



Full wwPDB EM Validation Report ⓘ

Sep 14, 2022 – 11:37 am BST

PDB ID : 7QIW
EMDB ID : EMD-14001
Title : Specific features and methylation sites of a plant ribosome. 60S ribosomal subunit.
Authors : Cottilli, P.; Itoh, Y.; Amunts, A.
Deposited on : 2021-12-16
Resolution : 2.35 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:

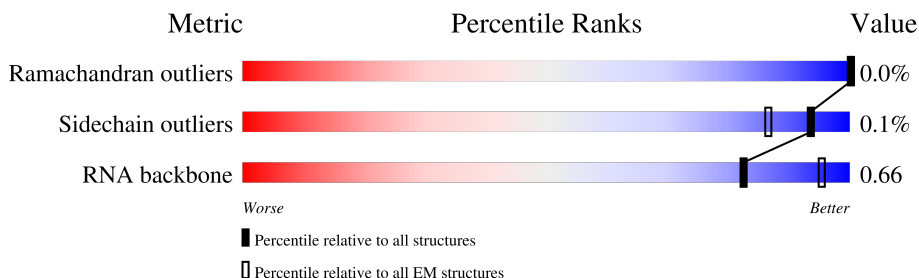
EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.30

1 Overall quality at a glance

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

The reported resolution of this entry is 2.35 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	D	260	<div> <div>96%</div> <div>5%</div> </div>
2	F	406	<div> <div>95%</div> <div>5%</div> </div>
3	E	389	<div> <div>99%</div> <div>14%</div> </div>
4	G	301	<div> <div>92%</div> <div>8%</div> </div>
5	H	229	<div> <div>88%</div> <div>12%</div> </div>
6	I	242	<div> <div>99%</div> <div>7%</div> </div>
7	J	258	<div> <div>89%</div> <div>11%</div> </div>
8	K	194	<div> <div>95%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
9	L	220	
10	M	181	
11	N	206	
12	O	133	
13	P	204	
14	Q	206	
15	R	173	
16	S	187	
17	T	213	
18	U	178	
19	V	164	
20	W	124	
21	X	140	
22	Y	165	
23	Z	154	
24	a	146	
25	b	135	
26	c	148	
27	d	60	
28	e	112	
29	f	120	
30	g	133	
31	h	112	
32	i	120	
33	j	123	

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Mol	Chain	Length	Quality of chain
34	k	110	
35	l	95	
36	m	69	
37	n	51	
38	o	128	
39	p	105	
40	q	92	
41	r	143	
42	s	2	
43	2	3391	
44	5	120	
45	8	165	

2 Entry composition [i](#)

There are 51 unique types of molecules in this entry. The entry contains 216806 atoms, of which 89115 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 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	251	Total	C	H	N	O	S	0	0
			3892	1201	1965	395	321	10		

- Molecule 2 is a protein called Ribos_L4_asso_C domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	F	385	Total	C	H	N	O	S	0	0
			6099	1892	3104	563	530	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	162	VAL	ILE	conflict	UNP A0A3Q7HW81
F	170	ASN	VAL	conflict	UNP A0A3Q7HW81
F	277	GLN	LEU	conflict	UNP A0A3Q7HW81
F	366	ALA	GLN	conflict	UNP A0A3Q7HW81

- Molecule 3 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	386	Total	C	H	N	O	S	0	0
			6343	1984	3237	578	530	14		

- Molecule 4 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	278	Total	C	H	N	O	S	0	0
			4537	1433	2278	409	412	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	51	PHE	LEU	conflict	UNP A0A3Q7H274

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Chain	Residue	Modelled	Actual	Comment	Reference
G	85	HIS	ARG	conflict	UNP A0A3Q7H274

- Molecule 5 is a protein called Ribosomal_L6e_N domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	201	Total	C	H	N	O	S	0	0
			3311	1030	1727	284	268	2		

- Molecule 6 is a protein called Thaliana 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	239	Total	C	H	N	O	S	0	0
			4024	1259	2068	358	335	4		

- Molecule 7 is a protein called Ribosomal_L7Ae domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	230	Total	C	H	N	O	S	0	0
			3845	1183	1999	341	314	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	10	SER	ALA	conflict	UNP A0A3Q7GV73
J	18	ALA	SER	conflict	UNP A0A3Q7GV73
J	21	LEU	VAL	conflict	UNP A0A3Q7GV73

- Molecule 8 is a protein called 60S ribosomal protein uL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	K	184	Total	C	H	N	O	S	0	0
			3023	932	1558	265	263	5		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	24	GLN	LEU	conflict	UNP A0A3Q7JDZ0
K	27	VAL	ILE	conflict	UNP A0A3Q7JDZ0
K	65	GLY	SER	conflict	UNP A0A3Q7JDZ0
K	69	THR	ALA	conflict	UNP A0A3Q7JDZ0
K	109	SER	THR	conflict	UNP A0A3Q7JDZ0

- Molecule 9 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	L	207	Total	C	H	N	O	S	0	0
			3362	1045	1709	327	271	10		

- Molecule 10 is a protein called 60S ribosomal protein uL5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	M	160	Total	C	H	N	O	S	0	0
			2642	819	1344	244	228	7		

- Molecule 11 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	N	204	Total	C	H	N	O	S	0	0
			3378	1036	1733	329	277	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	128	ARG	HIS	conflict	UNP A0A3Q7JCM5

- Molecule 12 is a protein called Ribosomal_L14e domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	O	132	Total	C	H	N	O	S	0	0
			2239	687	1167	200	181	4		

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	P	203	Total	C	H	N	O	S	0	0
			3471	1068	1770	354	276	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	135	VAL	ILE	conflict	UNP A0A3Q7HQB0
P	137	GLN	SER	conflict	UNP A0A3Q7HQB0

- Molecule 14 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Q	205	Total	C	H	N	O	S	0	0
			3418	1045	1775	320	270	8		

- Molecule 15 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	R	155	Total	C	H	N	O	S	0	0
			2506	773	1258	245	225	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	46	SER	ARG	conflict	UNP A0A3Q7FNQ5

- Molecule 16 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	S	186	Total	C	H	N	O	S	0	0
			3013	924	1561	277	248	3		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	17	THR	ILE	conflict	UNP A0A3Q7I5W4
S	37	ALA	SER	conflict	UNP A0A3Q7I5W4
S	60	PRO	ALA	conflict	UNP A0A3Q7I5W4
S	68	ILE	VAL	conflict	UNP A0A3Q7I5W4
S	71	ALA	MET	conflict	UNP A0A3Q7I5W4
S	75	GLY	GLU	conflict	UNP A0A3Q7I5W4
S	79	VAL	ALA	conflict	UNP A0A3Q7I5W4
S	81	LEU	VAL	conflict	UNP A0A3Q7I5W4
S	100	CYS	THR	conflict	UNP A0A3Q7I5W4
S	103	LYS	ARG	conflict	UNP A0A3Q7I5W4
S	136	LEU	VAL	conflict	UNP A0A3Q7I5W4
S	153	PRO	LYS	conflict	UNP A0A3Q7I5W4

- Molecule 17 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	T	146	Total	C	H	N	O	S	0	0
			2556	763	1337	257	191	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	178	LYS	GLU	conflict	UNP A0A3Q7GQ29
T	179	LYS	GLU	conflict	UNP A0A3Q7GQ29

- Molecule 18 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	U	177	Total	C	H	N	O	S	0	0
			3056	971	1553	273	251	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	73	THR	LYS	conflict	UNP A0A3Q7IGB1
U	104	ALA	GLY	conflict	UNP A0A3Q7IGB1

- Molecule 19 is a protein called 60S ribosomal protein eL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	V	163	Total	C	H	N	O	S	0	0
			2673	821	1365	258	226	3		

- Molecule 20 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	W	101	Total	C	H	N	O	S	0	0
			1663	518	849	144	149	3		

- Molecule 21 is a protein called 60S ribosomal protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	X	131	Total	C	H	N	O	S	0	0
			2032	623	1047	183	170	9		

- Molecule 22 is a protein called TRASH domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Y	62	Total	C	H	N	O	S	0	0
			1071	341	548	98	81	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	0	MET	-	initiating methionine	UNP A0A3Q7IN69

- Molecule 23 is a protein called Ribosomal_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Z	117	Total	C	H	N	O	S	0	0
			1981	610	1030	170	169	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	55	SER	ASN	conflict	UNP A0A3Q7INK3
Z	61	VAL	ILE	conflict	UNP A0A3Q7INK3
Z	73	ALA	GLN	conflict	UNP A0A3Q7INK3
Z	74	ILE	VAL	conflict	UNP A0A3Q7INK3
Z	77	TYR	CYS	conflict	UNP A0A3Q7INK3
Z	101	LYS	HIS	conflict	UNP A0A3Q7INK3

- Molecule 24 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	a	132	Total	C	H	N	O	S	0	0
			2207	657	1144	218	185	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	25	VAL	LEU	conflict	UNP A0A3Q7FBC6
a	43	ASN	SER	conflict	UNP A0A3Q7FBC6
a	99	ASN	HIS	conflict	UNP A0A3Q7FBC6
a	105	VAL	ILE	conflict	UNP A0A3Q7FBC6

- Molecule 25 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	b	134	Total	C	H	N	O	S	0	0
			2275	708	1177	206	182	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	117	PHE	LEU	conflict	UNP A0A3Q7GZ83

- Molecule 26 is a protein called Putative 60S ribosomal protein L27a-3-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	c	147	Total	C	H	N	O	S	0	0
			2358	739	1204	224	188	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	82	VAL	LEU	conflict	UNP A0A0V0H357
c	129	ILE	VAL	conflict	UNP A0A0V0H357

- Molecule 27 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	d	46	Total	C	H	N	O	S	0	0
			775	235	388	88	63	1		

- Molecule 28 is a protein called Ribosomal_L7Ae domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	e	95	Total	C	H	N	O	S	0	0
			1497	464	766	128	134	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	43	GLY	ALA	conflict	UNP A0A3Q7E9D6
e	55	LEU	ILE	conflict	UNP A0A3Q7E9D6
e	89	TYR	PHE	conflict	UNP A0A3Q7E9D6
e	92	SER	CYS	conflict	UNP A0A3Q7E9D6

- Molecule 29 is a protein called 60S ribosomal protein eL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	f	110	Total	C	H	N	O	S	0	0
			1841	558	951	171	159	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	76	VAL	ILE	conflict	UNP A0A3Q7JRW8

- Molecule 30 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	g	127	Total	C	H	N	O	S	0	0
			2173	662	1125	211	170	5		

- Molecule 31 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	h	111	Total	C	H	N	O	S	0	0
			1839	573	937	172	153	4		

- Molecule 32 is a protein called 60S ribosomal protein eL34.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	i	114	Total	C	H	N	O	S	0	0
			1942	580	1015	194	152	1		

- Molecule 33 is a protein called Similar to 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	j	122	Total	C	H	N	O	S	0	0
			2134	640	1137	191	165	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	67	ALA	LEU	conflict	UNP Q53U38
j	72	VAL	ALA	conflict	UNP Q53U38
j	100	SER	ALA	conflict	UNP Q53U38
j	112	MET	LEU	conflict	UNP Q53U38

- Molecule 34 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	k	100	Total	C	H	N	O	S	0	0
			1692	501	893	164	132	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	88	LYS	ARG	conflict	UNP A0A3Q7GUG2

- Molecule 35 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	l	87	Total	C	H	N	O	S	0	0
			1434	431	729	156	113	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	44	LEU	LYS	conflict	UNP A0A3Q7FV98

- Molecule 36 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	m	68	Total	C	H	N	O	S	0	0
			1163	358	605	99	98	3		

- Molecule 37 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	n	50	Total	C	H	N	O	S	0	0
			927	285	479	96	65	2		

- Molecule 38 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	o	52	Total	C	H	N	O	S	0	0
			901	268	470	91	66	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	113	ARG	LYS	conflict	UNP K4B017

- Molecule 39 is a protein called 60S ribosomal protein eL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	p	99	Total	C	H	N	O	S	0	0
			1653	500	857	159	132	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	76	GLY	SER	conflict	UNP A0A3Q7H1I0
p	80	VAL	MET	conflict	UNP A0A3Q7H1I0

- Molecule 40 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	q	91	Total	C	H	N	O	S	0	0
			1455	443	746	136	125	5		

- Molecule 41 is a protein called Ribosomal_L28e domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	r	142	Total	C	H	N	O	S	0	0
			2302	703	1185	210	202	2		

- Molecule 42 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	s	2	Total	C	H	N	O	P	0	0
			64	19	22	8	13	2		

- Molecule 43 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	2	3098	Total	C	H	N	O	P	0	0
			98740	29664	32316	12094	21568	3098		

- Molecule 44 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	5	120	Total	C	H	N	O	P	0	0
			3796	1142	1237	459	838	120		

- Molecule 45 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	8	159	Total	C	H	N	O	P	0	0
			5049	1517	1653	613	1107	159		

- Molecule 46 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
46	D	2	Total 2	K 2	0
46	E	1	Total 1	K 1	0
46	L	1	Total 1	K 1	0
46	N	2	Total 2	K 2	0
46	i	1	Total 1	K 1	0
46	p	1	Total 1	K 1	0
46	2	79	Total 79	K 79	0
46	8	3	Total 3	K 3	0

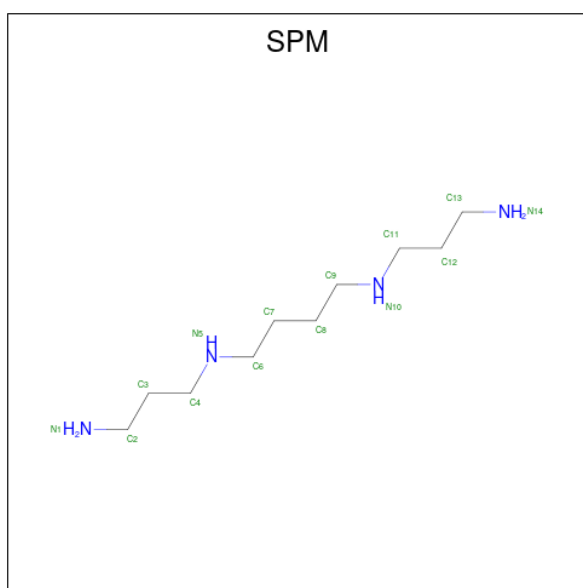
- Molecule 47 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
47	E	1	Total 1	Mg 1	0
47	I	1	Total 1	Mg 1	0
47	L	1	Total 1	Mg 1	0
47	N	1	Total 1	Mg 1	0
47	R	1	Total 1	Mg 1	0
47	T	1	Total 1	Mg 1	0
47	X	1	Total 1	Mg 1	0
47	1	1	Total 1	Mg 1	0
47	2	258	Total 258	Mg 258	0
47	5	5	Total 5	Mg 5	0
47	8	5	Total 5	Mg 5	0

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

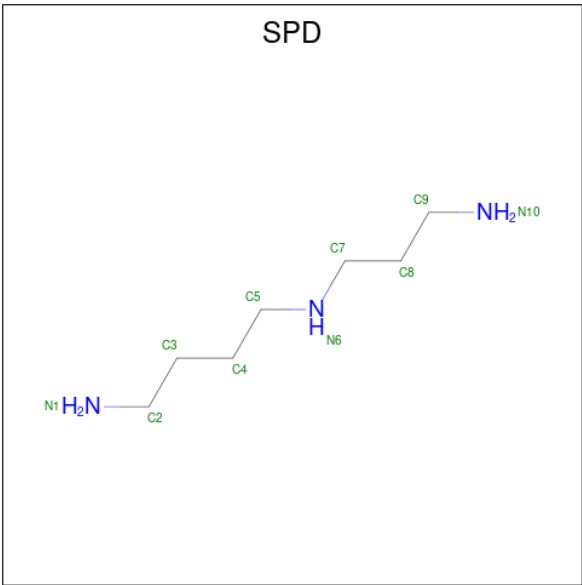
Mol	Chain	Residues	Atoms		AltConf
48	l	1	Total	Zn	0
			1	1	
48	o	1	Total	Zn	0
			1	1	
48	p	1	Total	Zn	0
			1	1	
48	q	1	Total	Zn	0
			1	1	

- Molecule 49 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
49	2	1	Total	C	H	N	0
			120	30	78	12	
49	2	1	Total	C	H	N	0
			120	30	78	12	
49	2	1	Total	C	H	N	0
			120	30	78	12	

- Molecule 50 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms				AltConf
50	2	1	Total	C	H	N	0
			29	7	19	3	

- Molecule 51 is water.

