



wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 11:35 am BST

PDB ID : 8BTK
EMDB ID : EMD-16232
Title : Structure of the TRAP complex with the Sec translocon and a translating ribosome
Authors : Jaskolowski, M.; Jomaa, A.; Gamedinger, M.; Shrestha, S.; Leibundgut, M.; Deuerling, E.; Ban, N.
Deposited on : 2022-11-29
Resolution : 3.50 Å(reported)

This is a wwPDB EM Validation Summary 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 : **FAILED**
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

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition i

There are 98 unique types of molecules in this entry. The entry contains 233722 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 RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	B5	3764	80772	36003	14762	26243	3764	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B7	119	2538	1131	451	837	119	0	0

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B8	156	3319	1481	585	1097	156	0	0

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	BA	253	1940	1214	396	324	6	0	0

- Molecule 5 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BB	398	3206	2042	605	546	13	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BC	362	2886	1814	577	481	14	0	0

- Molecule 7 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	BD	293	2391	1512	438	427	14	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	BE	243	1960	1258	378	321	3	0	0

- Molecule 9 is a protein called uL30,60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BF	226	1886	1211	362	304	9	0	0

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	BG	233	1877	1197	361	315	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	86	ALA	VAL	conflict	UNP G1STW0
BG	191	GLY	CYS	conflict	UNP G1STW0

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	BH	190	1516	954	284	272	6	0	0

- Molecule 12 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BI	213	1717	1086	332	285	14	0	0

- Molecule 13 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BJ	170	1362	861	254	241	6	0	0

- Molecule 14 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	BK	29	145	87	29	29	0	0

- Molecule 15 is a protein called L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	BL	210	1701	1065	354	278	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	74	ARG	HIS	conflict	UNP G1TKB3
BL	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 16 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	BM	138	1137	727	221	182	7	0	0

- Molecule 17 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BN	203	1701	1072	359	266	4	0	0

- Molecule 18 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	BO	199	1630	1051	319	255	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	174	LEU	ILE	conflict	UNP A0A0N8ETI8
BO	194	ASP	GLU	conflict	UNP A0A0N8ETI8

- Molecule 19 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	BP	159	1289	809	249	222	9	0	0

- Molecule 20 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	BQ	187	1515	946	315	250	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 21 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	BR	180	1508	933	328	238	9	0	0

- Molecule 22 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	BS	176	1457	924	288	234	11	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BS	1	MET	THR	conflict	UNP G1TTY7

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Chain	Residue	Modelled	Actual	Comment	Reference
BS	18	PRO	-	insertion	UNP G1TTY7
BS	19	THR	-	insertion	UNP G1TTY7
BS	20	PRO	SER	conflict	UNP G1TTY7
BS	49	SER	LEU	conflict	UNP G1TTY7
BS	50	GLN	GLU	conflict	UNP G1TTY7
BS	95	ARG	HIS	conflict	UNP G1TTY7
BS	101	THR	ILE	conflict	UNP G1TTY7
BS	102	THR	MET	conflict	UNP G1TTY7
BS	104	GLY	SER	conflict	UNP G1TTY7
BS	138	ARG	PRO	conflict	UNP G1TTY7
BS	168	SER	TYR	conflict	UNP G1TTY7

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	BT	159	1298	823	252	217	6	0	0

- Molecule 24 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	BU	99	806	516	141	147	2	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	GLY	ARG	conflict	UNP G1TSG1
BU	36	ALA	GLU	conflict	UNP G1TSG1
BU	39	PHE	SER	conflict	UNP G1TSG1
BU	54	GLY	ARG	conflict	UNP G1TSG1
BU	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 25 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	BV	139	1034	648	199	182	5	0	0

- Molecule 26 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 27 is a protein called Ribosomal_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 28 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 29 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 30 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ba	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bb	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 32 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bc	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 33 is a protein called Ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bd	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 34 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Be	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 35 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bf	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 36 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 37 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bh	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bi	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 39 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bj	88	Total	C	N	O	S	0	0
			721	443	160	113	5		

- Molecule 40 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Bk	69	569	366	103	99	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bk	24	LYS	ASN	conflict	UNP G1U001

- Molecule 41 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Bl	50	447	286	96	64	1	0	0

- Molecule 42 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Bm	52	432	269	90	67	6	0	0

- Molecule 43 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Bo	105	863	543	175	139	6	0	0

- Molecule 44 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Bp	91	708	445	136	120	7	0	0

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Br	126	1014	629	209	170	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Br	103	ARG	HIS	conflict	UNP G1U7L1

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Bs	196	1507	959	263	276	9	0	0

- Molecule 47 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Bt	156	1178	733	221	220	4	0	0

- Molecule 48 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Bv	212	1707	1092	308	299	8	0	0

- Molecule 49 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	SX	425	3317	2186	534	576	21	0	0

- Molecule 50 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	SY	62	494	326	86	79	3	0	0

- Molecule 51 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	SZ	29	229	157	36	34	2	0	0

- Molecule 52 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	A2	1770	37833	16911	6781	12371	1770	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 53 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AA	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 54 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AB	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 55 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AC	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 56 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AD	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 57 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AE	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 58 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AF	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 59 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AG	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 60 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AH	4	Total	C	N	O	P	0	0
			66	28	11	23	4		

- Molecule 61 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AT	75	Total	C	N	O	P	0	0
			1597	713	279	530	75		

- Molecule 62 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AZ	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 63 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Aa	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 64 is a protein called Ribosomal_S5_C domain-containing protein,40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Ab	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	2	ALA	VAL	conflict	UNP A0A5F9D8I1
Ab	36	ARG	CYS	conflict	UNP A0A5F9D8I1
Ab	38	ARG	GLY	conflict	UNP A0A5F9D8I1
Ab	39	GLY	LYS	conflict	UNP A0A5F9D8I1
Ab	40	ARG	ALA	conflict	UNP A0A5F9D8I1

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Chain	Residue	Modelled	Actual	Comment	Reference
Ab	42	ARG	ASP	conflict	UNP A0A5F9D8I1
Ab	73	MET	VAL	conflict	UNP G1TUT9
Ab	119	GLY	ALA	conflict	UNP G1TUT9
Ab	194	ARG	HIS	conflict	UNP G1TUT9
Ab	215	MET	LEU	conflict	UNP G1TUT9
Ab	227	ARG	TRP	conflict	UNP G1TUT9
Ab	228	GLY	SER	conflict	UNP G1TUT9

- Molecule 65 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	Ac	225	1751	1116	315	313	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	Ad	262	2076	1324	386	358	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ad	25	GLY	SER	conflict	UNP G1TK17
Ad	51	ARG	LYS	conflict	UNP G1TK17
Ad	78	THR	ALA	conflict	UNP G1TK17
Ad	156	VAL	MET	conflict	UNP G1TK17

- Molecule 67 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	Ae	191	1509	943	286	273	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Af	237	1923	1200	387	329	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ag	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ah	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 71 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ai	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 72 is a protein called Ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aj	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ak	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 74 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 75 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Am	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 76 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	136	Total	C	N	O	S	0	0
			1017	622	199	190	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	5F0	ASP	conflict	UNP G1U472

- Molecule 77 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ao	128	Total	C	N	O	S	0	0
			1048	665	197	179	7		

- Molecule 78 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ap	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 79 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Aq	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 80 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ar	148	Total	C	N	O	S	0	0
			1217	763	245	208	1		

- Molecule 81 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	As	143	1113	698	214	198	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
As	119	GLY	TRP	conflict	UNP G1TN62
As	142	ASN	LYS	conflict	UNP G1TN62

- Molecule 82 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	At	104	821	514	155	148	4	0	0

- Molecule 83 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	Au	83	640	394	117	124	5	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Au	3	ASN	SER	conflict	UNP G1TM82
Au	4	ASP	ASN	conflict	UNP G1TM82
Au	33	GLN	PRO	conflict	UNP G1TM82
Au	50	PHE	SER	conflict	UNP G1TM82

- Molecule 84 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	Av	129	1034	659	193	176	6	0	0

