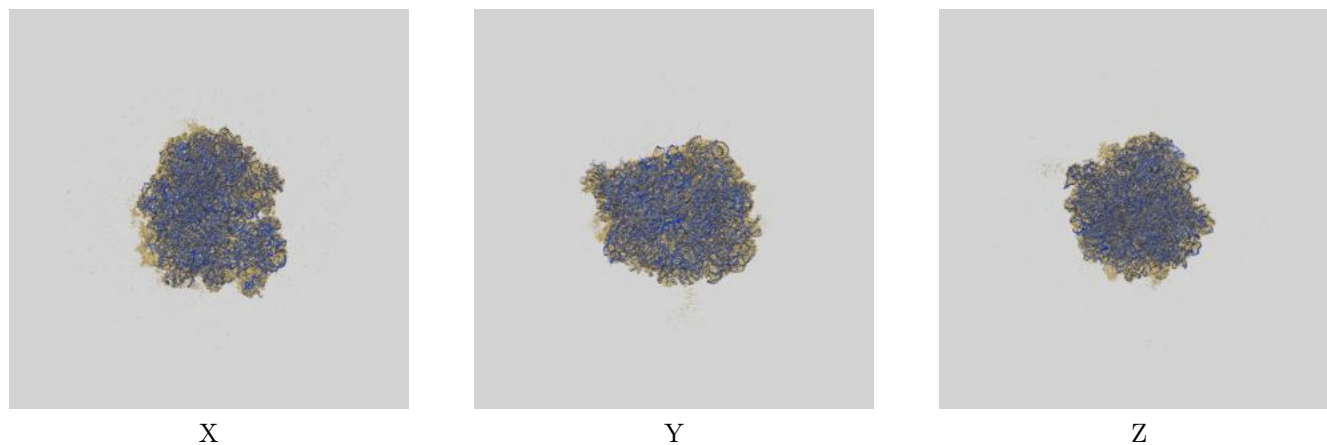
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.04	-	-
Author-provided FSC curve	2.04	2.63	2.09
Unmasked-calculated*	3.14	6.38	3.28

*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 3.14 differs from the reported value 2.04 by more than 10 %

9 Map-model fit [i](#)

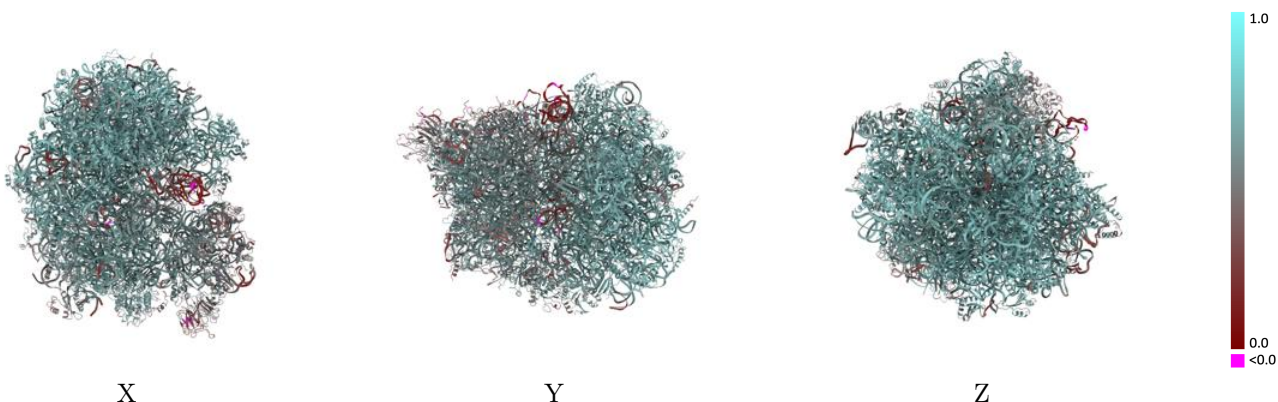
This section contains information regarding the fit between EMDB map EMD-16594 and PDB model 8CDR. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