Mol	Chain	Residues	Atoms		AltConf
51	D	45	Total	O	0
			45	45	
51	F	50	Total	O	0
			50	50	
51	E	66	Total	O	0
			66	66	
51	G	19	Total	O	0
			19	19	
51	H	2	Total	O	0
			2	2	
51	I	28	Total	O	0
			28	28	
51	J	9	Total	O	0
			9	9	
51	K	1	Total	O	0
			1	1	
51	L	3	Total	O	0
			3	3	
51	N	36	Total	O	0
			36	36	
51	O	7	Total	O	0
			7	7	

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Mol	Chain	Residues	Atoms		AltConf
51	P	52	Total 52	O 52	0
51	Q	19	Total 19	O 19	0
51	R	14	Total 14	O 14	0
51	S	16	Total 16	O 16	0
51	T	11	Total 11	O 11	0
51	U	9	Total 9	O 9	0
51	V	15	Total 15	O 15	0
51	X	7	Total 7	O 7	0
51	Y	3	Total 3	O 3	0
51	Z	4	Total 4	O 4	0
51	a	9	Total 9	O 9	0
51	b	4	Total 4	O 4	0
51	c	30	Total 30	O 30	0
51	d	10	Total 10	O 10	0
51	f	10	Total 10	O 10	0
51	g	26	Total 26	O 26	0
51	h	15	Total 15	O 15	0
51	i	11	Total 11	O 11	0
51	j	7	Total 7	O 7	0
51	k	5	Total 5	O 5	0
51	l	31	Total 31	O 31	0

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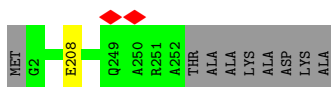
Mol	Chain	Residues	Atoms		AltConf
51	n	6	Total 6	O 6	0
51	o	2	Total 2	O 2	0
51	p	14	Total 14	O 14	0
51	q	8	Total 8	O 8	0
51	r	8	Total 8	O 8	0
51	s	4	Total 4	O 4	0
51	2	3147	Total 3147	O 3147	0
51	5	60	Total 60	O 60	0
51	8	112	Total 112	O 112	0

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.

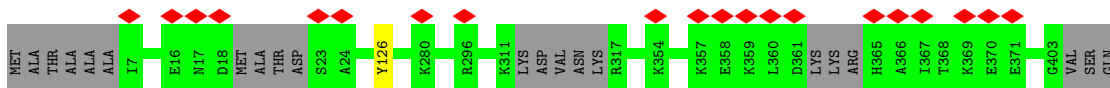
- Molecule 1: 60S ribosomal protein L8

Chain D:  96%



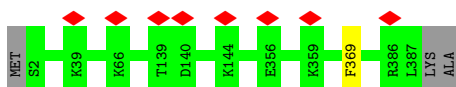
- Molecule 2: Ribos_L4_asso_C domain-containing protein

Chain F:  5% 95% 5%

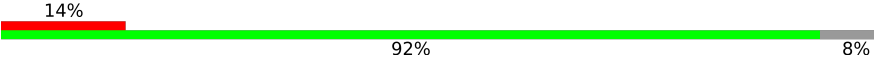


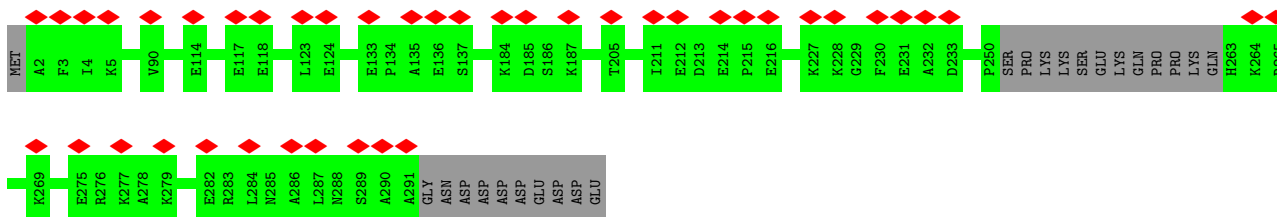
- Molecule 3: Ribosomal protein L3

Chain E:  99%



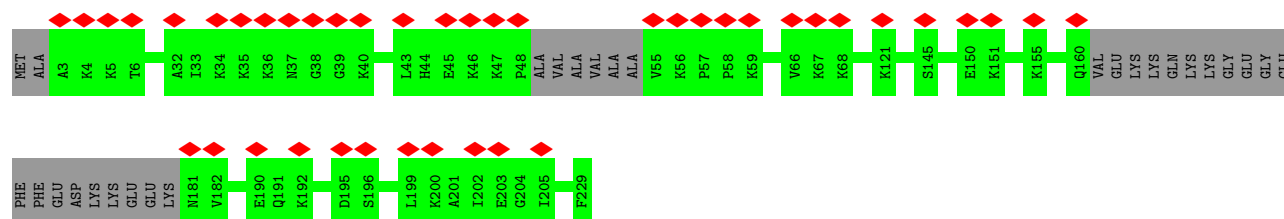
- Molecule 4: Ribosomal_L18_c domain-containing protein

Chain G:  14% 92% 8%

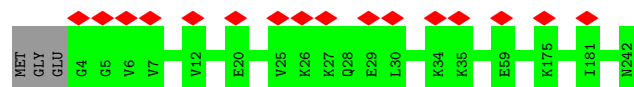


- Molecule 5: Ribosomal_L6e_N domain-containing protein

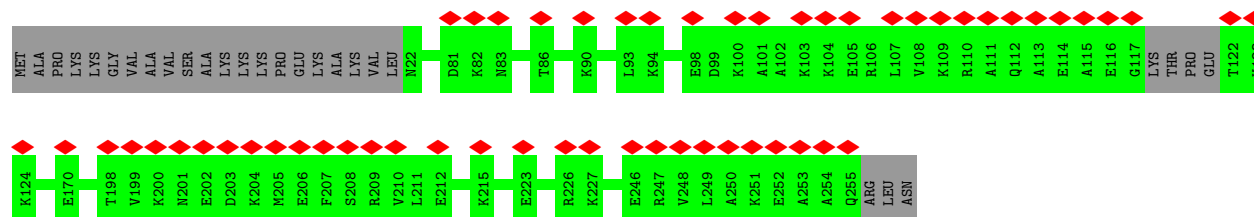
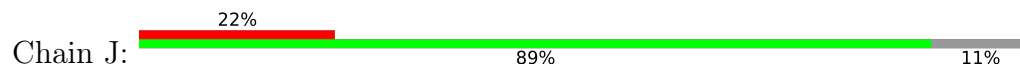
Chain H:  18% 88% 12%



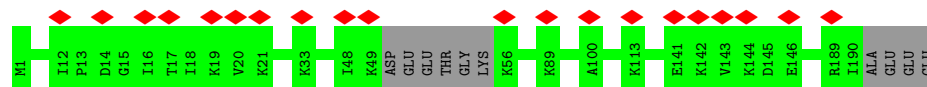
- Molecule 6: Thaliana 60S ribosomal protein L7



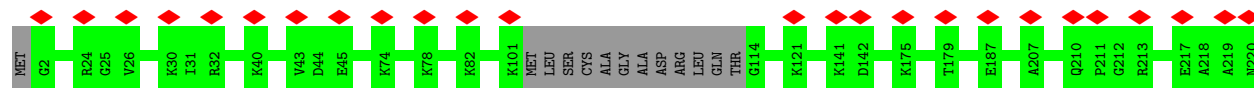
- Molecule 7: Ribosomal_L7Ae domain-containing protein



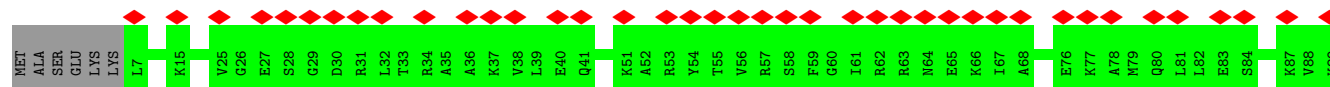
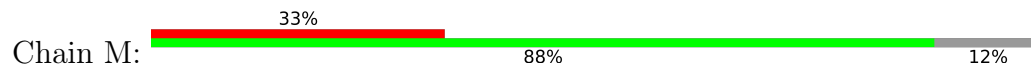
- Molecule 8: 60S ribosomal protein uL6

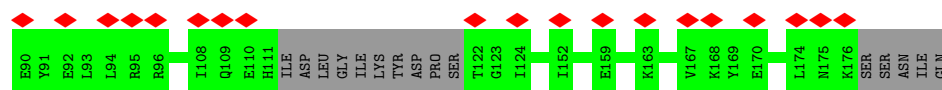


- Molecule 9: 60S ribosomal protein L10

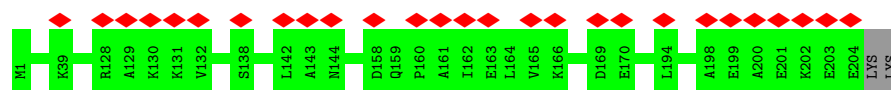


- Molecule 10: 60S ribosomal protein uL5

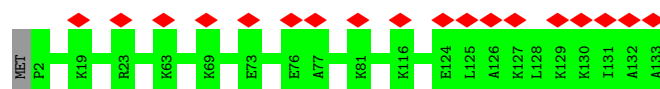




- Molecule 11: 60S ribosomal protein L13



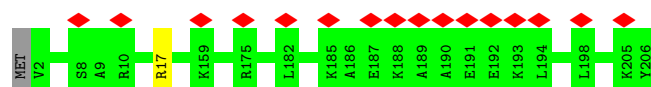
- Molecule 12: Ribosomal_L14e domain-containing protein



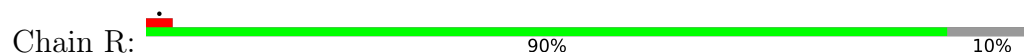
- Molecule 13: Ribosomal protein L15



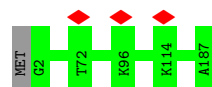
- Molecule 14: 60S ribosomal protein uL13



- Molecule 15: 50S ribosomal protein L22, chloroplastic



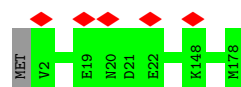
- Molecule 16: Ribosomal_L18e/L15P domain-containing protein



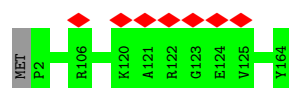
- Molecule 17: Ribosomal protein L19




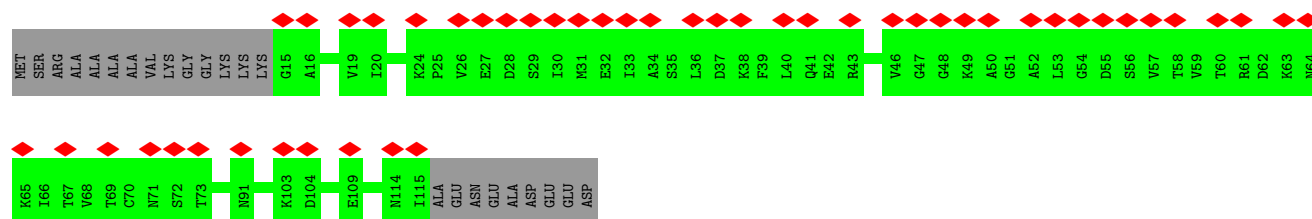
- Chain U:  99%



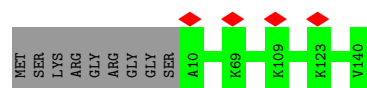
- Chain V:  99%



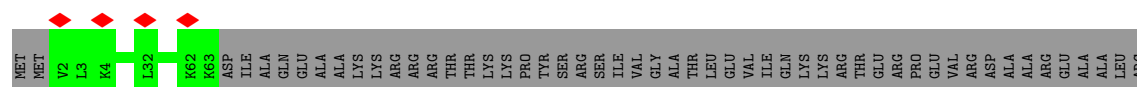
- Chain W: 



- Chain X: 94% 6%



- Chain Y:  38% 62%



GLU
ILE
LYS
GLU
ARG
ILE
LYS
LYS
THR
LYS
ASP
GLU
LYS
LYS
LYS
ALA
LYS
LYS
GLN
ALA
VAL
GLN
ALA
LYS
LYS
SER
GLN
LYS
ALA
GLY
GLY
LYS
LYS
GLY
ASN
MET
SER
LYS
SER
GLY
GLY
ALA
SER
LYS
GLY
PRO
LYS
LYS
LEU
GLY
GLY
GLY
GLY
LYS
ARG

- Molecule 23: Ribosomal_L23eN domain-containing protein

Chain Z: 5% 76% 24%

MET
ALA
PRO
ALA
LYS
VAL
ASP
LEU
THR
LYS
LYS
ASP
PRO
LYS
ALA
GLN
ALA
VAL
LYS
LYS
ALA
LYS
LYS
SER
VAL
LYS
SER
GLY
SER
THR
PHE
LYS
LYS
LYS
SER
SER
LYS
LYS
I38
L50
D90
K112
I119
L345
K150
I154