- Molecule 85 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Aw	141	1099	693	219	184	3	0	0

- Molecule 86 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	Ax	125	1015	642	199	169	5	0	0

- Molecule 87 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
87	Ay	85	683	439	128	115	1	0	0

- Molecule 88 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
88	Az	25	239	145	64	27	3	0	0

- Molecule 89 is a protein called Translocon-associated protein subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
89	TA	172	1372	888	219	261	4	0	0

- Molecule 90 is a protein called Translocon-associated protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
90	TB	161	1254	807	210	235	2	0	0

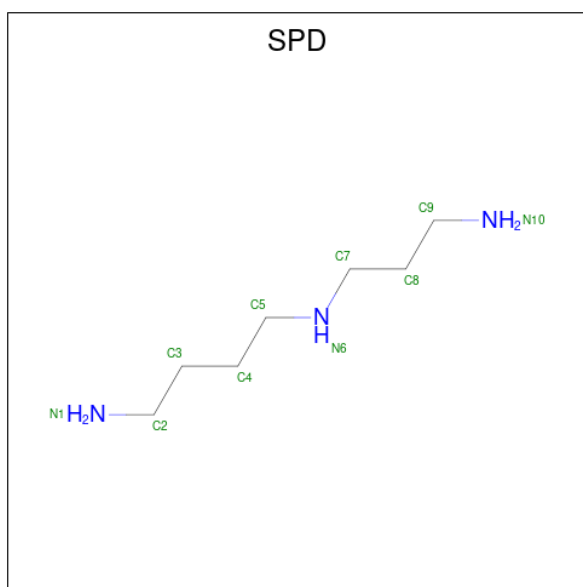
- Molecule 91 is a protein called Signal sequence receptor subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
91	TC	160	1295	853	212	227	3	0	0

- Molecule 92 is a protein called Translocon-associated protein subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
92	TD	150	1185	755	199	228	3	0	0

- Molecule 93 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



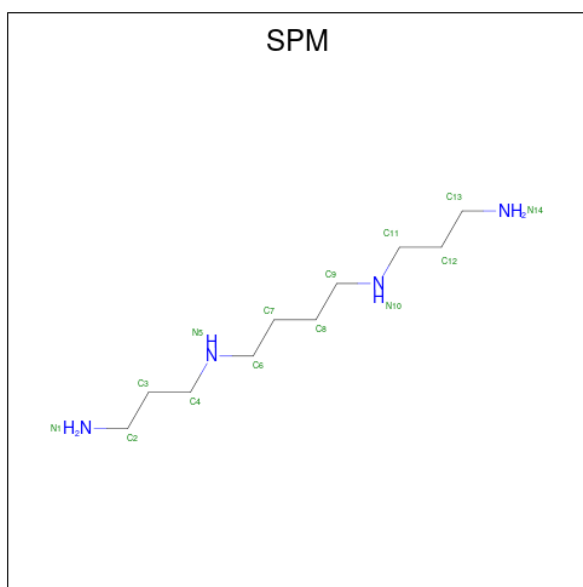
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	B5	1	10	7	3	0
93	BN	1	10	7	3	0
93	A2	1	10	7	3	0
93	A2	1	10	7	3	0
93	A2	1	10	7	3	0
93	A2	1	10	7	3	0
93	A2	1	10	7	3	0
93	A2	1	10	7	3	0
93	A2	1	10	7	3	0
93	A2	1	10	7	3	0

- Molecule 94 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
94	B5	1	Total	C	N	0
			14	10	4	
94	B5	1	Total	C	N	0
			14	10	4	
94	A2	1	Total	C	N	0
			14	10	4	

- Molecule 95 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
95	B5	510	Total	Mg	0
			510	510	
95	B7	15	Total	Mg	0
			15	15	
95	B8	16	Total	Mg	0
			16	16	
95	BA	4	Total	Mg	0
			4	4	
95	BB	3	Total	Mg	0
			3	3	
95	BC	1	Total	Mg	0
			1	1	
95	BH	1	Total	Mg	0
			1	1	
95	BI	2	Total	Mg	0
			2	2	
95	BL	1	Total	Mg	0
			1	1	

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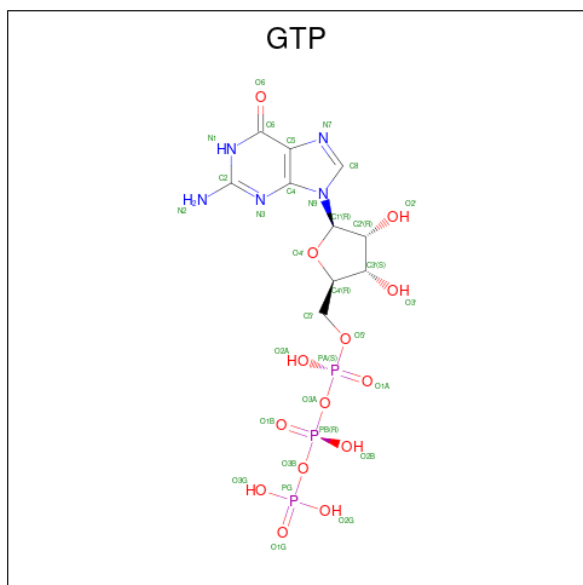
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
95	BN	1	1	1	0
95	BP	1	1	1	0
95	BQ	2	2	2	0
95	BR	1	1	1	0
95	BT	2	2	2	0
95	BV	1	1	1	0
95	Ba	1	1	1	0
95	Bb	1	1	1	0
95	Be	2	2	2	0
95	Bf	1	1	1	0
95	Bj	1	1	1	0
95	Bl	1	1	1	0
95	Bo	1	1	1	0
95	A2	167	167	167	0
95	AH	1	1	1	0
95	AT	7	7	7	0
95	Ad	1	1	1	0
95	Ae	1	1	1	0
95	Ak	1	1	1	0
95	An	1	1	1	0
95	Ar	1	1	1	0

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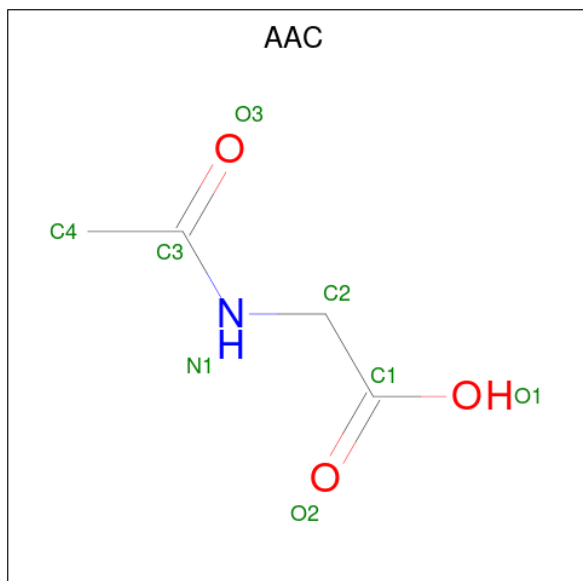
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
95	As	1	1	1	0

- Molecule 96 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
96	B7	1	32	10	5	14	3	0

- Molecule 97 is ACETYLAMINO-ACETIC ACID (three-letter code: AAC) (formula: $C_4H_7NO_3$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
97	BD	1	7	4	1	2	0

- Molecule 98 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
98	Bg	1	1	1	0
98	Bj	1	1	1	0
98	Bm	1	1	1	0
98	Bo	1	1	1	0
98	Bp	1	1	1	0
98	AC	1	1	1	0
98	AE	1	1	1	0
98	AG	1	1	1	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22643	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