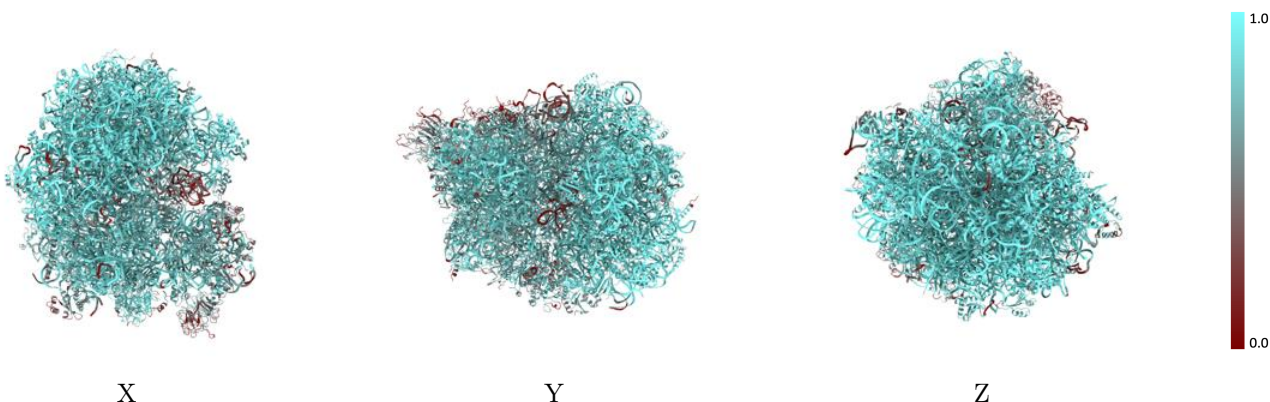
The images above show the 3D surface view of the map at the recommended contour level 0.157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



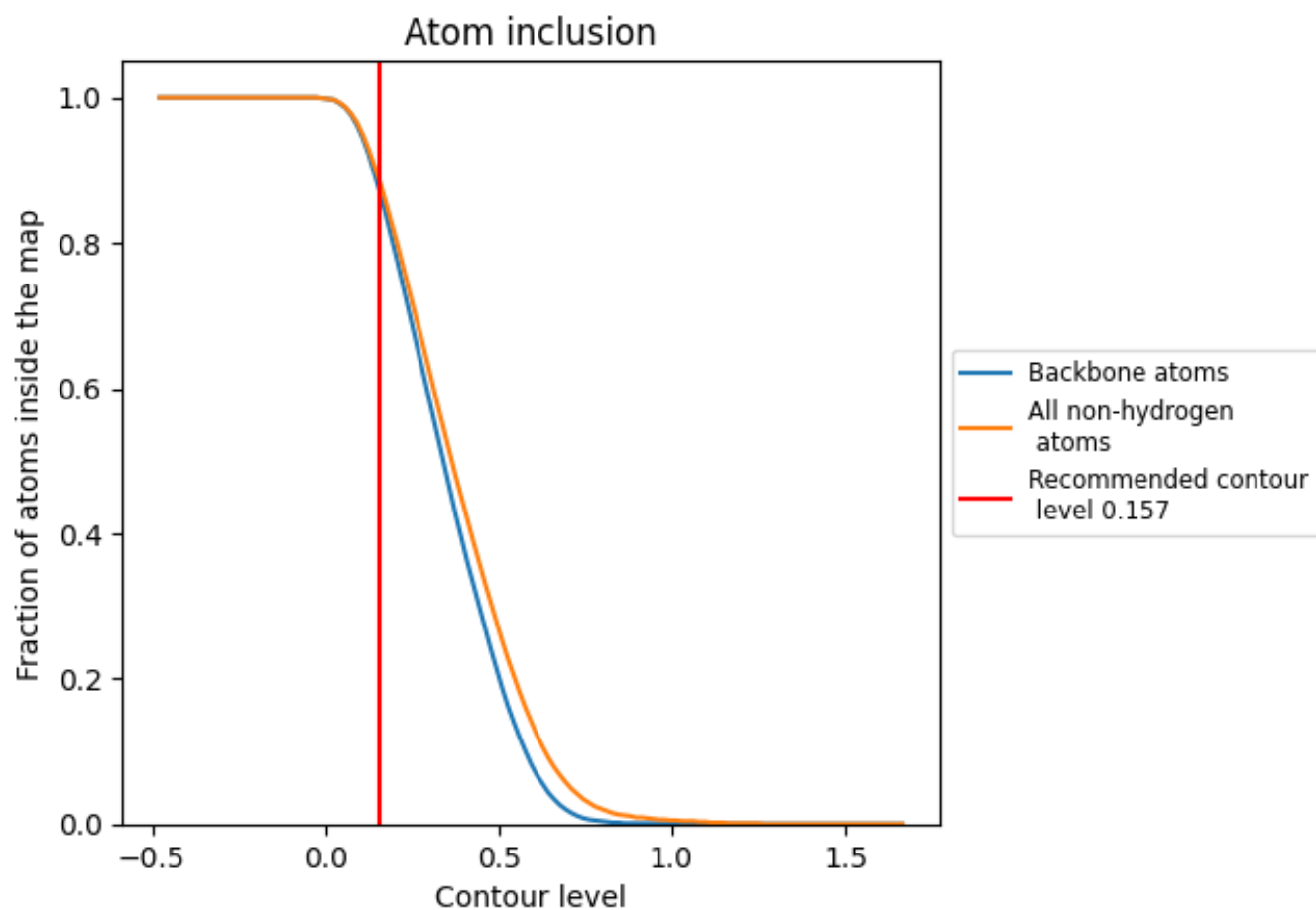
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.157).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 88% 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 (0.157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.6150
0	 0.7560	 0.5420
1	 0.1240	 0.3180
2	 0.8820	 0.6330
3	 0.7450	 0.5570
4	 0.6370	 0.5200
5	 0.9110	 0.5950
6	 0.7620	 0.5400
7	 0.4680	 0.4030
8	 0.3900	 0.3190
A	 0.9740	 0.6970
AA	 0.9430	 0.6410
Aa	 0.7810	 0.5890
B	 0.9780	 0.7080
BB	 0.9830	 0.6560
Bb	 0.5780	 0.4790
C	 0.9790	 0.7000
CC	 0.9770	 0.6650
Cc	 0.7320	 0.4630
D	 0.9080	 0.6670
DD	 0.7110	 0.5560
Dd	 0.8080	 0.5250
E	 0.9590	 0.6890
EE	 0.9680	 0.6990
Ee	 0.3580	 0.4190
F	 0.9310	 0.6720
FF	 0.9640	 0.6960
G	 0.8880	 0.6190
GG	 0.9630	 0.6920
H	 0.9730	 0.7000
HH	 0.8700	 0.6260
I	 0.9510	 0.6910
II	 0.9340	 0.6690
J	 0.9460	 0.6800
JJ	 0.9570	 0.6910



