- Molecule 24: KOW domain-containing protein

Chain a: 7% 89% 10%

M1
K2
K41
Y73
K107
K123
A126
A127
A128
D129
K130
D131
K132
GLY
THR
LYS
PHE
THR
THR
GLU
GLU
ILE
MET
GLN
ALA
ILE
ASP

- Molecule 25: 60S ribosomal protein L27

Chain b: 13% 99% 0%

MET
V2
E31
R34
K56
K60
D88
V89
D90
L91
K92
D93
V94
D98
V99
L100
Q101
A102
R103
D104
K105
K106
V107
E119
K125
F135

- Molecule 26: Putative 60S ribosomal protein L27a-3-like

Chain c: 0% 98% 2%

MET
T2
V15
Y60
K89
A92
V93
K94
T96
A146

- Molecule 27: 60S ribosomal protein L29

Chain d: 0% 77% 23%

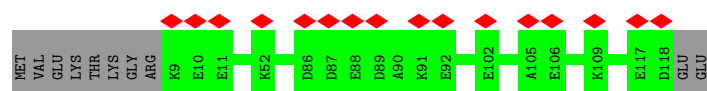
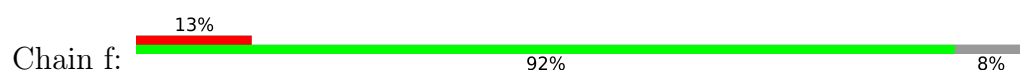
MET
ALA
LYS
SER
LYS
N6
K51
LYS
ASN
GLY
GLU
THR
ALA
G95
GLU
GLU

- Molecule 28: Ribosomal_L7Ae domain-containing protein

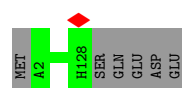
Chain e: 8% 85% 15%

MET
VAL
ALA
ALA
LYS
LYS
THR
LYS
LYS
THR
HIS
GLU
S13
L20
K26
K42
K68
S102
I105
K106
S107
LEU
PRO
SER
ASP
GLN

- Molecule 29: 60S ribosomal protein eL31



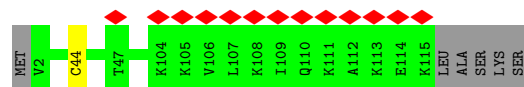
- Molecule 30: 60S ribosomal protein eL32



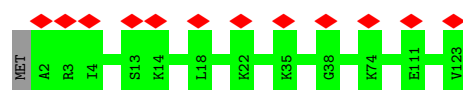
- Molecule 31: 60S ribosomal protein eL33



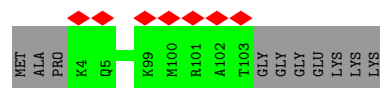
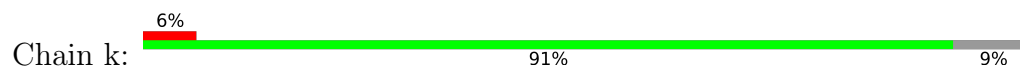
- Molecule 32: 60S ribosomal protein eL34



- Molecule 33: Similar to 60S ribosomal protein L35

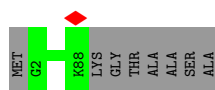


- Molecule 34: 60S ribosomal protein L36

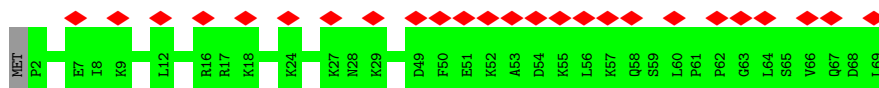


- Molecule 35: Ribosomal protein L37





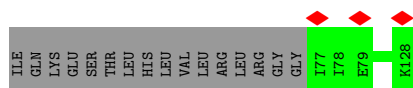
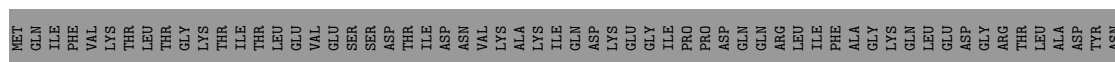
- Molecule 36: 60S ribosomal protein L38



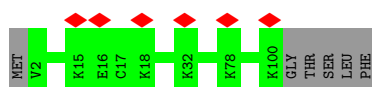
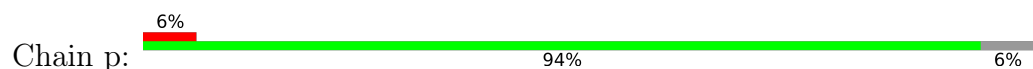
- Molecule 37: 60S ribosomal protein eL39



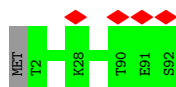
- Molecule 38: Ubiquitin-like domain-containing protein



- Molecule 39: 60S ribosomal protein eL42

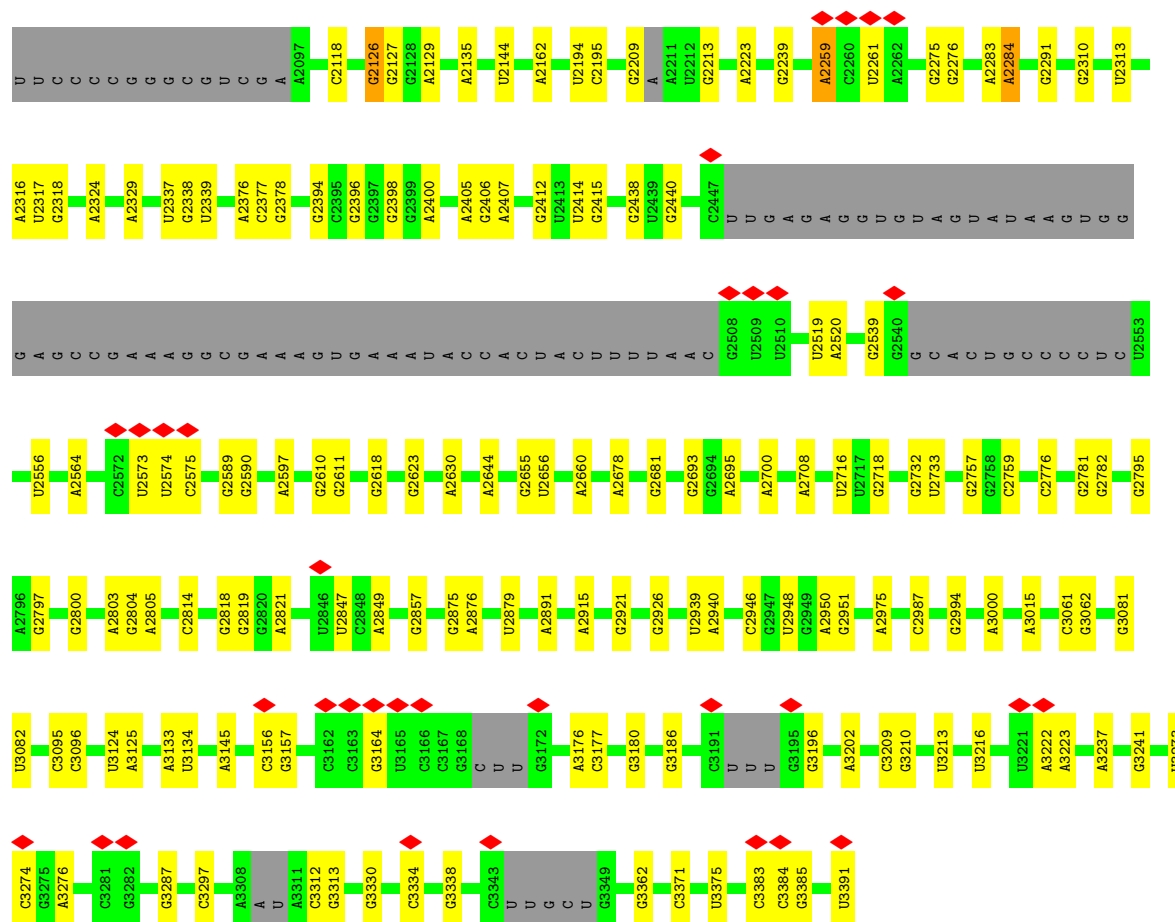


- Molecule 40: 60S ribosomal protein eL43



- Molecule 41: Ribosomal_L28e domain-containing protein

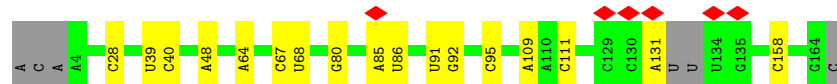
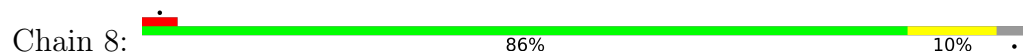




• Molecule 44: 5S rRNA



• Molecule 45: 5.8S rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335806	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 ($e^-/\text{\AA}^2$)	30.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.642	Depositor
Minimum map value	-0.311	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0328	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, HIC, OMU, OMG, K, THC, SPM, 5MC, 1MA, ZN, SPD, PSU, A2M, OMC, MG

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	D	0.24	0/1972	0.56	0/2651
2	F	0.23	0/3056	0.49	0/4123
3	E	0.24	0/3160	0.51	0/4230
4	G	0.24	0/2301	0.49	0/3087
5	H	0.24	0/1615	0.44	0/2163
6	I	0.24	0/1991	0.47	0/2669
7	J	0.23	0/1876	0.46	0/2513
8	K	0.23	0/1483	0.48	0/1982
9	L	0.24	0/1689	0.52	0/2258
10	M	0.23	0/1317	0.52	0/1758
11	N	0.24	0/1677	0.53	0/2249
12	O	0.23	0/1085	0.50	0/1448
13	P	0.23	0/1739	0.59	0/2330
14	Q	0.23	0/1672	0.50	0/2238
15	R	0.24	0/1273	0.52	0/1709
16	S	0.24	0/1477	0.53	0/1980
17	T	0.22	0/1236	0.55	0/1633
18	U	0.24	0/1543	0.49	0/2070
19	V	0.24	0/1332	0.54	0/1784
20	W	0.24	0/825	0.48	0/1106
21	X	0.25	0/1001	0.53	0/1345
22	Y	0.25	0/537	0.47	0/715
23	Z	0.23	0/966	0.47	0/1297
24	a	0.23	0/1076	0.57	0/1436
25	b	0.24	0/1118	0.50	0/1492
26	c	0.24	0/1183	0.50	0/1583
27	d	0.24	0/397	0.51	0/526
28	e	0.24	0/742	0.45	0/999
29	f	0.23	0/900	0.53	0/1202
30	g	0.23	0/1066	0.54	0/1425
31	h	0.25	0/922	0.53	0/1234
32	i	0.23	0/940	0.56	0/1253

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	j	0.23	0/1007	0.49	0/1339
34	k	0.23	0/808	0.52	0/1069
35	l	0.24	0/718	0.64	0/954
36	m	0.23	0/566	0.46	0/752
37	n	0.23	0/460	0.57	0/609
38	o	0.23	0/437	0.54	0/576
39	p	0.24	0/810	0.48	0/1069
40	q	0.23	0/718	0.53	0/952
41	r	0.23	0/1124	0.46	0/1504
42	s	0.22	0/46	0.68	0/69
43	2	0.21	0/71398	0.68	1/111346 (0.0%)
44	5	0.27	1/2860 (0.0%)	0.66	0/4454
45	8	0.19	0/3699	0.67	0/5762
All	All	0.22	1/129818 (0.0%)	0.63	1/190943 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	5	1	G	OP3-P	-10.64	1.48	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2	1565	C	C2-N1-C1'	5.50	124.86	118.80

There are no chirality outliers.

There are no planarity outliers.

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	D	249/260 (96%)	241 (97%)	8 (3%)	0	100	100
2	F	377/406 (93%)	373 (99%)	4 (1%)	0	100	100
3	E	383/389 (98%)	377 (98%)	6 (2%)	0	100	100
4	G	274/301 (91%)	273 (100%)	1 (0%)	0	100	100
5	H	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
6	I	237/242 (98%)	232 (98%)	5 (2%)	0	100	100
7	J	226/258 (88%)	225 (100%)	1 (0%)	0	100	100
8	K	180/194 (93%)	180 (100%)	0	0	100	100
9	L	203/220 (92%)	202 (100%)	1 (0%)	0	100	100
10	M	156/181 (86%)	155 (99%)	1 (1%)	0	100	100
11	N	202/206 (98%)	196 (97%)	6 (3%)	0	100	100
12	O	130/133 (98%)	127 (98%)	3 (2%)	0	100	100
13	P	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
14	Q	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
15	R	153/173 (88%)	150 (98%)	3 (2%)	0	100	100
16	S	184/187 (98%)	181 (98%)	3 (2%)	0	100	100
17	T	144/213 (68%)	144 (100%)	0	0	100	100
18	U	175/178 (98%)	175 (100%)	0	0	100	100
19	V	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
20	W	99/124 (80%)	99 (100%)	0	0	100	100
21	X	129/140 (92%)	127 (98%)	2 (2%)	0	100	100
22	Y	60/165 (36%)	60 (100%)	0	0	100	100
23	Z	115/154 (75%)	114 (99%)	1 (1%)	0	100	100
24	a	130/146 (89%)	129 (99%)	1 (1%)	0	100	100
25	b	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
26	c	145/148 (98%)	139 (96%)	5 (3%)	1 (1%)	22	23
27	d	44/60 (73%)	44 (100%)	0	0	100	100
28	e	93/112 (83%)	92 (99%)	1 (1%)	0	100	100
29	f	108/120 (90%)	107 (99%)	1 (1%)	0	100	100
30	g	125/133 (94%)	122 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	h	109/112 (97%)	109 (100%)	0	0	100	100
32	i	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
33	j	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
34	k	98/110 (89%)	98 (100%)	0	0	100	100
35	l	85/95 (90%)	84 (99%)	1 (1%)	0	100	100
36	m	66/69 (96%)	66 (100%)	0	0	100	100
37	n	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
38	o	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
39	p	97/105 (92%)	96 (99%)	1 (1%)	0	100	100
40	q	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
41	r	140/143 (98%)	138 (99%)	2 (1%)	0	100	100
All	All	6227/6929 (90%)	6146 (99%)	80 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	c	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	194/199 (98%)	193 (100%)	1 (0%)	88	94
2	F	316/332 (95%)	315 (100%)	1 (0%)	92	96
3	E	330/332 (99%)	329 (100%)	1 (0%)	92	96
4	G	232/254 (91%)	232 (100%)	0	100	100
5	H	174/196 (89%)	174 (100%)	0	100	100
6	I	208/210 (99%)	208 (100%)	0	100	100
7	J	198/221 (90%)	198 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	162/170 (95%)	162 (100%)	0	100	100
9	L	170/180 (94%)	170 (100%)	0	100	100
10	M	140/159 (88%)	140 (100%)	0	100	100
11	N	168/170 (99%)	168 (100%)	0	100	100
12	O	114/115 (99%)	114 (100%)	0	100	100
13	P	176/177 (99%)	176 (100%)	0	100	100
14	Q	174/176 (99%)	173 (99%)	1 (1%)	86	93
15	R	135/150 (90%)	135 (100%)	0	100	100
16	S	153/154 (99%)	153 (100%)	0	100	100
17	T	130/179 (73%)	130 (100%)	0	100	100
18	U	163/164 (99%)	163 (100%)	0	100	100
19	V	139/140 (99%)	139 (100%)	0	100	100
20	W	91/106 (86%)	91 (100%)	0	100	100
21	X	103/109 (94%)	103 (100%)	0	100	100
22	Y	57/135 (42%)	57 (100%)	0	100	100
23	Z	106/135 (78%)	106 (100%)	0	100	100
24	a	118/130 (91%)	116 (98%)	2 (2%)	60	72
25	b	115/116 (99%)	115 (100%)	0	100	100
26	c	118/119 (99%)	117 (99%)	1 (1%)	81	89
27	d	41/51 (80%)	41 (100%)	0	100	100
28	e	82/97 (84%)	82 (100%)	0	100	100
29	f	96/105 (91%)	96 (100%)	0	100	100
30	g	115/121 (95%)	115 (100%)	0	100	100
31	h	97/98 (99%)	97 (100%)	0	100	100
32	i	99/104 (95%)	98 (99%)	1 (1%)	76	85
33	j	109/110 (99%)	109 (100%)	0	100	100
34	k	86/92 (94%)	86 (100%)	0	100	100
35	l	72/76 (95%)	72 (100%)	0	100	100
36	m	64/65 (98%)	64 (100%)	0	100	100
37	n	47/48 (98%)	47 (100%)	0	100	100
38	o	47/114 (41%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	p	87/92 (95%)	87 (100%)	0	100	100
40	q	73/74 (99%)	73 (100%)	0	100	100
41	r	122/123 (99%)	122 (100%)	0	100	100
All	All	5421/5898 (92%)	5413 (100%)	8 (0%)	93	97