226 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	$\# Z > 2$
1	A2M	B5	4317	1	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
1	OMU	B5	4244	1,95	19,22,23	1.19	2 (10%)	26,31,34	1.69	5 (19%)
42	M3L	Bm	98	42	10,11,12	0.82	0	9,14,16	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	A2M	A2	159	52	18,25,26	1.02	1 (5%)	18,36,39	1.31	2 (11%)
52	PSU	A2	218	52	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	3447	1	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	PSU	A2	1057	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	UY1	B5	3550	1,95	19,22,23	1.40	3 (15%)	22,31,34	1.87	5 (22%)
1	A2M	B5	3456	1	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
1	OMC	B5	2265	1,95	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
1	A2M	B5	1270	1	18,25,26	0.99	1 (5%)	18,36,39	1.23	2 (11%)
1	OMC	B5	3433	1,95	19,22,23	0.79	0	26,31,34	0.75	0
1	OMC	B5	1820	1,95	19,22,23	0.79	0	26,31,34	0.79	0
1	PSU	B5	4217	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4298	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	4383	1,95	18,26,27	0.94	1 (5%)	19,38,41	1.10	2 (10%)
1	PSU	B5	1632	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
1	PSU	B5	4740	1,95	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	816	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	MA6	A2	1851	52	18,26,27	1.09	2 (11%)	19,38,41	1.99	3 (15%)
1	OMG	B5	2207	1	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
1	OMU	B5	2258	1	19,22,23	1.23	4 (21%)	26,31,34	1.68	4 (15%)
3	PSU	B8	69	3	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4188	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
43	MLZ	B _o	53	43	8,9,10	0.49	0	4,9,11	0.11	0
1	OMU	B5	4366	1	19,22,23	1.22	3 (15%)	26,31,34	1.73	4 (15%)
1	PSU	B5	3371	1	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	B5	1718	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	B5	400	1	18,25,26	1.03	1 (5%)	18,36,39	1.24	2 (11%)
1	PSU	B5	3369	1,95	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
45	SAC	Br	2	45	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
1	OMG	B5	4116	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
1	PSU	B5	4267	1,95	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	B5	3450	1	18,25,26	1.02	1 (5%)	18,36,39	1.20	2 (11%)
1	PSU	B5	3494	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4419	1,95	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	OMC	A2	1704	52	19,22,23	0.82	0	26,31,34	0.81	0
1	PSU	B5	3652	1,95	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	B5	2351	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	B5	3973	1	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
1	OMC	B5	3573	1	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
52	PSU	A2	109	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	PSU	A2	573	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	A2M	A2	1679	52	18,25,26	1.02	1 (5%)	18,36,39	1.29	2 (11%)
52	A2M	A2	166	52	18,25,26	1.06	1 (5%)	18,36,39	1.22	2 (11%)
52	PSU	A2	1175	52,95	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	OMU	A2	429	52	19,22,23	1.20	3 (15%)	26,31,34	1.68	4 (15%)
1	PSU	B5	4177	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMU	B5	3657	1	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
52	OMG	A2	602	52	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
1	A2M	B5	3492	1,52,95	18,25,26	1.01	1 (5%)	18,36,39	1.39	2 (11%)
1	A2M	B5	3599	1	18,25,26	1.00	1 (5%)	18,36,39	1.20	2 (11%)
1	OMG	B5	4138	1	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
52	PSU	A2	93	52	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
52	OMU	A2	116	52	19,22,23	1.20	2 (10%)	26,31,34	1.68	4 (15%)
1	A2M	B5	2658	1,95	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
52	OMU	A2	1805	52,95	19,22,23	1.22	3 (15%)	26,31,34	1.68	5 (19%)
1	A2M	B5	4336	1	18,25,26	1.04	1 (5%)	18,36,39	1.23	2 (11%)
1	A2M	B5	2206	1,95	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	B5	4435	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
52	A2M	A2	27	52,95	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
52	PSU	A2	1348	52	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	B5	4278	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
52	PSU	A2	1082	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
76	5F0	An	138	76	8,8,9	1.49	2 (25%)	7,9,11	1.70	1 (14%)
1	PSU	B5	4374	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	4202	1	19,22,23	0.82	0	26,31,34	0.82	0
52	PSU	A2	36	52	18,21,22	1.33	2 (11%)	22,30,33	1.84	3 (13%)
52	OMU	A2	1443	52,95	19,22,23	1.23	3 (15%)	26,31,34	1.69	5 (19%)
1	OMU	B5	2680	1,95	19,22,23	1.22	2 (10%)	26,31,34	1.72	4 (15%)
1	PSU	B5	3490	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
62	SAC	AZ	2	62	7,8,9	0.54	0	8,9,11	0.86	1 (12%)
52	OMG	A2	510	52,95	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	HY3	Aw	62	85	6,8,9	2.00	1 (16%)	5,10,12	1.11	1 (20%)
1	PSU	B5	4322	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	4203	1	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
52	OMC	A2	174	52,95	19,22,23	0.81	0	26,31,34	0.78	0
1	PSU	B5	4382	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
31	MLZ	Bb	5	31,95	8,9,10	0.49	0	4,9,11	0.16	0
1	1MA	B5	1266	1,95	16,25,26	1.59	2 (12%)	18,37,40	1.05	2 (11%)
1	OMG	B5	4369	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
52	PSU	A2	610	52	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
1	OMC	B5	3601	1	19,22,23	0.81	0	26,31,34	0.83	0
52	OMG	A2	645	52	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
61	PSU	AT	54	61	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
52	OMG	A2	684	52	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
1	OMC	B5	3619	1	19,22,23	0.81	0	26,31,34	0.85	0
83	AME	Au	1	83	9,10,11	0.48	0	9,11,13	0.86	1 (11%)
52	PSU	A2	967	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	3502	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	A2M	A2	513	52	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
81	NMM	As	67	81	9,11,12	0.60	0	6,12,14	0.39	0
1	OMG	B5	3942	1,61	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
1	OMG	B5	2719	1	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
52	PSU	A2	652	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4099	1,95	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	OMG	A2	1448	52	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
52	OMU	A2	628	52	19,22,23	1.18	2 (10%)	26,31,34	1.70	5 (19%)
1	OMC	B5	2667	1	19,22,23	0.81	0	26,31,34	0.86	1 (3%)
52	PSU	A2	1239	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4749	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	B5	3517	1	18,25,26	0.97	1 (5%)	18,36,39	1.34	2 (11%)
1	PSU	B5	4169	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
52	OMG	A2	868	52	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
52	PSU	A2	1693	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	3616	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	4711	1,95	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	802	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	OMG	B5	1477	1	18,26,27	0.95	1 (5%)	19,38,41	1.08	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	PSU	A2	1178	52,95	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1638	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1799	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	1233	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	4364	1,95	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
80	SAC	Ar	2	80	7,8,9	0.53	0	8,9,11	0.92	1 (12%)
1	PSU	B5	4166	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	1801	1,95	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	2647	1	19,22,23	0.81	0	26,31,34	0.85	1 (3%)
1	5MC	B5	4193	1,95	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
1	A2M	B5	3562	1	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
52	OMC	A2	463	52	19,22,23	0.82	0	26,31,34	0.79	0
52	PSU	A2	1626	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	1491	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	4039	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3427	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
52	4AC	A2	1338	52	21,24,25	1.03	1 (4%)	29,34,37	1.26	3 (10%)
1	PSU	B5	4058	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	OMC	A2	518	52	19,22,23	0.82	0	26,31,34	0.83	0