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Chain	Atom inclusion	Q-score
K	 0.9520	 0.6870
KK	 0.8880	 0.6370
L	 0.9120	 0.6420
LL	 0.9320	 0.6700
M	 0.9620	 0.6890
MM	 0.9280	 0.6820
N	 0.9030	 0.6320
NN	 0.7930	 0.5660
O	 0.9070	 0.6510
OO	 0.9210	 0.6630
P	 0.8960	 0.6550
PP	 0.9530	 0.6860
Pp	 0.3160	 0.2890
Q	 0.9700	 0.7090
QQ	 0.9880	 0.7060
R	 0.9950	 0.7190
S	 0.9380	 0.6800
T	 0.9420	 0.6680
U	 0.9060	 0.6300
V	 0.9910	 0.7090
W	 0.8530	 0.6230
X	 0.9610	 0.6740
Y	 0.9600	 0.7030
Z	 0.9290	 0.6690
a	 0.9380	 0.6710
b	 0.9280	 0.6840
c	 0.9010	 0.5740
d	 0.8470	 0.5870
e	 0.7500	 0.5550
f	 0.8990	 0.6350
g	 0.7410	 0.5340
h	 0.8560	 0.5890
i	 0.6190	 0.4820
j	 0.6500	 0.4930
k	 0.6000	 0.5090
l	 0.8390	 0.5910
m	 0.8540	 0.5900
n	 0.6960	 0.4970
o	 0.8480	 0.6120
p	 0.8840	 0.6280
q	 0.8510	 0.5880
r	 0.7220	 0.5050

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Chain	Atom inclusion	Q-score
s	 0.7670	 0.5310
t	 0.6290	 0.4870
u	 0.5780	 0.4640
v	 0.7020	 0.4920
w	 0.6790	 0.5170
x	 0.8600	 0.6140
y	 0.9520	 0.6610
z	 0.9120	 0.6480