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	208	GLU
2	F	126	TYR
3	E	369	PHE
14	Q	17	ARG
24	a	2	LYS
24	a	73	TYR
26	c	60	TYR
32	i	44	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	123	GLN
9	L	123	GLN
15	R	143	HIS
17	T	40	ASN
25	b	96	ASN
41	r	103	ASN
41	r	104	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
42	s	1/2 (50%)	1 (100%)	0
43	2	3083/3391 (90%)	314 (10%)	2 (0%)
44	5	119/120 (99%)	8 (6%)	0
45	8	157/165 (95%)	15 (9%)	0
All	All	3360/3678 (91%)	338 (10%)	2 (0%)

All (338) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
42	s	2	A
43	2	38	A
43	2	41	A
43	2	47	A
43	2	58	A
43	2	63	A
43	2	64	A
43	2	68	PSU
43	2	84	G
43	2	90	G
43	2	97	A
43	2	109	C
43	2	114	C
43	2	133	C
43	2	134	G
43	2	154	G
43	2	155	A
43	2	162	U
43	2	167	A
43	2	168	G
43	2	187	U
43	2	197	G
43	2	216	A
43	2	228	U
43	2	235	A
43	2	258	G
43	2	262	A
43	2	283	U
43	2	292	A
43	2	302	U
43	2	320	A
43	2	326	U
43	2	373	G
43	2	394	A
43	2	396	A
43	2	398	U
43	2	418	G
43	2	419	A
43	2	436	C
43	2	445	C
43	2	446	C
43	2	458	G
43	2	465	G

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Mol	Chain	Res	Type
43	2	483	U
43	2	484	C
43	2	488	U
43	2	489	C
43	2	525	A
43	2	538	C
43	2	539	G
43	2	542	A
43	2	544	G
43	2	550	G
43	2	571	U
43	2	589	U
43	2	590	C
43	2	591	C
43	2	592	G
43	2	600	U
43	2	603	G
43	2	607	C
43	2	608	U
43	2	609	G
43	2	620	A
43	2	629	U
43	2	632	G
43	2	647	C
43	2	660	A2M
43	2	671	A
43	2	688	A
43	2	692	A
43	2	693	A
43	2	700	A
43	2	701	G
43	2	728	A
43	2	729	U
43	2	730	U
43	2	732	G
43	2	745	G
43	2	771	A
43	2	777	U
43	2	781	A
43	2	791	G
43	2	795	G
43	2	809	G

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Mol	Chain	Res	Type
43	2	827	A2M
43	2	840	G
43	2	856	A
43	2	859	C
43	2	871	C
43	2	884	U
43	2	889	U
43	2	917	G
43	2	918	OMG
43	2	924	A
43	2	926	G
43	2	927	A
43	2	931	A
43	2	947	G
43	2	954	C
43	2	969	C
43	2	970	PSU
43	2	984	G
43	2	987	C
43	2	1013	C
43	2	1014	A
43	2	1022	G
43	2	1032	G
43	2	1059	A
43	2	1076	A
43	2	1093	U
43	2	1107	G
43	2	1108	G
43	2	1109	A
43	2	1114	A
43	2	1115	G
43	2	1128	G
43	2	1142	G
43	2	1166	C
43	2	1170	A
43	2	1185	G
43	2	1191	C
43	2	1192	U
43	2	1202	C
43	2	1205	A
43	2	1213	C
43	2	1220	U

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Mol	Chain	Res	Type
43	2	1233	A
43	2	1234	G
43	2	1297	G
43	2	1299	A
43	2	1319	G
43	2	1321	U
43	2	1328	U
43	2	1329	A
43	2	1360	A
43	2	1361	A
43	2	1362	G
43	2	1363	U
43	2	1364	G
43	2	1365	C
43	2	1366	C
43	2	1410	U
43	2	1430	G
43	2	1445	G
43	2	1448	OMC
43	2	1454	G
43	2	1457	A
43	2	1466	U
43	2	1492	A
43	2	1513	G
43	2	1518	G
43	2	1547	G
43	2	1566	A
43	2	1571	G
43	2	1585	U
43	2	1592	A
43	2	1594	A
43	2	1598	A
43	2	1602	G
43	2	1625	C
43	2	1633	U
43	2	1647	A
43	2	1649	G
43	2	1661	C
43	2	1691	U
43	2	1696	G
43	2	1729	G
43	2	1755	A

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Mol	Chain	Res	Type
43	2	1756	G
43	2	1763	G
43	2	1803	A
43	2	1820	A
43	2	1827	C
43	2	1848	A
43	2	1856	A
43	2	1872	C
43	2	1884	G
43	2	1885	A
43	2	1886	U
43	2	1899	G
43	2	1912	G
43	2	1949	C
43	2	1959	G
43	2	2118	C
43	2	2126	OMG
43	2	2135	A
43	2	2144	U
43	2	2162	A
43	2	2194	PSU
43	2	2195	C
43	2	2209	G
43	2	2213	G
43	2	2259	A2M
43	2	2261	PSU
43	2	2275	G
43	2	2276	G
43	2	2283	A
43	2	2284	A2M
43	2	2310	G
43	2	2313	U
43	2	2316	A
43	2	2318	G
43	2	2337	U
43	2	2338	G
43	2	2339	U
43	2	2376	A
43	2	2377	C
43	2	2378	G
43	2	2396	G
43	2	2400	A

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Mol	Chain	Res	Type
43	2	2405	A
43	2	2406	G
43	2	2407	A
43	2	2414	U
43	2	2415	G
43	2	2438	G
43	2	2440	G
43	2	2519	U
43	2	2520	A
43	2	2539	G
43	2	2556	U
43	2	2564	A
43	2	2573	U
43	2	2574	U
43	2	2575	C
43	2	2589	G
43	2	2590	G
43	2	2597	A
43	2	2610	G
43	2	2611	G
43	2	2618	G
43	2	2630	A
43	2	2656	U
43	2	2660	A
43	2	2678	A
43	2	2681	G
43	2	2693	G
43	2	2695	A
43	2	2700	A
43	2	2708	A
43	2	2718	G
43	2	2732	G
43	2	2733	OMU
43	2	2757	G
43	2	2759	C
43	2	2776	C
43	2	2781	G
43	2	2782	G
43	2	2800	G
43	2	2803	A
43	2	2804	G
43	2	2805	A

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Mol	Chain	Res	Type
43	2	2814	C
43	2	2818	G
43	2	2821	A
43	2	2849	A
43	2	2857	G
43	2	2875	G
43	2	2876	A
43	2	2879	U
43	2	2891	A
43	2	2939	U
43	2	2940	A
43	2	2946	C
43	2	2951	G
43	2	2975	A
43	2	2987	C
43	2	2994	G
43	2	3000	A
43	2	3015	A
43	2	3061	C
43	2	3062	G
43	2	3081	G
43	2	3082	U
43	2	3095	C
43	2	3096	C
43	2	3125	A
43	2	3133	A
43	2	3134	U
43	2	3145	A
43	2	3156	C
43	2	3157	G
43	2	3164	G
43	2	3176	A
43	2	3177	C
43	2	3180	G
43	2	3186	G
43	2	3196	G
43	2	3202	A
43	2	3209	C
43	2	3210	G
43	2	3213	U
43	2	3216	U
43	2	3222	A

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Mol	Chain	Res	Type
43	2	3223	A
43	2	3237	A
43	2	3241	G
43	2	3273	U
43	2	3274	C
43	2	3276	A
43	2	3287	G
43	2	3297	C
43	2	3312	C
43	2	3313	G
43	2	3330	G
43	2	3334	C
43	2	3338	G
43	2	3362	G
43	2	3371	C
43	2	3375	U
43	2	3383	C
43	2	3384	C
43	2	3385	G
43	2	3391	U
44	5	7	G
44	5	25	G
44	5	38	U
44	5	53	U
44	5	54	A
44	5	64	G
44	5	110	G
44	5	120	U
45	8	28	C
45	8	39	U
45	8	40	C
45	8	64	A
45	8	67	C
45	8	68	U
45	8	85	A
45	8	86	U
45	8	91	U
45	8	92	G
45	8	95	C
45	8	109	A
45	8	111	C
45	8	131	A

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Mol	Chain	Res	Type
45	8	158	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
43	2	926	G
43	2	3124	U