1	UR3	B5	4276	1	19,22,23	0.99	1 (5%)	26,32,35	1.42	1 (3%)
52	OMC	A2	1392	52	19,22,23	0.83	0	26,31,34	0.85	1 (3%)
1	OMG	B5	3631	1	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
1	5MC	B5	3514	1,95	18,22,23	0.97	2 (11%)	26,32,35	1.19	3 (11%)
30	V5N	Ba	39	30	4,11,12	0.77	0	5,14,16	1.48	1 (20%)
61	5MC	AT	48	61	18,22,23	0.95	2 (11%)	26,32,35	1.11	2 (7%)
52	PSU	A2	1046	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	823	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	4AC	A2	1843	52,95	21,24,25	1.09	2 (9%)	29,34,37	1.24	3 (10%)
52	OMU	A2	1289	52	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
1	PSU	B5	4107	1,95	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	1731	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
61	5MU	AT	53	61	19,22,23	1.42	5 (26%)	28,32,35	2.00	5 (17%)
1	OMU	B5	4052	1	19,22,23	1.22	3 (15%)	26,31,34	1.69	5 (19%)
52	OMU	A2	355	52,95	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
1	PSU	B5	1720	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	B5	4246	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	A2M	A2	669	52,95	18,25,26	1.00	1 (5%)	18,36,39	1.34	2 (11%)
3	PSU	B8	55	3	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	650	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	OMG	A2	1491	52,95	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
1	OMC	B5	1284	1	19,22,23	0.81	0	26,31,34	0.78	0
1	OMG	B5	1260	1	18,26,27	0.93	1 (5%)	19,38,41	1.11	2 (10%)
1	OMC	B5	2194	1,95	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
52	A2M	A2	1032	52	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
1	OMC	B5	2704	1	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
1	OMG	B5	3676	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
52	A2M	A2	577	52	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
4	V5N	BA	216	4	4,11,12	0.80	0	5,14,16	1.52	1 (20%)
1	A2M	B5	3557	1	18,25,26	1.04	1 (5%)	18,36,39	1.23	2 (11%)
1	OMC	B5	4282	1,95	19,22,23	0.82	0	26,31,34	0.84	0
52	PSU	A2	119	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	OMG	A2	437	52	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	A2M	B5	2630	1,95	18,25,26	1.00	1 (5%)	18,36,39	1.36	2 (11%)
52	PSU	A2	1047	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	1644	52,95	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	B5	1721	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	3476	1	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
1	6MZ	B5	3966	1	18,25,26	0.90	1 (5%)	16,36,39	2.01	4 (25%)
52	OMU	A2	172	52	19,22,23	1.19	3 (15%)	26,31,34	1.70	5 (19%)
52	PSU	A2	1368	52	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	3500	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	B5	2208	1,95	19,22,23	0.81	0	26,31,34	0.81	0
1	A2M	B5	398	1	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	B5	3585	1,95	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1005	52	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
52	PSU	A2	34	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	PSU	A2	687	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	105	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	A2M	A2	469	52	18,25,26	1.05	1 (5%)	18,36,39	1.22	2 (11%)
52	PSU	A2	864	52	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	OMU	A2	121	52	19,22,23	1.21	3 (15%)	26,31,34	1.66	4 (15%)
52	PSU	A2	210	52	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	OMG	A2	1329	52,95	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
52	A2M	A2	1384	52	18,25,26	1.03	1 (5%)	18,36,39	1.25	2 (11%)
6	AYA	BC	2	6	6,7,8	0.72	0	5,8,10	0.33	0
52	6MZ	A2	1833	52,95	18,25,26	0.92	1 (5%)	16,36,39	1.92	4 (25%)
52	B8N	A2	1249	52	24,29,30	1.29	3 (12%)	29,42,45	1.27	3 (10%)
1	PSU	B5	3554	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	867	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	OMU	A2	1327	52,95	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
1	A2M	B5	1489	1,95	18,25,26	1.01	1 (5%)	18,36,39	1.36	2 (11%)
52	PSU	A2	1446	52	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	B5	3359	1	18,26,27	0.94	1 (5%)	19,38,41	1.10	2 (10%)
1	PSU	B5	4042	1	18,21,22	1.32	2 (11%)	22,30,33	1.90	3 (13%)
3	OMG	B8	75	3	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
52	A2M	A2	591	52	18,25,26	1.06	1 (5%)	18,36,39	1.23	2 (11%)
1	PSU	B5	3576	1	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
52	A2M	A2	485	52	18,25,26	1.03	1 (5%)	18,36,39	1.26	2 (11%)
1	PSU	B5	2475	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	B5	3974	1	18,26,27	0.91	1 (5%)	19,38,41	1.12	2 (10%)
1	PSU	B5	1537	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	1245	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	3462	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	3466	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	B5	1580	1,95	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
52	PSU	A2	407	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3496	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4045	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
52	G7M	A2	1640	52,61	20,26,27	3.02	7 (35%)	17,39,42	0.95	1 (5%)
1	OMC	B5	3540	1	19,22,23	0.82	0	26,31,34	0.81	0
1	OMG	B5	2267	1	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
1	A2M	B5	1479	1	18,25,26	1.02	1 (5%)	18,36,39	1.24	2 (11%)
1	PSU	B5	4325	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	B5	4269	1,95	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
1	A2M	B5	1810	1,95	18,25,26	1.04	1 (5%)	18,36,39	1.24	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	B5	2244	1,95	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
1	OMG	B5	3524	1	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
1	OMG	B5	4240	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
52	PSU	A2	682	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4149	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
1	PSU	B5	1683	1,95	18,21,22	1.32	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	4245	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
52	PSU	A2	815	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	MA6	A2	1852	52	18,26,27	1.09	1 (5%)	19,38,41	1.93	3 (15%)
52	A2M	A2	99	52,95	18,25,26	1.04	1 (5%)	18,36,39	1.20	2 (11%)
1	PSU	B5	3583	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
5	HIC	BB	245	5	8,11,12	0.87	0	6,14,16	0.83	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
1	A2M	B5	4317	1	-	1/5/27/28	0/3/3/3
1	OMU	B5	4244	1,95	-	0/9/27/28	0/2/2/2
42	M3L	Bm	98	42	-	0/9/10/12	-
52	A2M	A2	159	52	-	0/5/27/28	0/3/3/3
52	PSU	A2	218	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3447	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1057	52	-	0/7/25/26	0/2/2/2
1	UY1	B5	3550	1,95	-	1/9/27/28	0/2/2/2
1	A2M	B5	3456	1	-	0/5/27/28	0/3/3/3
1	OMC	B5	2265	1,95	-	0/9/27/28	0/2/2/2
1	A2M	B5	1270	1	-	0/5/27/28	0/3/3/3
1	OMC	B5	3433	1,95	-	4/9/27/28	0/2/2/2
1	OMC	B5	1820	1,95	-	1/9/27/28	0/2/2/2
1	PSU	B5	4217	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4298	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4383	1,95	-	0/5/27/28	0/3/3/3
1	PSU	B5	1632	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4740	1,95	-	0/7/25/26	0/2/2/2
52	PSU	A2	816	52	-	0/7/25/26	0/2/2/2
52	MA6	A2	1851	52	-	0/7/29/30	0/3/3/3
1	OMG	B5	2207	1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	B5	2258	1	-	0/9/27/28	0/2/2/2
3	PSU	B8	69	3	-	0/7/25/26	0/2/2/2
1	PSU	B5	4188	1	-	0/7/25/26	0/2/2/2
43	MLZ	Bo	53	43	-	0/7/8/10	-
1	OMU	B5	4366	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	3371	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1718	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	400	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3369	1,95	-	0/7/25/26	0/2/2/2
45	SAC	Br	2	45	-	0/7/8/10	-
1	OMG	B5	4116	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4267	1,95	-	0/7/25/26	0/2/2/2
1	A2M	B5	3450	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3494	1	-	1/7/25/26	0/2/2/2
1	PSU	B5	4419	1,95	-	0/7/25/26	0/2/2/2
52	OMC	A2	1704	52	-	1/9/27/28	0/2/2/2
1	PSU	B5	3652	1,95	-	0/7/25/26	0/2/2/2
1	PSU	B5	2351	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	3973	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	3573	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	109	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	573	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	1679	52	-	1/5/27/28	0/3/3/3
52	A2M	A2	166	52	-	0/5/27/28	0/3/3/3
52	PSU	A2	1175	52,95	-	0/7/25/26	0/2/2/2
52	OMU	A2	429	52	-	4/9/27/28	0/2/2/2
1	PSU	B5	4177	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	3657	1	-	1/9/27/28	0/2/2/2
52	OMG	A2	602	52	-	0/5/27/28	0/3/3/3
1	A2M	B5	3492	1,52,95	-	1/5/27/28	0/3/3/3
1	A2M	B5	3599	1	-	1/5/27/28	0/3/3/3
1	OMG	B5	4138	1	-	0/5/27/28	0/3/3/3
52	PSU	A2	93	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	116	52	-	0/9/27/28	0/2/2/2
1	A2M	B5	2658	1,95	-	0/5/27/28	0/3/3/3
52	OMU	A2	1805	52,95	-	0/9/27/28	0/2/2/2
1	A2M	B5	4336	1	-	1/5/27/28	0/3/3/3
1	A2M	B5	2206	1,95	-	0/5/27/28	0/3/3/3
1	PSU	B5	4435	1	-	0/7/25/26	0/2/2/2
52	A2M	A2	27	52,95	-	2/5/27/28	0/3/3/3
52	PSU	A2	1348	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4278	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	A2	1082	52	-	0/7/25/26	0/2/2/2
76	5F0	An	138	76	-	4/9/9/10	-
1	PSU	B5	4374	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	4202	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	36	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	1443	52,95	-	1/9/27/28	0/2/2/2
1	OMU	B5	2680	1,95	-	1/9/27/28	0/2/2/2
1	PSU	B5	3490	1	-	0/7/25/26	0/2/2/2
62	SAC	AZ	2	62	-	2/7/8/10	-
52	OMG	A2	510	52,95	-	1/5/27/28	0/3/3/3
85	HY3	Aw	62	85	-	1/1/12/14	0/1/1/1
1	PSU	B5	4322	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4203	1	-	0/7/25/26	0/2/2/2
52	OMC	A2	174	52,95	-	0/9/27/28	0/2/2/2
1	PSU	B5	4382	1	-	4/7/25/26	0/2/2/2
31	MLZ	Bb	5	31,95	-	2/7/8/10	-
1	1MA	B5	1266	1,95	-	0/3/25/26	0/3/3/3
1	OMG	B5	4369	1	-	0/5/27/28	0/3/3/3
52	PSU	A2	610	52	-	0/7/25/26	0/2/2/2
1	OMC	B5	3601	1	-	0/9/27/28	0/2/2/2
52	OMG	A2	645	52	-	3/5/27/28	0/3/3/3
61	PSU	AT	54	61	-	0/7/25/26	0/2/2/2
52	OMG	A2	684	52	-	1/5/27/28	0/3/3/3
1	OMC	B5	3619	1	-	1/9/27/28	0/2/2/2
83	AME	Au	1	83	-	2/9/10/12	-
52	PSU	A2	967	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3502	1	-	0/7/25/26	0/2/2/2
52	A2M	A2	513	52	-	2/5/27/28	0/3/3/3
81	NMM	As	67	81	-	0/9/11/13	-
1	OMG	B5	3942	1,61	-	0/5/27/28	0/3/3/3
1	OMG	B5	2719	1	-	0/5/27/28	0/3/3/3
52	PSU	A2	652	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4099	1,95	-	0/7/25/26	0/2/2/2
52	OMG	A2	1448	52	-	2/5/27/28	0/3/3/3
52	OMU	A2	628	52	-	4/9/27/28	0/2/2/2
1	OMC	B5	2667	1	-	1/9/27/28	0/2/2/2
52	PSU	A2	1239	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4749	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3517	1	-	2/5/27/28	0/3/3/3
1	PSU	B5	4169	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	OMG	A2	868	52	-	1/5/27/28	0/3/3/3
52	PSU	A2	1693	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3616	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4711	1,95	-	0/7/25/26	0/2/2/2
52	PSU	A2	802	52	-	2/7/25/26	0/2/2/2
1	OMG	B5	1477	1	-	0/5/27/28	0/3/3/3
52	PSU	A2	1178	52,95	-	0/7/25/26	0/2/2/2
1	PSU	B5	1638	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1799	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1233	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	4364	1,95	-	0/5/27/28	0/3/3/3
80	SAC	Ar	2	80	-	0/7/8/10	-
1	PSU	B5	4166	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1801	1,95	-	0/7/25/26	0/2/2/2
1	OMC	B5	2647	1	-	0/9/27/28	0/2/2/2
1	5MC	B5	4193	1,95	-	4/7/25/26	0/2/2/2
1	A2M	B5	3562	1	-	0/5/27/28	0/3/3/3
52	OMC	A2	463	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	1626	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	1491	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4039	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3427	1	-	0/7/25/26	0/2/2/2
52	4AC	A2	1338	52	-	4/11/29/30	0/2/2/2
1	PSU	B5	4058	1	-	0/7/25/26	0/2/2/2
52	OMC	A2	518	52	-	0/9/27/28	0/2/2/2
1	UR3	B5	4276	1	-	0/7/25/26	0/2/2/2
52	OMC	A2	1392	52	-	0/9/27/28	0/2/2/2
1	OMG	B5	3631	1	-	1/5/27/28	0/3/3/3
1	5MC	B5	3514	1,95	-	0/7/25/26	0/2/2/2
30	V5N	Ba	39	30	-	0/5/10/12	0/1/1/1
61	5MC	AT	48	61	-	0/7/25/26	0/2/2/2
52	PSU	A2	1046	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	823	52	-	0/7/25/26	0/2/2/2
52	4AC	A2	1843	52,95	-	4/11/29/30	0/2/2/2
52	OMU	A2	1289	52	-	0/9/27/28	0/2/2/2
1	PSU	B5	4107	1,95	-	0/7/25/26	0/2/2/2
1	PSU	B5	1731	1	-	0/7/25/26	0/2/2/2
61	5MU	AT	53	61	-	0/7/25/26	0/2/2/2
1	OMU	B5	4052	1	-	1/9/27/28	0/2/2/2
52	OMU	A2	355	52,95	-	0/9/27/28	0/2/2/2
1	PSU	B5	1720	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	4246	1	-	1/7/25/26	0/2/2/2
52	A2M	A2	669	52,95	-	2/5/27/28	0/3/3/3
3	PSU	B8	55	3	-	0/7/25/26	0/2/2/2
52	PSU	A2	650	52	-	0/7/25/26	0/2/2/2
52	OMG	A2	1491	52,95	-	0/5/27/28	0/3/3/3
1	OMC	B5	1284	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	1260	1	-	0/5/27/28	0/3/3/3
1	OMC	B5	2194	1,95	-	2/9/27/28	0/2/2/2
52	A2M	A2	1032	52	-	0/5/27/28	0/3/3/3
1	OMC	B5	2704	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	3676	1	-	0/5/27/28	0/3/3/3
52	A2M	A2	577	52	-	2/5/27/28	0/3/3/3
4	V5N	BA	216	4	-	1/5/10/12	0/1/1/1
1	A2M	B5	3557	1	-	0/5/27/28	0/3/3/3
1	OMC	B5	4282	1,95	-	1/9/27/28	0/2/2/2
52	PSU	A2	119	52	-	0/7/25/26	0/2/2/2
52	OMG	A2	437	52	-	0/5/27/28	0/3/3/3
1	A2M	B5	2630	1,95	-	0/5/27/28	0/3/3/3
52	PSU	A2	1047	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1644	52,95	-	0/7/25/26	0/2/2/2
1	PSU	B5	1721	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3476	1	-	1/5/27/28	0/3/3/3
1	6MZ	B5	3966	1	-	0/5/27/28	0/3/3/3
52	OMU	A2	172	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	1368	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3500	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2208	1,95	-	0/9/27/28	0/2/2/2
1	A2M	B5	398	1	-	4/5/27/28	0/3/3/3
1	PSU	B5	3585	1,95	-	0/7/25/26	0/2/2/2
52	PSU	A2	1005	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	34	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	687	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	105	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	469	52	-	2/5/27/28	0/3/3/3
52	PSU	A2	864	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	121	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	210	52	-	0/7/25/26	0/2/2/2
52	OMG	A2	1329	52,95	-	0/5/27/28	0/3/3/3
52	A2M	A2	1384	52	-	0/5/27/28	0/3/3/3
6	AYA	BC	2	6	-	3/4/6/8	-
52	6MZ	A2	1833	52,95	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	B8N	A2	1249	52	-	4/16/34/35	0/2/2/2
1	PSU	B5	3554	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	867	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	1327	52,95	-	0/9/27/28	0/2/2/2
1	A2M	B5	1489	1,95	-	2/5/27/28	0/3/3/3
52	PSU	A2	1446	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	3359	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4042	1	-	0/7/25/26	0/2/2/2
3	OMG	B8	75	3	-	0/5/27/28	0/3/3/3
52	A2M	A2	591	52	-	0/5/27/28	0/3/3/3
1	PSU	B5	3576	1	-	1/7/25/26	0/2/2/2
52	A2M	A2	485	52	-	0/5/27/28	0/3/3/3
1	PSU	B5	2475	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3974	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	1537	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1245	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3462	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3466	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	1580	1,95	-	0/5/27/28	0/3/3/3
52	PSU	A2	407	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3496	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4045	1	-	0/7/25/26	0/2/2/2
52	G7M	A2	1640	52,61	-	2/3/25/26	0/3/3/3
1	OMC	B5	3540	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	2267	1	-	1/5/27/28	0/3/3/3
1	A2M	B5	1479	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4325	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	4269	1,95	-	0/5/27/28	0/3/3/3
1	A2M	B5	1810	1,95	-	0/5/27/28	0/3/3/3
1	A2M	B5	2244	1,95	-	0/5/27/28	0/3/3/3
1	OMG	B5	3524	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	4240	1	-	0/5/27/28	0/3/3/3
52	PSU	A2	682	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4149	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1683	1,95	-	0/7/25/26	0/2/2/2
1	OMG	B5	4245	1	-	0/5/27/28	0/3/3/3
52	PSU	A2	815	52	-	0/7/25/26	0/2/2/2
52	MA6	A2	1852	52	-	4/7/29/30	0/3/3/3
52	A2M	A2	99	52,95	-	2/5/27/28	0/3/3/3
1	PSU	B5	3583	1	-	0/7/25/26	0/2/2/2
5	HIC	BB	245	5	-	2/5/6/8	0/1/1/1