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

129 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$
43	PSU	2	2617	43	18,21,22	0.49	0	22,30,33	0.56	0
43	PSU	2	2263	43	18,21,22	0.48	0	22,30,33	0.56	0
43	PSU	2	1482	43	18,21,22	0.50	0	22,30,33	0.55	0
43	OMG	2	2398	43	18,26,27	0.90	1 (5%)	19,38,41	0.70	0
43	OMG	2	2127	43	18,26,27	0.94	1 (5%)	19,38,41	0.72	0
43	PSU	2	2352	47,43	18,21,22	0.50	0	22,30,33	0.56	0
43	OMG	2	2795	43	18,26,27	0.94	2 (11%)	19,38,41	0.61	0
43	A2M	2	1144	47,43	18,25,26	0.67	0	18,36,39	0.87	1 (5%)
43	A2M	2	2329	43	18,25,26	0.67	0	18,36,39	0.83	1 (5%)
45	A2M	8	48	45	18,25,26	0.68	0	18,36,39	0.83	1 (5%)
43	PSU	2	2979	43	18,21,22	0.48	0	22,30,33	0.57	0
43	PSU	2	2869	43	18,21,22	0.49	0	22,30,33	0.57	0
43	A2M	2	2223	43	18,25,26	0.67	0	18,36,39	0.80	1 (5%)
43	OMU	2	1894	46,43	19,22,23	0.31	0	26,31,34	0.65	0
43	PSU	2	1133	43	18,21,22	0.46	0	22,30,33	0.54	0
43	PSU	2	2257	43	18,21,22	0.47	0	22,30,33	0.57	0
43	OMC	2	2963	43	19,22,23	0.30	0	26,31,34	0.47	0
43	OMC	2	2686	43	19,22,23	0.27	0	26,31,34	0.44	0
43	PSU	2	2317	46,43	18,21,22	0.45	0	22,30,33	0.60	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	OMU	2	1068	43	19,22,23	0.30	0	26,31,34	0.55	0
43	OMU	2	675	43	19,22,23	0.29	0	26,31,34	0.51	0
43	A2M	2	827	47,43	18,25,26	0.65	0	18,36,39	0.87	1 (5%)
43	PSU	2	1230	43	18,21,22	0.45	0	22,30,33	0.59	0
43	PSU	2	2435	43	18,21,22	0.47	0	22,30,33	0.56	0
43	OMU	2	2350	46,43	19,22,23	0.31	0	26,31,34	0.42	0
43	A2M	2	1460	47,43	18,25,26	0.68	0	18,36,39	0.77	1 (5%)
43	PSU	2	2716	43	18,21,22	0.52	0	22,30,33	0.62	1 (4%)
43	OMC	2	2368	43	19,22,23	0.29	0	26,31,34	0.42	0
43	PSU	2	35	43	18,21,22	0.45	0	22,30,33	0.56	0
43	PSU	2	1474	43	18,21,22	0.48	0	22,30,33	0.56	0
43	A2M	2	817	43	18,25,26	0.66	0	18,36,39	0.76	1 (5%)
43	PSU	2	2194	43	18,21,22	0.53	0	22,30,33	0.52	0
43	OMC	2	2340	43	19,22,23	0.28	0	26,31,34	0.45	0
43	OMU	2	2413	46,43	19,22,23	0.29	0	26,31,34	0.39	0
45	PSU	8	23	45,43	18,21,22	0.48	0	22,30,33	0.53	0
43	5MC	2	2874	46,43	18,22,23	0.44	0	26,32,35	0.53	0
43	PSU	2	2269	43	18,21,22	0.46	0	22,30,33	0.57	0
43	A2M	2	2644	43	18,25,26	0.66	0	18,36,39	0.71	1 (5%)
43	OMU	2	2116	43	19,22,23	0.25	0	26,31,34	0.41	0
43	OMU	2	2887	43	19,22,23	0.30	0	26,31,34	0.55	0
43	OMG	2	2623	47,43	18,26,27	0.91	2 (11%)	19,38,41	0.60	0
43	PSU	2	2996	43	18,21,22	0.55	0	22,30,33	0.50	0
43	PSU	2	378	43	18,21,22	0.48	0	22,30,33	0.57	0
43	OMC	2	1480	43	19,22,23	0.24	0	26,31,34	0.38	0
43	PSU	2	1909	47,46,43	18,21,22	0.47	0	22,30,33	0.53	0
43	OMG	2	1857	46,43	18,26,27	0.95	2 (11%)	19,38,41	0.62	0
43	OMC	2	2952	43	19,22,23	0.28	0	26,31,34	0.37	0
43	PSU	2	2321	47,43	18,21,22	0.49	0	22,30,33	0.53	0
43	PSU	2	2748	43	18,21,22	0.48	0	22,30,33	0.55	0
43	PSU	2	1134	43	18,21,22	0.47	0	22,30,33	0.59	0
43	OMG	2	399	43	18,26,27	0.90	1 (5%)	19,38,41	0.70	0
43	PSU	2	3114	43	18,21,22	0.48	0	22,30,33	0.56	0
43	OMC	2	2296	43	19,22,23	0.28	0	26,31,34	0.43	0
43	PSU	2	2419	47,43	18,21,22	0.49	0	22,30,33	0.57	0
43	1MA	2	656	47,43	16,25,26	1.15	3 (18%)	18,37,40	0.82	1 (5%)
43	PSU	2	2139	43	18,21,22	0.50	0	22,30,33	0.55	0
43	OMC	2	2840	43	19,22,23	0.27	0	26,31,34	0.36	0
43	OMU	2	48	43	19,22,23	0.27	0	26,31,34	0.40	0
43	A2M	2	2915	43	18,25,26	0.65	0	18,36,39	0.76	1 (5%)
43	OMU	2	2925	47,43	19,22,23	0.28	0	26,31,34	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	A2M	2	369	43	18,25,26	0.65	0	18,36,39	0.71	1 (5%)
43	OMU	2	44	46,43	19,22,23	0.27	0	26,31,34	0.39	0
43	OMC	2	1852	47,43	19,22,23	0.27	0	26,31,34	0.41	0
43	A2M	2	660	43	18,25,26	0.66	0	18,36,39	0.75	1 (5%)
43	PSU	2	2898	43	18,21,22	0.51	0	22,30,33	0.53	0
43	PSU	2	2830	43	18,21,22	0.50	0	22,30,33	0.56	0
43	OMC	2	1862	43	19,22,23	0.29	0	26,31,34	0.40	0
43	OMU	2	804	43	19,22,23	0.29	0	26,31,34	0.50	0
43	PSU	2	2847	43	18,21,22	0.47	0	22,30,33	0.59	1 (4%)
43	OMC	2	1448	47,43	19,22,23	0.30	0	26,31,34	0.40	0
43	OMG	2	2797	43	18,26,27	0.93	1 (5%)	19,38,41	0.63	0
43	OMC	2	2883	43	19,22,23	0.28	0	26,31,34	0.39	0
3	HIC	E	246	3	8,11,12	0.80	0	6,14,16	0.58	0
43	PSU	2	970	43	18,21,22	0.52	0	22,30,33	0.65	1 (4%)
43	PSU	2	2214	43	18,21,22	0.49	0	22,30,33	0.55	0
43	OMU	2	2424	43	19,22,23	0.30	0	26,31,34	0.53	0
43	OMU	2	2733	43	19,22,23	0.30	0	26,31,34	0.45	0
43	PSU	2	2261	43	18,21,22	0.50	0	22,30,33	0.54	0
43	OMG	2	918	46,43	18,26,27	0.97	2 (11%)	19,38,41	0.60	0
45	PSU	8	79	45	18,21,22	0.47	0	22,30,33	0.56	0
43	OMG	2	2126	43	18,26,27	0.96	1 (5%)	19,38,41	0.68	0
43	PSU	2	1002	43	18,21,22	0.47	0	22,30,33	0.58	0
43	OMU	2	2739	47,43	19,22,23	0.30	0	26,31,34	0.46	0
43	OMC	2	674	43	19,22,23	0.27	0	26,31,34	0.45	0
43	OMC	2	2200	46,43	19,22,23	0.26	0	26,31,34	0.59	0
43	PSU	2	2858	43	18,21,22	0.49	0	22,30,33	0.55	0
43	PSU	2	2927	43	18,21,22	0.45	0	22,30,33	0.59	0
43	PSU	2	2521	43	18,21,22	0.50	0	22,30,33	0.58	0
43	PSU	2	1135	43	18,21,22	0.45	0	22,30,33	0.59	0
43	PSU	2	2959	43	18,21,22	0.49	0	22,30,33	0.55	0
43	A2M	2	886	43	18,25,26	0.66	0	18,36,39	0.74	1 (5%)
43	PSU	2	1054	43	18,21,22	0.46	0	22,30,33	0.58	0
43	OMG	2	815	43	18,26,27	0.93	2 (11%)	19,38,41	0.65	0
43	PSU	2	895	43	18,21,22	0.53	0	22,30,33	0.55	0
43	A2M	2	946	43	18,25,26	0.66	0	18,36,39	0.76	1 (5%)
43	OMU	2	2654	43	19,22,23	0.29	0	26,31,34	0.43	0
45	OMG	8	80	45	18,26,27	0.91	1 (5%)	19,38,41	0.62	0
43	A2M	2	2129	43	18,25,26	0.68	0	18,36,39	0.74	1 (5%)
41	THC	r	2	41	8,9,10	0.27	0	9,11,13	0.50	0
43	OMU	2	1537	46,43	19,22,23	0.24	0	26,31,34	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	OMG	2	2926	43	18,26,27	0.91	1 (5%)	19,38,41	0.64	0
43	OMG	2	2239	43	18,26,27	0.91	1 (5%)	19,38,41	0.62	0
43	OMG	2	2412	47,43	18,26,27	0.90	1 (5%)	19,38,41	0.64	0
43	A2M	2	2284	43	18,25,26	0.68	0	18,36,39	0.88	1 (5%)
43	A2M	2	2324	43	18,25,26	0.67	0	18,36,39	0.82	1 (5%)
43	UR3	2	2957	43	19,22,23	0.30	0	26,32,35	0.33	0
43	OMG	2	2394	43	18,26,27	0.95	1 (5%)	19,38,41	0.60	0
43	OMG	2	2291	43	18,26,27	0.93	2 (11%)	19,38,41	0.59	0
43	OMU	2	2721	43	19,22,23	0.29	0	26,31,34	0.46	0
43	PSU	2	1064	46,43	18,21,22	0.44	0	22,30,33	0.58	0
43	OMG	2	1461	43	18,26,27	0.93	1 (5%)	19,38,41	0.66	0
43	5MC	2	2281	47,43	18,22,23	0.30	0	26,32,35	0.43	0
43	OMG	2	2819	43	18,26,27	0.89	1 (5%)	19,38,41	0.61	0
43	PSU	2	2884	43	18,21,22	0.50	0	22,30,33	0.55	0
43	A2M	2	2950	47,46,43	18,25,26	0.69	0	18,36,39	0.92	1 (5%)
43	OMU	2	3305	43	19,22,23	0.30	0	26,31,34	0.41	0
43	OMG	2	2655	43	18,26,27	0.93	2 (11%)	19,38,41	0.70	0
43	PSU	2	2137	46,43	18,21,22	0.45	0	22,30,33	0.60	0
43	OMG	2	2921	43	18,26,27	0.95	2 (11%)	19,38,41	0.64	0
43	PSU	2	2228	43	18,21,22	0.53	0	22,30,33	0.51	0
43	OMC	2	1849	43	19,22,23	0.27	0	26,31,34	0.40	0
43	PSU	2	829	43	18,21,22	0.49	0	22,30,33	0.59	0
43	PSU	2	68	43	18,21,22	0.51	0	22,30,33	0.58	0
43	A2M	2	2259	43	18,25,26	0.65	0	18,36,39	0.72	1 (5%)
43	PSU	2	2267	43	18,21,22	0.47	0	22,30,33	0.56	0
43	PSU	2	2948	47,46,43	18,21,22	0.51	0	22,30,33	0.61	1 (4%)
43	OMU	2	144	43	19,22,23	0.25	0	26,31,34	0.40	0
43	PSU	2	1016	46,43	18,21,22	0.48	0	22,30,33	0.58	0
43	A2M	2	1378	47,43	18,25,26	0.65	0	18,36,39	0.72	1 (5%)

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
43	PSU	2	2617	43	-	0/7/25/26	0/2/2/2
43	PSU	2	2263	43	-	0/7/25/26	0/2/2/2
43	PSU	2	1482	43	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	OMG	2	2398	43	-	0/5/27/28	0/3/3/3
43	OMG	2	2127	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2352	47,43	-	0/7/25/26	0/2/2/2
43	OMG	2	2795	43	-	0/5/27/28	0/3/3/3
43	A2M	2	1144	47,43	-	0/5/27/28	0/3/3/3
43	A2M	2	2329	43	-	0/5/27/28	0/3/3/3
45	A2M	8	48	45	-	0/5/27/28	0/3/3/3
43	PSU	2	2979	43	-	0/7/25/26	0/2/2/2
43	PSU	2	2869	43	-	0/7/25/26	0/2/2/2
43	A2M	2	2223	43	-	0/5/27/28	0/3/3/3
43	OMU	2	1894	46,43	-	0/9/27/28	0/2/2/2
43	PSU	2	1133	43	-	0/7/25/26	0/2/2/2
43	PSU	2	2257	43	-	0/7/25/26	0/2/2/2
43	OMC	2	2963	43	-	0/9/27/28	0/2/2/2
43	OMC	2	2686	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2317	46,43	-	1/7/25/26	0/2/2/2
43	OMU	2	1068	43	-	0/9/27/28	0/2/2/2
43	OMU	2	675	43	-	0/9/27/28	0/2/2/2
43	A2M	2	827	47,43	-	2/5/27/28	0/3/3/3
43	PSU	2	1230	43	-	0/7/25/26	0/2/2/2
43	PSU	2	2435	43	-	0/7/25/26	0/2/2/2
43	OMU	2	2350	46,43	-	0/9/27/28	0/2/2/2
43	A2M	2	1460	47,43	-	0/5/27/28	0/3/3/3
43	PSU	2	2716	43	-	0/7/25/26	0/2/2/2
43	OMC	2	2368	43	-	0/9/27/28	0/2/2/2
43	PSU	2	35	43	-	0/7/25/26	0/2/2/2
43	PSU	2	1474	43	-	0/7/25/26	0/2/2/2
43	A2M	2	817	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2194	43	-	2/7/25/26	0/2/2/2
43	OMC	2	2340	43	-	0/9/27/28	0/2/2/2
43	OMU	2	2413	46,43	-	0/9/27/28	0/2/2/2
45	PSU	8	23	45,43	-	0/7/25/26	0/2/2/2
43	5MC	2	2874	46,43	-	2/7/25/26	0/2/2/2
43	PSU	2	2269	43	-	0/7/25/26	0/2/2/2
43	A2M	2	2644	43	-	0/5/27/28	0/3/3/3
43	OMU	2	2116	43	-	0/9/27/28	0/2/2/2
43	OMU	2	2887	43	-	0/9/27/28	0/2/2/2
43	OMG	2	2623	47,43	-	0/5/27/28	0/3/3/3
43	PSU	2	2996	43	-	0/7/25/26	0/2/2/2
43	PSU	2	378	43	-	0/7/25/26	0/2/2/2
43	OMC	2	1480	43	-	0/9/27/28	0/2/2/2
43	PSU	2	1909	47,46,43	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	OMG	2	1857	46,43	-	0/5/27/28	0/3/3/3
43	OMC	2	2952	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2321	47,43	-	0/7/25/26	0/2/2/2
43	PSU	2	2748	43	-	0/7/25/26	0/2/2/2
43	PSU	2	1134	43	-	0/7/25/26	0/2/2/2
43	OMG	2	399	43	-	0/5/27/28	0/3/3/3
43	PSU	2	3114	43	-	0/7/25/26	0/2/2/2
43	OMC	2	2296	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2419	47,43	-	0/7/25/26	0/2/2/2
43	1MA	2	656	47,43	-	0/3/25/26	0/3/3/3
43	PSU	2	2139	43	-	0/7/25/26	0/2/2/2
43	OMC	2	2840	43	-	0/9/27/28	0/2/2/2
43	OMU	2	48	43	-	0/9/27/28	0/2/2/2
43	A2M	2	2915	43	-	1/5/27/28	0/3/3/3
43	OMU	2	2925	47,43	-	0/9/27/28	0/2/2/2
43	A2M	2	369	43	-	0/5/27/28	0/3/3/3
43	OMU	2	44	46,43	-	0/9/27/28	0/2/2/2
43	OMC	2	1852	47,43	-	2/9/27/28	0/2/2/2
43	A2M	2	660	43	-	1/5/27/28	0/3/3/3
43	PSU	2	2898	43	-	0/7/25/26	0/2/2/2
43	PSU	2	2830	43	-	0/7/25/26	0/2/2/2
43	OMC	2	1862	43	-	0/9/27/28	0/2/2/2
43	OMU	2	804	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2847	43	-	0/7/25/26	0/2/2/2
43	OMC	2	1448	47,43	-	1/9/27/28	0/2/2/2
43	OMG	2	2797	43	-	0/5/27/28	0/3/3/3
43	OMC	2	2883	43	-	0/9/27/28	0/2/2/2
3	HIC	E	246	3	-	0/5/6/8	0/1/1/1
43	PSU	2	970	43	-	2/7/25/26	0/2/2/2
43	PSU	2	2214	43	-	0/7/25/26	0/2/2/2
43	OMU	2	2424	43	-	0/9/27/28	0/2/2/2
43	OMU	2	2733	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2261	43	-	2/7/25/26	0/2/2/2
43	OMG	2	918	46,43	-	1/5/27/28	0/3/3/3
45	PSU	8	79	45	-	0/7/25/26	0/2/2/2
43	OMG	2	2126	43	-	3/5/27/28	0/3/3/3
43	PSU	2	1002	43	-	0/7/25/26	0/2/2/2
43	OMU	2	2739	47,43	-	0/9/27/28	0/2/2/2
43	OMC	2	674	43	-	0/9/27/28	0/2/2/2
43	OMC	2	2200	46,43	-	4/9/27/28	0/2/2/2
43	PSU	2	2858	43	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	PSU	2	2927	43	-	1/7/25/26	0/2/2/2
43	PSU	2	2521	43	-	0/7/25/26	0/2/2/2
43	PSU	2	1135	43	-	0/7/25/26	0/2/2/2
43	PSU	2	2959	43	-	0/7/25/26	0/2/2/2
43	A2M	2	886	43	-	0/5/27/28	0/3/3/3
43	PSU	2	1054	43	-	0/7/25/26	0/2/2/2
43	OMG	2	815	43	-	0/5/27/28	0/3/3/3
43	PSU	2	895	43	-	0/7/25/26	0/2/2/2
43	A2M	2	946	43	-	0/5/27/28	0/3/3/3
43	OMU	2	2654	43	-	0/9/27/28	0/2/2/2
45	OMG	8	80	45	-	0/5/27/28	0/3/3/3
43	A2M	2	2129	43	-	0/5/27/28	0/3/3/3
41	THC	r	2	41	-	4/8/10/12	-
43	OMU	2	1537	46,43	-	0/9/27/28	0/2/2/2
43	OMG	2	2926	43	-	0/5/27/28	0/3/3/3
43	OMG	2	2239	43	-	0/5/27/28	0/3/3/3
43	OMG	2	2412	47,43	-	0/5/27/28	0/3/3/3
43	A2M	2	2284	43	-	2/5/27/28	0/3/3/3
43	A2M	2	2324	43	-	0/5/27/28	0/3/3/3
43	UR3	2	2957	43	-	0/7/25/26	0/2/2/2
43	OMG	2	2394	43	-	0/5/27/28	0/3/3/3
43	OMG	2	2291	43	-	0/5/27/28	0/3/3/3
43	OMU	2	2721	43	-	0/9/27/28	0/2/2/2
43	PSU	2	1064	46,43	-	0/7/25/26	0/2/2/2
43	OMG	2	1461	43	-	1/5/27/28	0/3/3/3
43	5MC	2	2281	47,43	-	0/7/25/26	0/2/2/2
43	OMG	2	2819	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2884	43	-	0/7/25/26	0/2/2/2
43	A2M	2	2950	47,46,43	-	0/5/27/28	0/3/3/3
43	OMU	2	3305	43	-	0/9/27/28	0/2/2/2
43	OMG	2	2655	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2137	46,43	-	0/7/25/26	0/2/2/2
43	OMG	2	2921	43	-	1/5/27/28	0/3/3/3
43	PSU	2	2228	43	-	1/7/25/26	0/2/2/2
43	OMC	2	1849	43	-	0/9/27/28	0/2/2/2
43	PSU	2	829	43	-	0/7/25/26	0/2/2/2
43	PSU	2	68	43	-	2/7/25/26	0/2/2/2
43	A2M	2	2259	43	-	1/5/27/28	0/3/3/3
43	PSU	2	2267	43	-	0/7/25/26	0/2/2/2
43	PSU	2	2948	47,46,43	-	0/7/25/26	0/2/2/2
43	OMU	2	144	43	-	1/9/27/28	0/2/2/2
43	PSU	2	1016	46,43	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A2M	2	1378	47,43	-	0/5/27/28	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	656	1MA	C6-N6	2.95	1.35	1.27
43	2	2795	OMG	C5-C6	-2.38	1.42	1.47
43	2	918	OMG	C5-C6	-2.38	1.42	1.47
43	2	2126	OMG	C5-C6	-2.35	1.42	1.47
43	2	1857	OMG	C5-C6	-2.32	1.42	1.47
43	2	2394	OMG	C5-C6	-2.29	1.42	1.47
43	2	2127	OMG	C5-C6	-2.27	1.42	1.47
43	2	2921	OMG	C5-C6	-2.26	1.42	1.47
43	2	2797	OMG	C5-C6	-2.24	1.42	1.47
43	2	2291	OMG	C5-C6	-2.23	1.42	1.47
43	2	2655	OMG	C5-C6	-2.19	1.43	1.47
43	2	2239	OMG	C5-C6	-2.19	1.43	1.47
45	8	80	OMG	C5-C6	-2.18	1.43	1.47
43	2	2623	OMG	C5-C6	-2.17	1.43	1.47
43	2	815	OMG	C5-C6	-2.14	1.43	1.47
43	2	2412	OMG	C5-C6	-2.14	1.43	1.47
43	2	1461	OMG	C5-C6	-2.14	1.43	1.47
43	2	2926	OMG	C5-C6	-2.12	1.43	1.47
43	2	918	OMG	C8-N7	-2.11	1.31	1.35
43	2	656	1MA	C5-C4	-2.10	1.37	1.43
43	2	656	1MA	C8-N7	-2.10	1.31	1.35
43	2	1857	OMG	C8-N7	-2.08	1.31	1.35
43	2	2921	OMG	C8-N7	-2.07	1.31	1.35
43	2	2623	OMG	C8-N7	-2.07	1.31	1.35
43	2	815	OMG	C8-N7	-2.05	1.31	1.35
43	2	2291	OMG	C8-N7	-2.04	1.31	1.35
43	2	2398	OMG	C5-C4	-2.03	1.37	1.43
43	2	2795	OMG	C8-N7	-2.02	1.31	1.35
43	2	399	OMG	C5-C6	-2.01	1.43	1.47
43	2	2819	OMG	C5-C6	-2.01	1.43	1.47
43	2	2655	OMG	C5-C4	-2.00	1.38	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2	886	A2M	C5-C6-N6	2.40	124.00	120.35
43	2	827	A2M	C5-C6-N6	2.37	123.95	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2	2915	A2M	C5-C6-N6	2.36	123.94	120.35
43	2	1378	A2M	C5-C6-N6	2.36	123.93	120.35
43	2	2223	A2M	C5-C6-N6	2.35	123.92	120.35
43	2	946	A2M	C5-C6-N6	2.34	123.91	120.35
43	2	2324	A2M	C5-C6-N6	2.33	123.89	120.35
43	2	660	A2M	C5-C6-N6	2.33	123.89	120.35
43	2	369	A2M	C5-C6-N6	2.33	123.89	120.35
43	2	2950	A2M	C5-C6-N6	2.32	123.88	120.35
43	2	2259	A2M	C5-C6-N6	2.31	123.87	120.35
43	2	2284	A2M	C5-C6-N6	2.31	123.86	120.35
45	8	48	A2M	C5-C6-N6	2.29	123.83	120.35
43	2	2129	A2M	C5-C6-N6	2.28	123.82	120.35
43	2	2329	A2M	C5-C6-N6	2.28	123.82	120.35
43	2	2644	A2M	C5-C6-N6	2.28	123.82	120.35
43	2	817	A2M	C5-C6-N6	2.28	123.82	120.35
43	2	1460	A2M	C5-C6-N6	2.27	123.80	120.35
43	2	1144	A2M	C5-C6-N6	2.25	123.77	120.35
43	2	2948	PSU	O4'-C1'-C2'	2.19	108.23	105.14
43	2	2716	PSU	O4'-C1'-C2'	2.18	108.22	105.14
43	2	970	PSU	O4'-C1'-C2'	2.11	108.12	105.14
43	2	2847	PSU	O4'-C1'-C2'	2.03	108.00	105.14
43	2	2317	PSU	O4'-C1'-C2'	2.01	107.98	105.14
43	2	656	1MA	N1-C6-N6	2.00	124.87	119.77