The worst 5 of 341 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1640	G7M	C5-C4	7.48	1.54	1.39
52	A2	1640	G7M	O6-C6	7.33	1.38	1.23
1	B5	1266	1MA	C2-N3	4.89	1.34	1.29
85	Aw	62	HY3	C3-CA	-4.52	1.50	1.55
52	A2	1640	G7M	C2-N2	4.48	1.44	1.34

The worst 5 of 554 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B5	4325	PSU	N1-C2-N3	6.04	121.97	115.13
1	B5	4322	PSU	N1-C2-N3	6.03	121.96	115.13
1	B5	3369	PSU	N1-C2-N3	6.03	121.96	115.13
1	B5	3616	PSU	N1-C2-N3	6.02	121.95	115.13
1	B5	4435	PSU	N1-C2-N3	6.02	121.95	115.13

There are no chirality outliers.

5 of 111 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B5	2207	OMG	O4'-C4'-C5'-O5'
1	B5	3433	OMC	C2'-C1'-N1-C2
1	B5	3433	OMC	C2'-C1'-N1-C6
1	B5	4193	5MC	C2'-C1'-N1-C6
1	B5	4382	PSU	O4'-C1'-C5-C4

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 793 ligands modelled in this entry, 758 are monoatomic - leaving 35 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	$\# Z > 2$
93	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.19	0
93	SPD	B5	4916	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	B5	4905	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4918	-	9,9,9	0.15	0	8,8,8	0.21	0
93	SPD	B5	4908	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	B5	4909	-	9,9,9	0.16	0	8,8,8	0.17	0
96	GTP	B7	201	2	26,34,34	0.95	2 (7%)	32,54,54	0.79	0
93	SPD	A2	1903	-	9,9,9	0.16	0	8,8,8	0.16	0
93	SPD	B5	4903	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1901	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	A2	1902	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	A2	1908	-	9,9,9	0.16	0	8,8,8	0.19	0
93	SPD	B5	4920	-	9,9,9	0.16	0	8,8,8	0.19	0
93	SPD	B5	4902	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1906	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4913	-	9,9,9	0.15	0	8,8,8	0.18	0
97	AAC	BD	301	7	6,6,7	0.89	0	6,6,8	1.11	1 (16%)
93	SPD	B5	4910	-	9,9,9	0.15	0	8,8,8	0.16	0
94	SPM	A2	1909	-	13,13,13	0.14	0	12,12,12	0.16	0
93	SPD	B5	4912	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1905	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPM	B5	4914	-	13,13,13	0.15	0	12,12,12	0.15	0
93	SPD	B5	4915	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	B5	4917	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	B5	4907	-	9,9,9	0.16	0	8,8,8	0.16	0
93	SPD	B5	4922	-	9,9,9	0.16	0	8,8,8	0.19	0
93	SPD	B5	4923	-	9,9,9	0.16	0	8,8,8	0.15	0
93	SPD	B5	4919	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1904	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4904	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4901	-	9,9,9	0.15	0	8,8,8	0.14	0
94	SPM	B5	4911	-	13,13,13	0.15	0	12,12,12	0.18	0
93	SPD	BN	301	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4906	-	9,9,9	0.15	0	8,8,8	0.20	0
93	SPD	B5	4921	-	9,9,9	0.15	0	8,8,8	0.20	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
93	SPD	A2	1907	-	-	1/7/7/7	-
93	SPD	B5	4916	-	-	0/7/7/7	-
93	SPD	B5	4905	-	-	1/7/7/7	-
93	SPD	B5	4918	-	-	0/7/7/7	-
93	SPD	B5	4908	-	-	0/7/7/7	-
93	SPD	B5	4909	-	-	1/7/7/7	-
96	GTP	B7	201	2	-	0/18/38/38	0/3/3/3
93	SPD	A2	1903	-	-	0/7/7/7	-
93	SPD	B5	4903	-	-	1/7/7/7	-
93	SPD	A2	1901	-	-	1/7/7/7	-
93	SPD	A2	1902	-	-	0/7/7/7	-
93	SPD	A2	1908	-	-	0/7/7/7	-
93	SPD	B5	4920	-	-	0/7/7/7	-
93	SPD	B5	4902	-	-	2/7/7/7	-
93	SPD	A2	1906	-	-	0/7/7/7	-
93	SPD	B5	4913	-	-	0/7/7/7	-
97	AAC	BD	301	7	-	0/3/4/5	-
93	SPD	B5	4910	-	-	0/7/7/7	-
94	SPM	A2	1909	-	-	1/11/11/11	-
93	SPD	B5	4912	-	-	0/7/7/7	-
93	SPD	A2	1905	-	-	0/7/7/7	-
94	SPM	B5	4914	-	-	0/11/11/11	-
93	SPD	B5	4915	-	-	0/7/7/7	-
93	SPD	B5	4917	-	-	0/7/7/7	-
93	SPD	B5	4907	-	-	0/7/7/7	-
93	SPD	B5	4922	-	-	0/7/7/7	-
93	SPD	B5	4923	-	-	1/7/7/7	-
93	SPD	B5	4919	-	-	1/7/7/7	-
93	SPD	A2	1904	-	-	0/7/7/7	-
93	SPD	B5	4904	-	-	0/7/7/7	-
93	SPD	B5	4901	-	-	2/7/7/7	-
94	SPM	B5	4911	-	-	1/11/11/11	-
93	SPD	BN	301	-	-	1/7/7/7	-
93	SPD	B5	4906	-	-	0/7/7/7	-
93	SPD	B5	4921	-	-	1/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
96	B7	201	GTP	C5-C6	-2.61	1.42	1.47
96	B7	201	GTP	C8-N7	-2.05	1.31	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	BD	301	AAC	O2-C1-C2	-2.27	118.86	125.42

There are no chirality outliers.

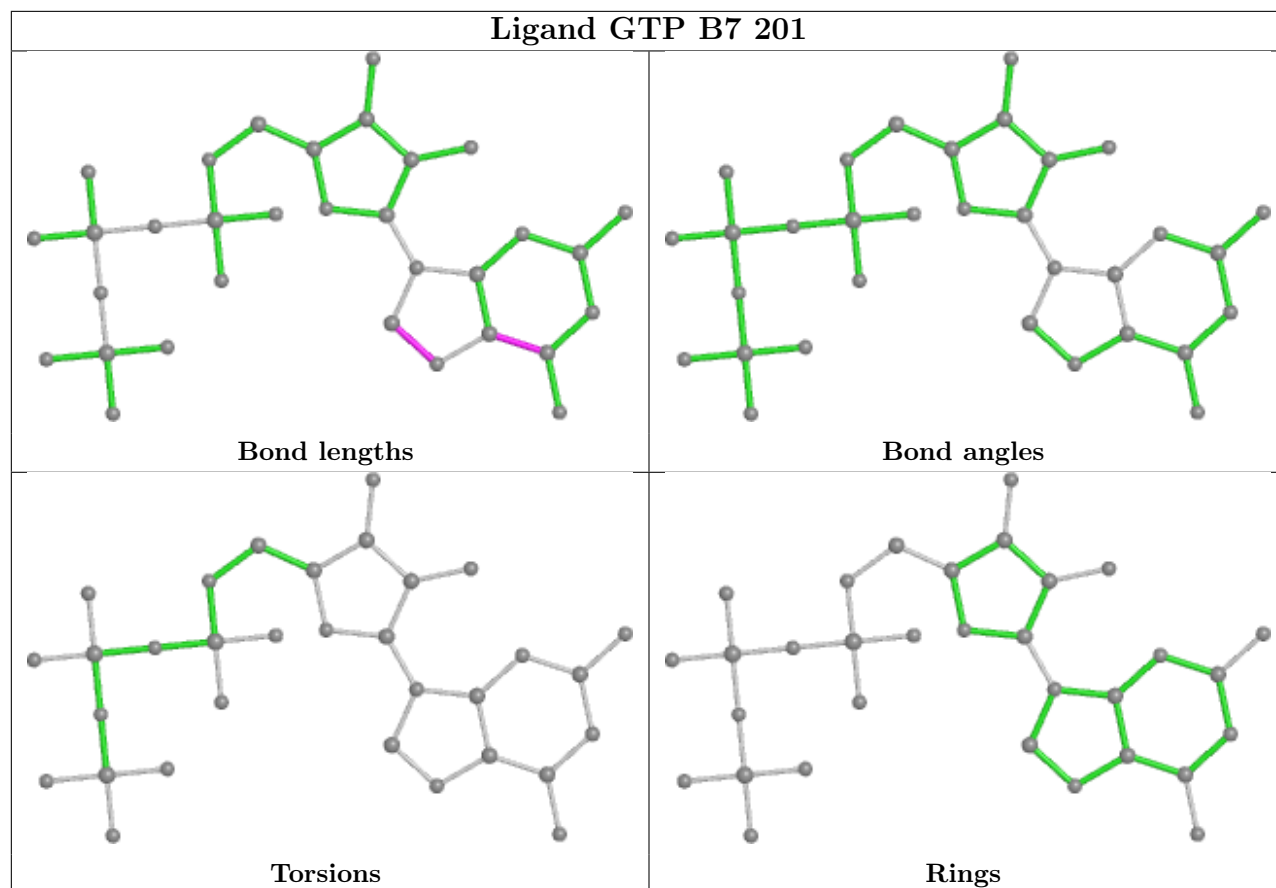
5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
94	A2	1909	SPM	C8-C9-N10-C11
93	B5	4902	SPD	C2-C3-C4-C5
93	B5	4921	SPD	C2-C3-C4-C5
94	B5	4911	SPM	C6-C7-C8-C9
93	A2	1901	SPD	C2-C3-C4-C5

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.



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

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

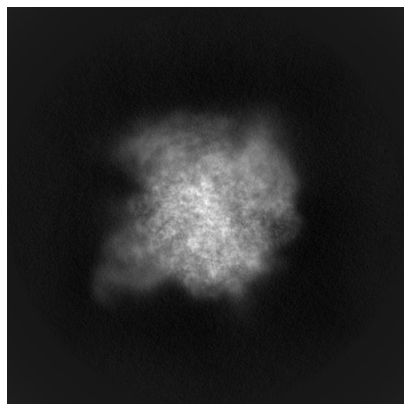
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16232. These allow visual inspection of the internal detail of the map and identification of artifacts.

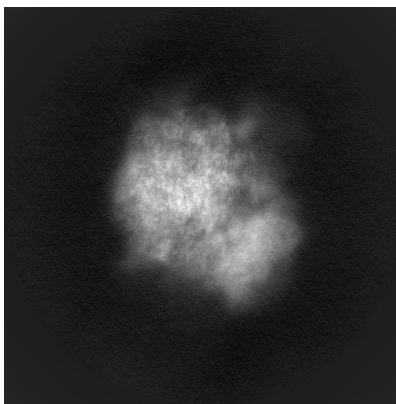
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

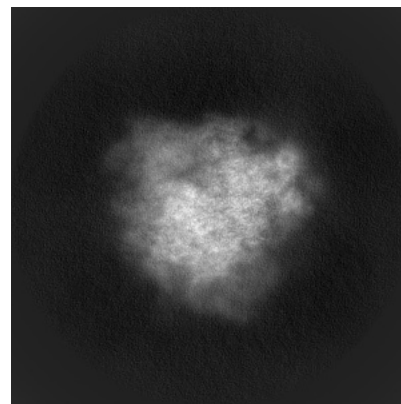
5.1.1 Primary map



X

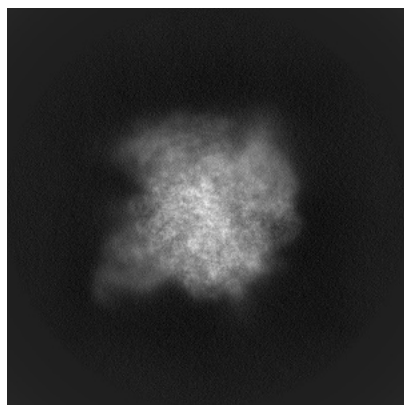


Y

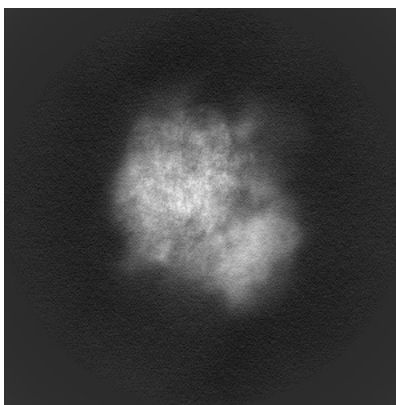


Z

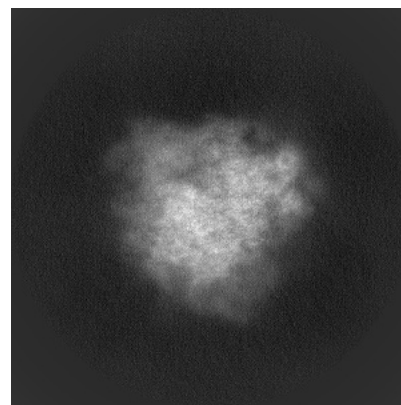
5.1.2 Raw map



X



Y

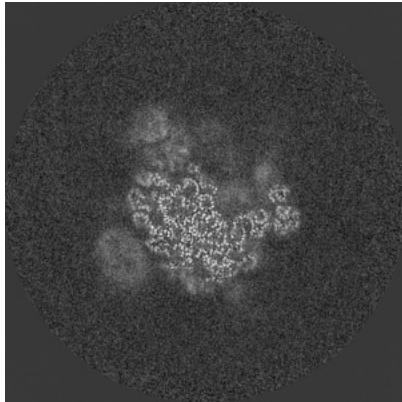


Z

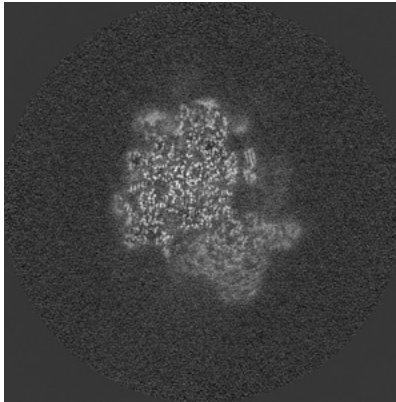
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