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	r	2	THC	N-CA-CB-OG1
41	r	2	THC	N-CA-CB-CG2
41	r	2	THC	C-CA-CB-OG1
41	r	2	THC	C-CA-CB-CG2
43	2	918	OMG	C3'-C2'-O2'-CM2
43	2	970	PSU	C2'-C1'-C5-C6
43	2	1852	OMC	C1'-C2'-O2'-CM2
43	2	2194	PSU	C3'-C4'-C5'-O5'
43	2	2259	A2M	O4'-C4'-C5'-O5'
43	2	2261	PSU	C3'-C4'-C5'-O5'
43	2	2915	A2M	C1'-C2'-O2'-CM'
43	2	68	PSU	O4'-C4'-C5'-O5'
43	2	2126	OMG	O4'-C4'-C5'-O5'
43	2	2194	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
43	2	2261	PSU	O4'-C4'-C5'-O5'
43	2	68	PSU	C3'-C4'-C5'-O5'
43	2	2126	OMG	C3'-C4'-C5'-O5'
43	2	2200	OMC	C2'-C1'-N1-C6
43	2	2200	OMC	C2'-C1'-N1-C2
43	2	2284	A2M	O4'-C4'-C5'-O5'
43	2	2284	A2M	C3'-C4'-C5'-O5'
43	2	2317	PSU	C4'-C5'-O5'-P
43	2	2200	OMC	O4'-C1'-N1-C2
43	2	2200	OMC	O4'-C1'-N1-C6
43	2	827	A2M	C4'-C5'-O5'-P
43	2	2927	PSU	C4'-C5'-O5'-P
43	2	1461	OMG	O4'-C4'-C5'-O5'
43	2	660	A2M	C4'-C5'-O5'-P
43	2	2126	OMG	C4'-C5'-O5'-P
43	2	2228	PSU	C3'-C4'-C5'-O5'
43	2	144	OMU	O4'-C4'-C5'-O5'
43	2	827	A2M	O4'-C4'-C5'-O5'
43	2	2874	5MC	O4'-C1'-N1-C6
43	2	2874	5MC	C2'-C1'-N1-C6
43	2	970	PSU	O4'-C1'-C5-C6
43	2	1448	OMC	O4'-C4'-C5'-O5'
43	2	2921	OMG	C3'-C2'-O2'-CM2
43	2	1852	OMC	O4'-C1'-N1-C6

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 374 ligands modelled in this entry, 370 are monoatomic - leaving 4 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	$\# Z > 2$
49	SPM	2	3483	-	13,13,13	0.29	0	12,12,12	0.95	0
49	SPM	2	3480	-	13,13,13	0.29	0	12,12,12	0.90	0
50	SPD	2	3482	-	9,9,9	0.27	0	8,8,8	0.88	0
49	SPM	2	3481	-	13,13,13	0.31	0	12,12,12	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	SPM	2	3483	-	-	3/11/11/11	-
49	SPM	2	3480	-	-	1/11/11/11	-
50	SPD	2	3482	-	-	0/7/7/7	-
49	SPM	2	3481	-	-	0/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	2	3483	SPM	N5-C6-C7-C8
49	2	3480	SPM	C7-C8-C9-N10
49	2	3483	SPM	C3-C4-N5-C6
49	2	3483	SPM	C7-C6-N5-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

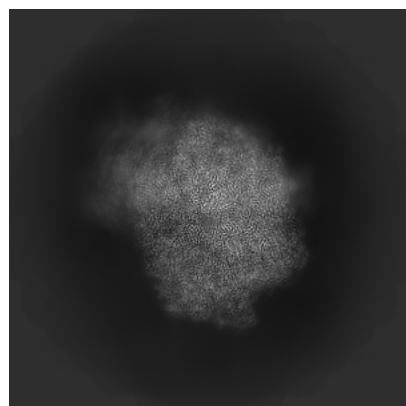
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14001. These allow visual inspection of the internal detail of the map and identification of artifacts.

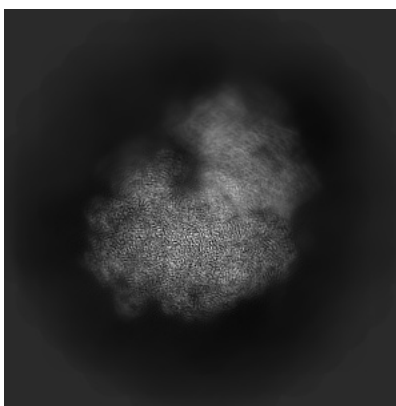
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

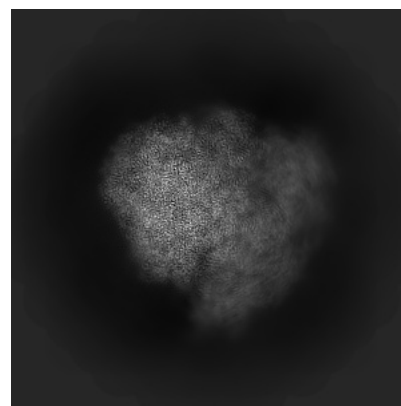
6.1.1 Primary map



X

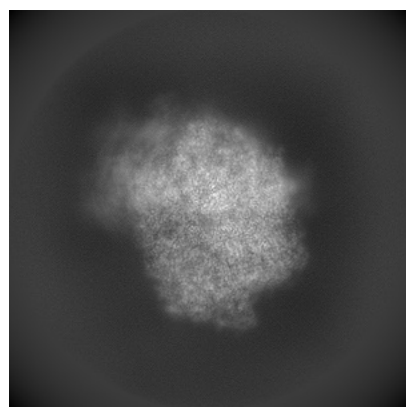


Y

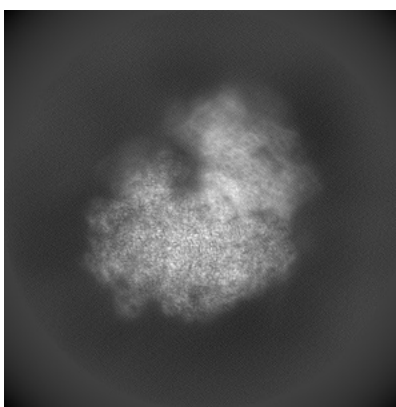


Z

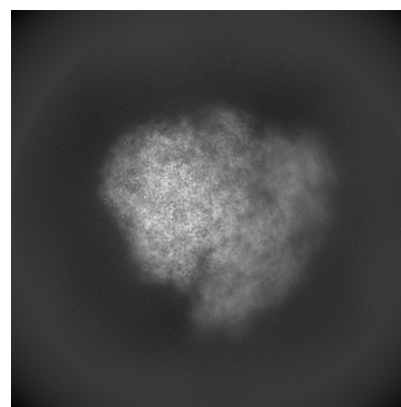
6.1.2 Raw map



X



Y

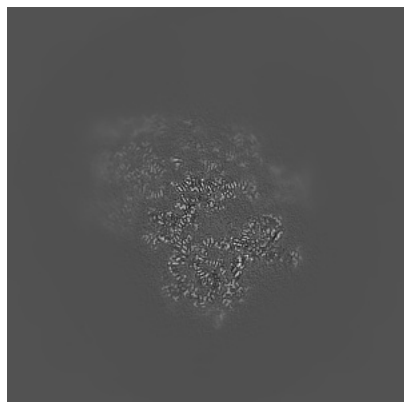


Z

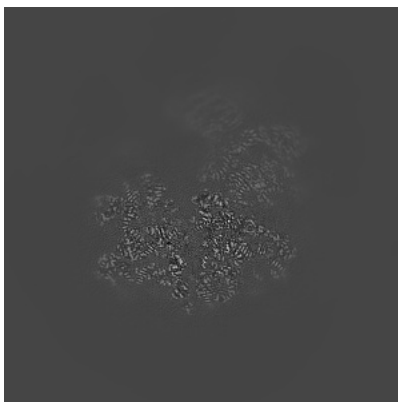
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

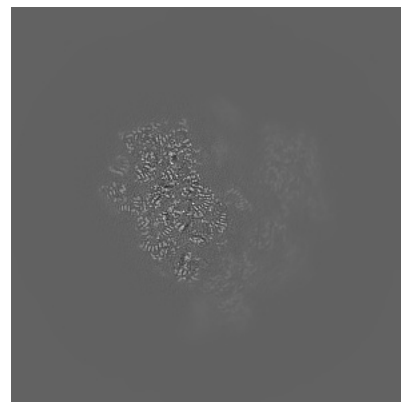
6.2.1 Primary map



X Index: 270

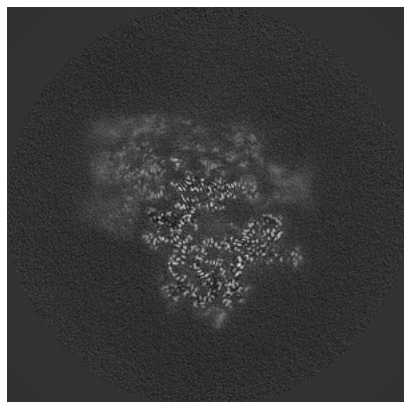


Y Index: 270

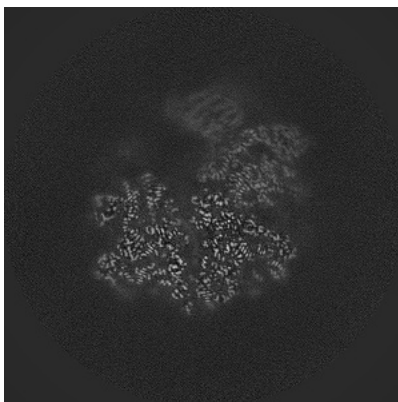


Z Index: 270

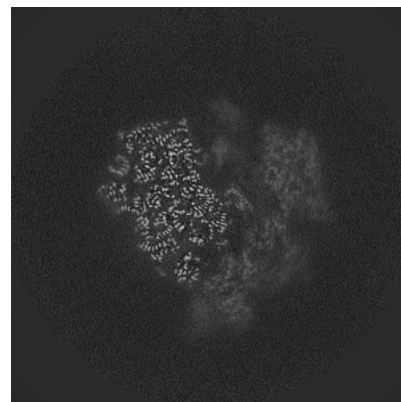
6.2.2 Raw map



X Index: 270



Y Index: 270

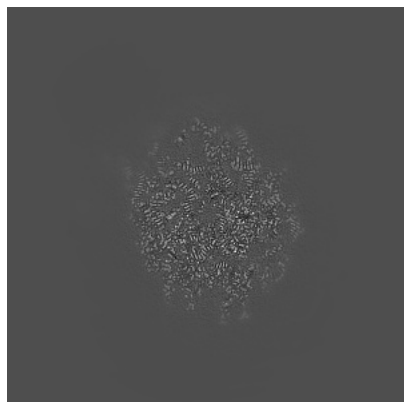


Z Index: 270

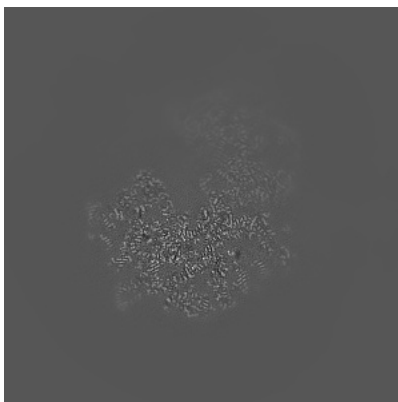
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

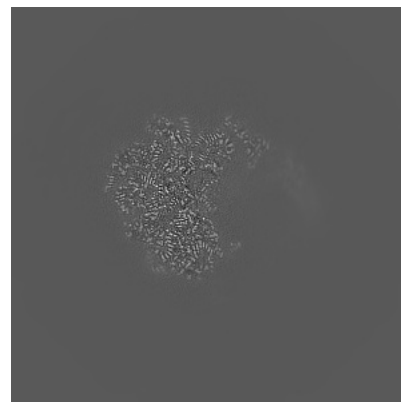
6.3.1 Primary map



X Index: 232

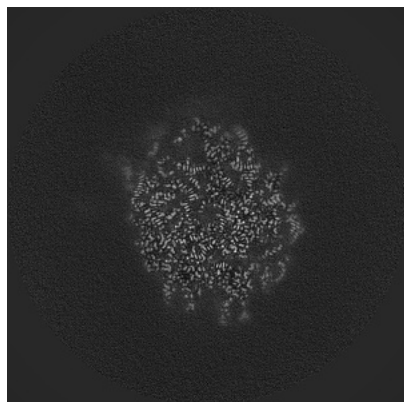


Y Index: 289

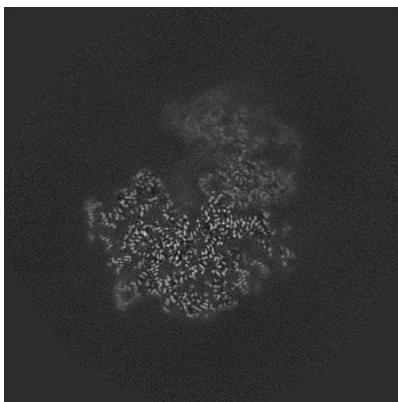


Z Index: 228

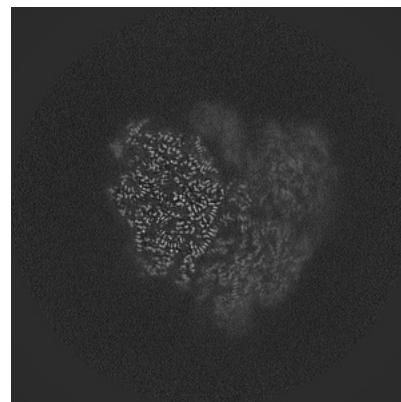
6.3.2 Raw map



X Index: 232



Y Index: 288

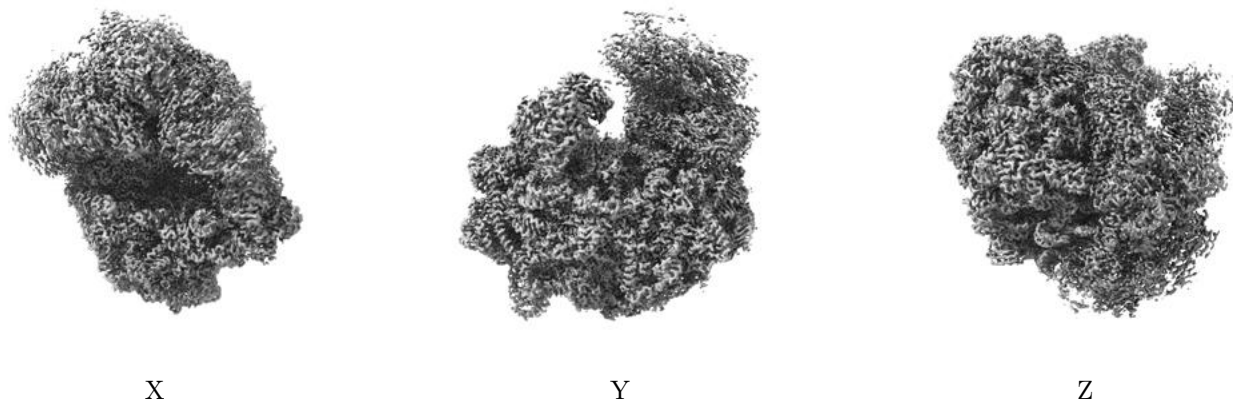


Z Index: 294

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

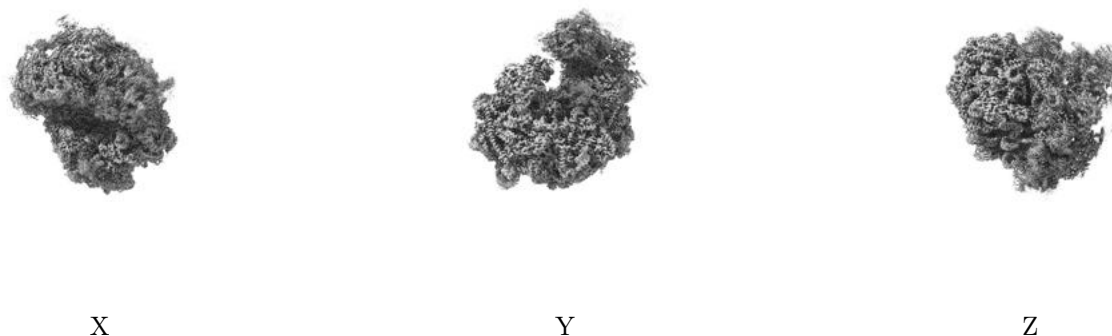
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0328. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

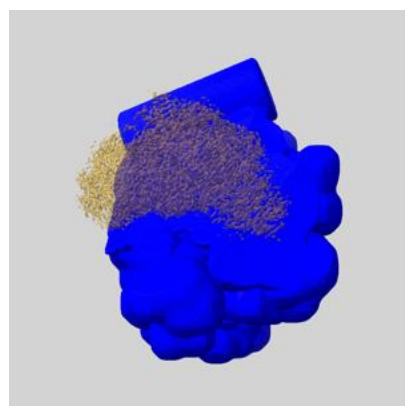
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

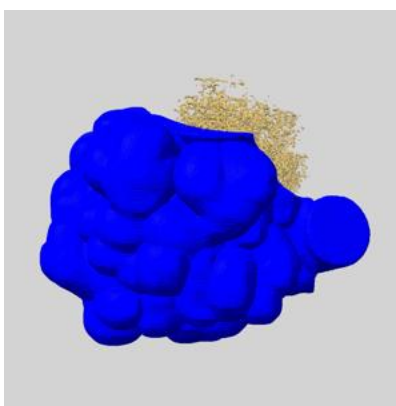
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

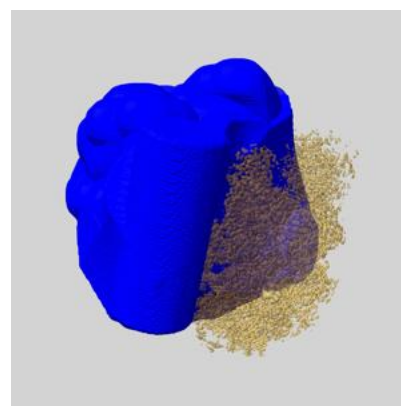
6.5.1 emd_14001_msk_1.map [i](#)



X



Y

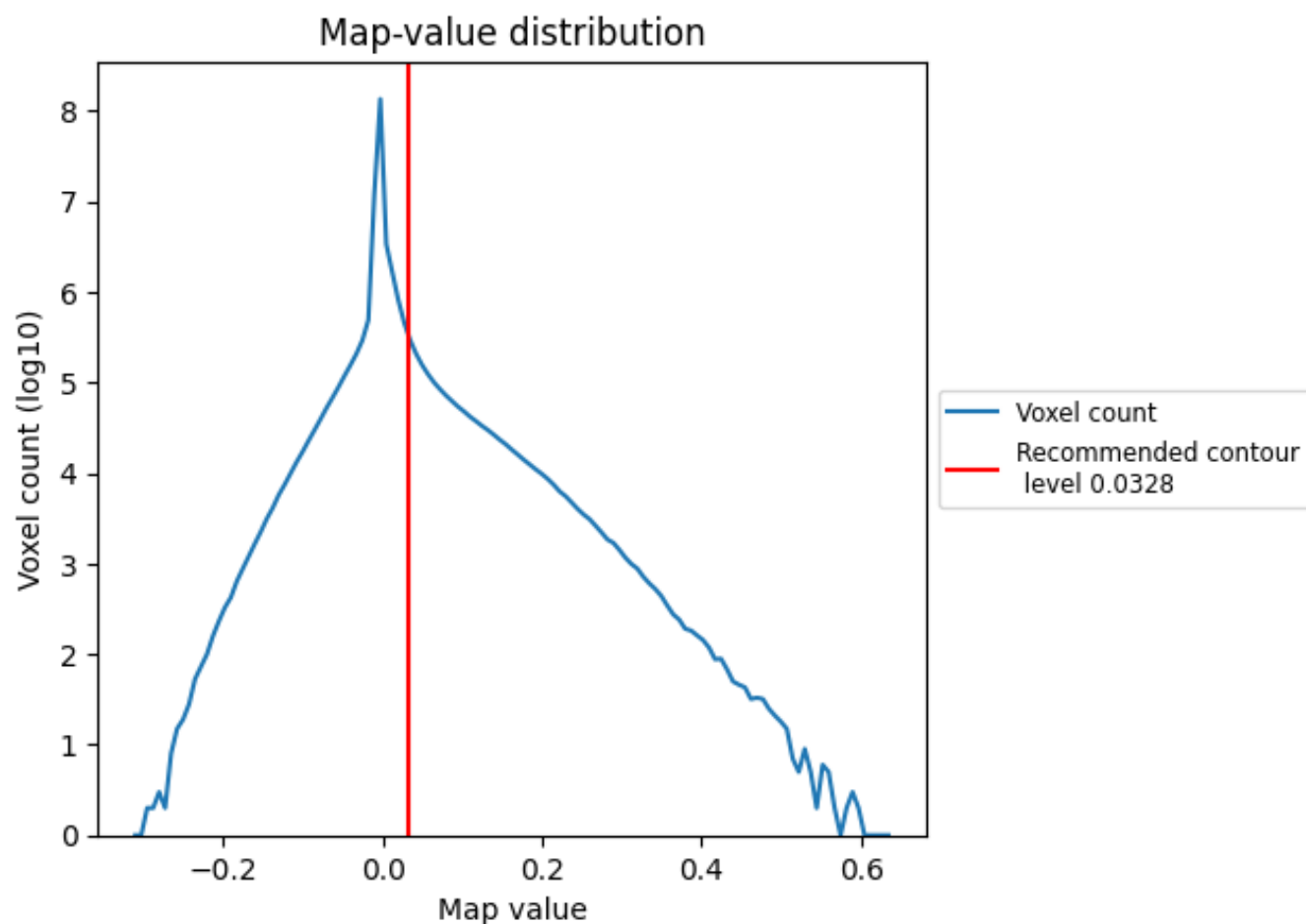


Z

7 Map analysis [i](#)

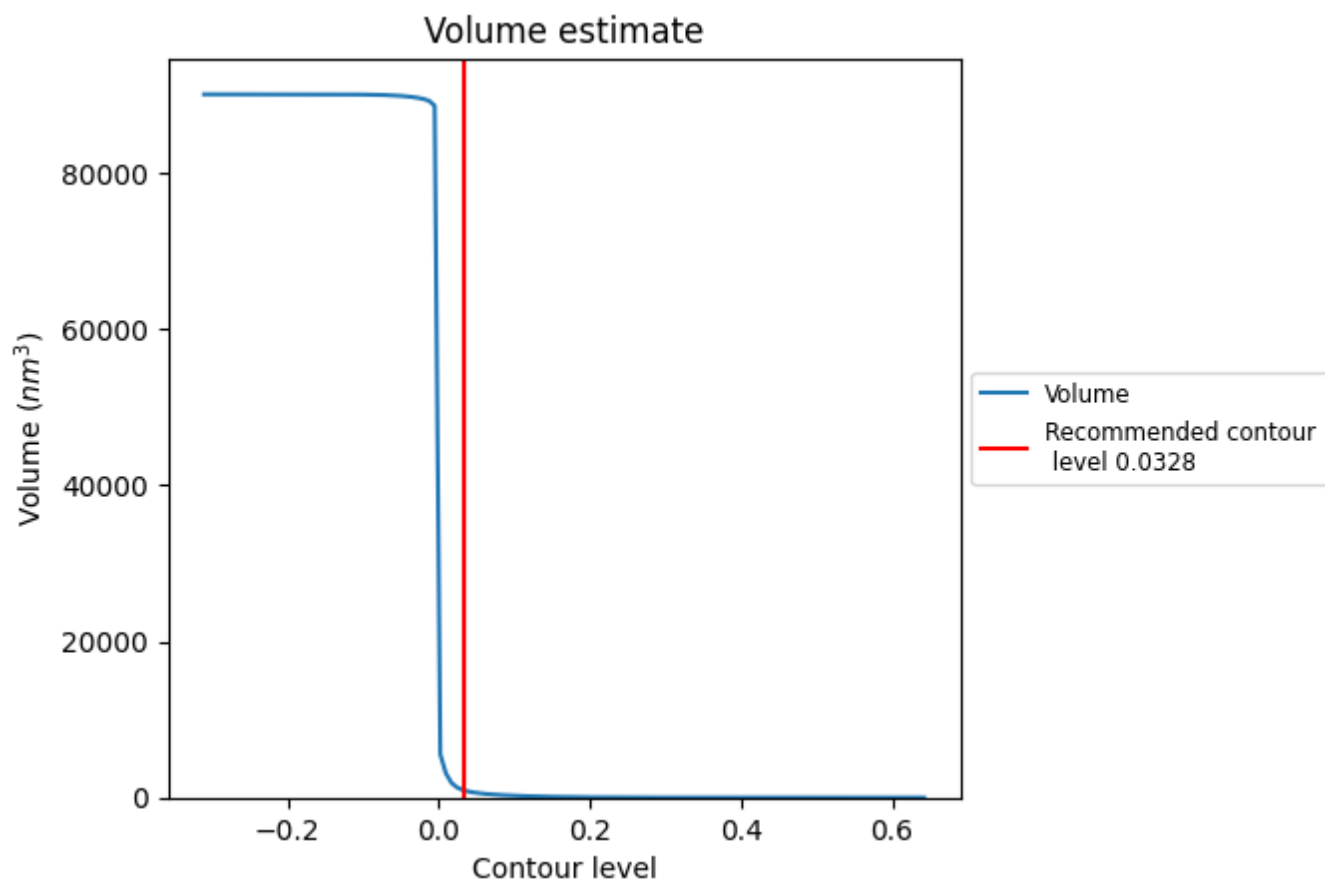
This section contains the results of statistical analysis of the map.

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.

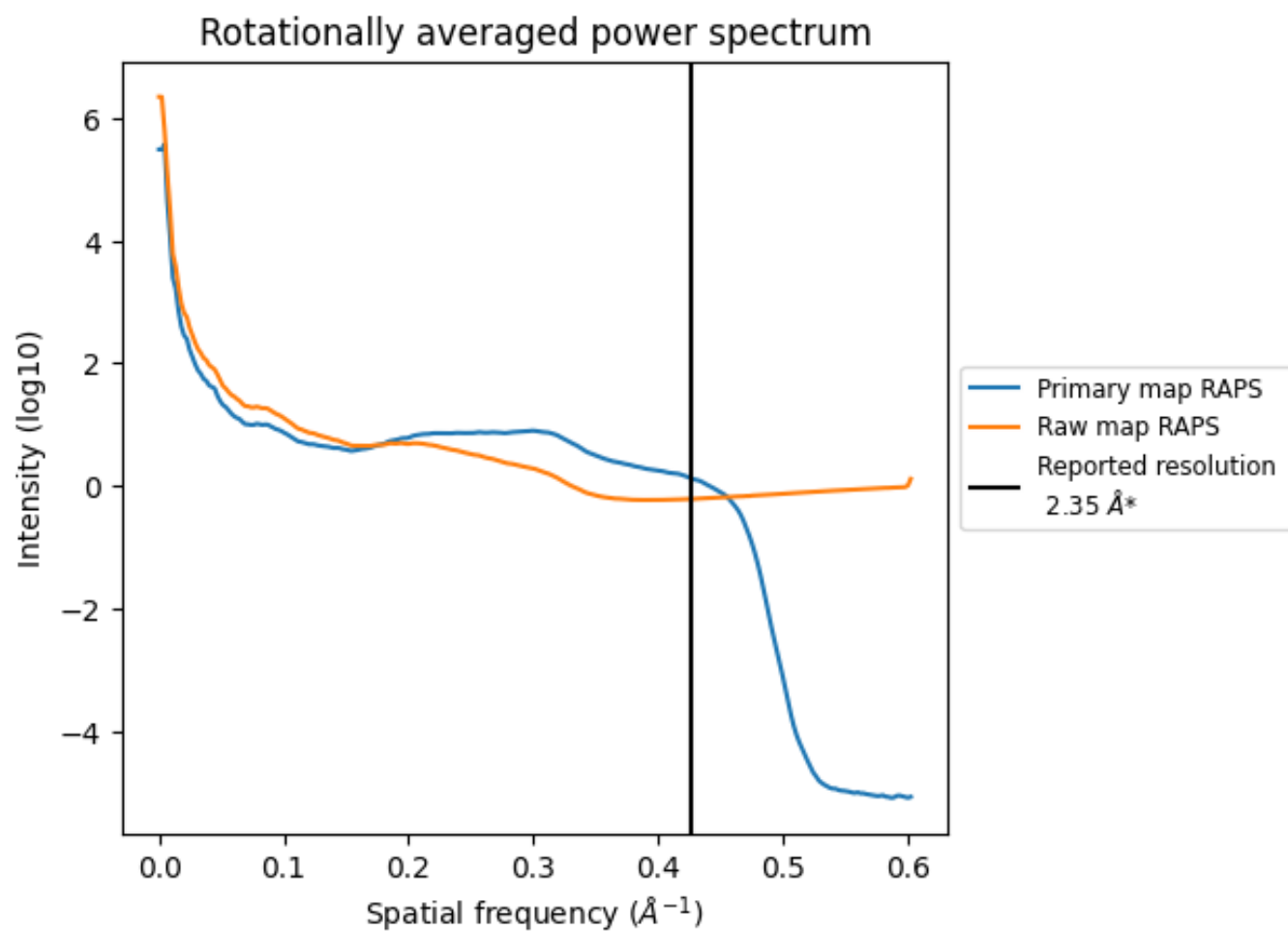
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 941 nm³; this corresponds to an approximate mass of 850 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

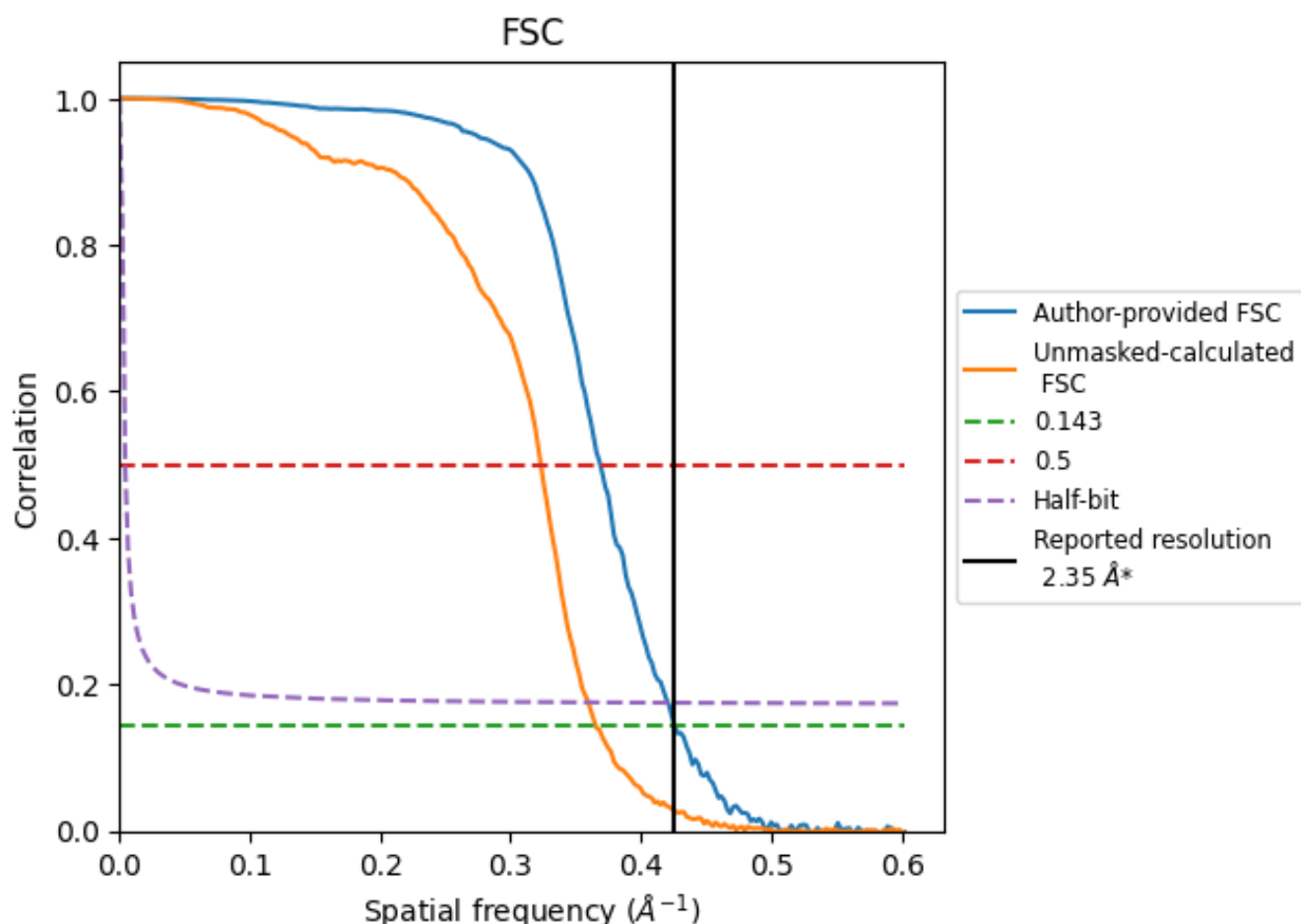


*Reported resolution corresponds to spatial frequency of 0.426 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.426 \AA^{-1}

8.2 Resolution estimates [i](#)

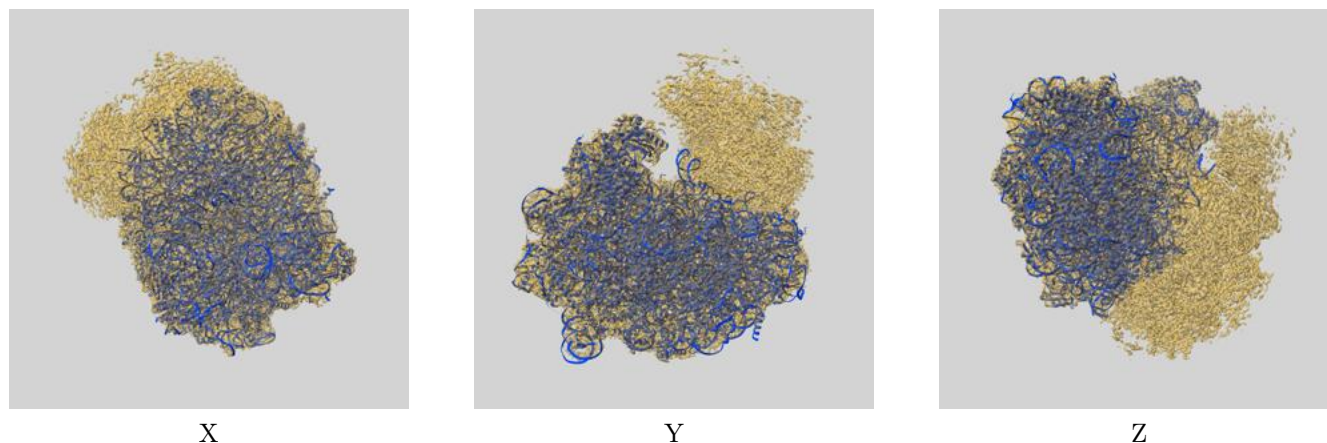
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.35	2.71	2.38
Unmasked-calculated*	2.74	3.09	2.78

*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 2.74 differs from the reported value 2.35 by more than 10 %

9 Map-model fit [i](#)

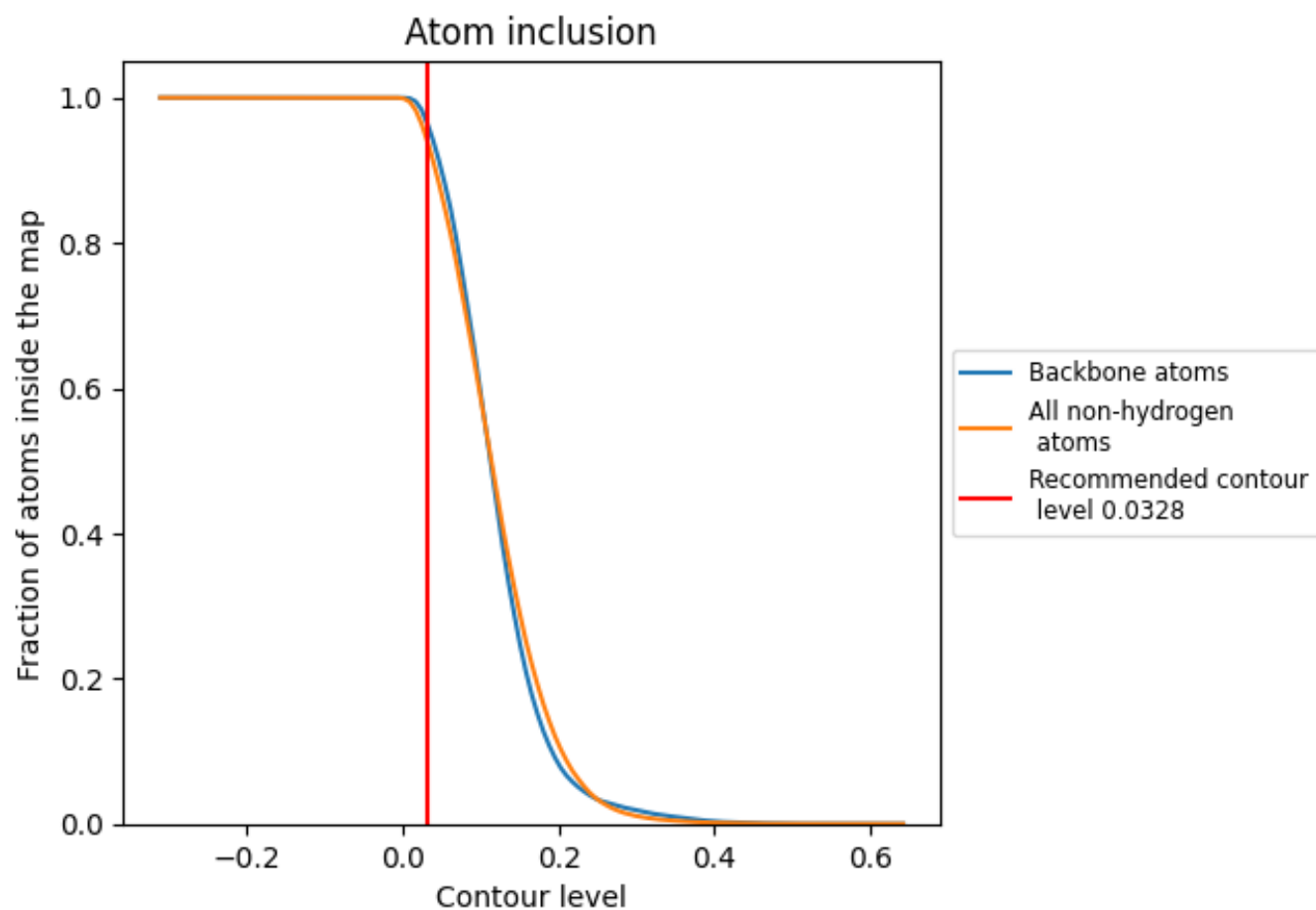
This section contains information regarding the fit between EMDB map EMD-14001 and PDB model 7QIW. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0328 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 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.