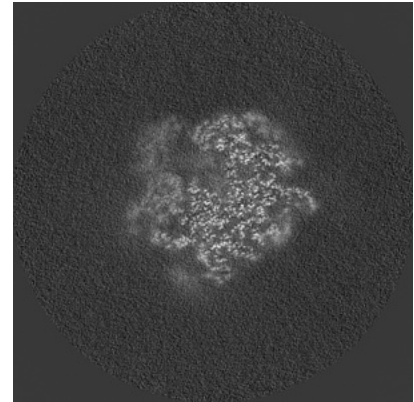
5.2.1 Primary map



X Index: 256

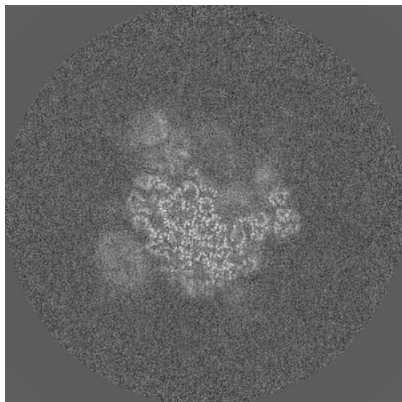


Y Index: 256

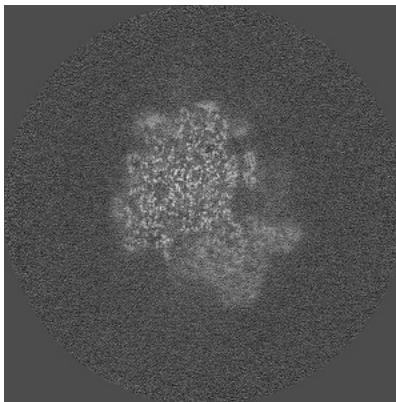


Z Index: 256

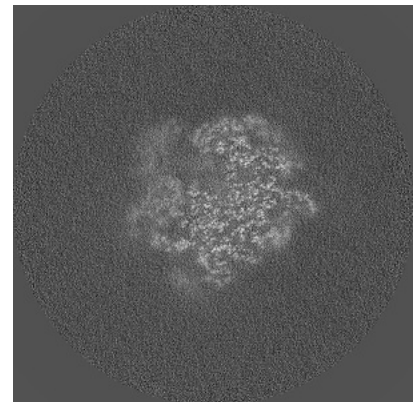
5.2.2 Raw map



X Index: 256



Y Index: 256

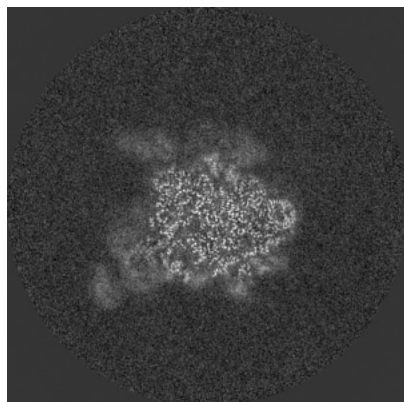


Z Index: 256

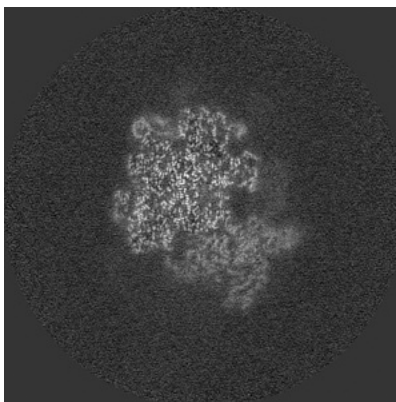
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

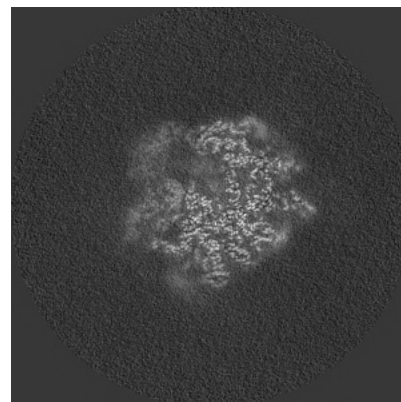
5.3.1 Primary map



X Index: 283

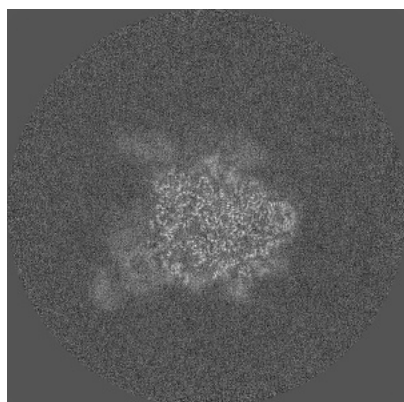


Y Index: 261

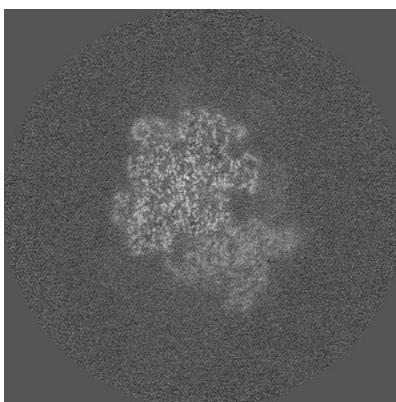


Z Index: 259

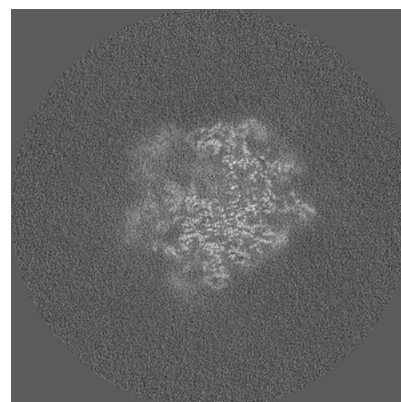
5.3.2 Raw map



X Index: 283



Y Index: 261

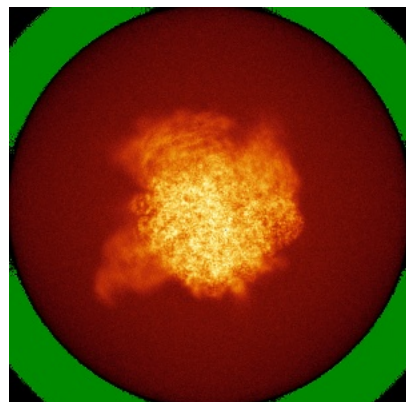


Z Index: 260

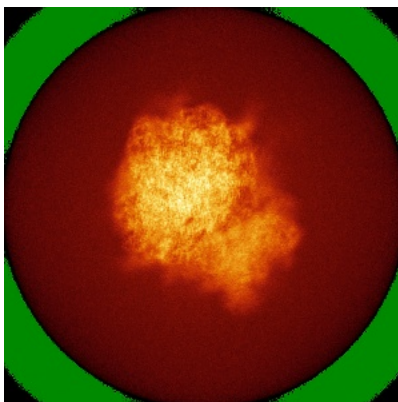
The images above show the largest variance slices of the map in three orthogonal directions.

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

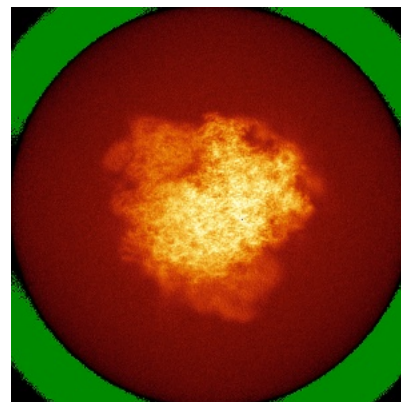
5.4.1 Primary map



X

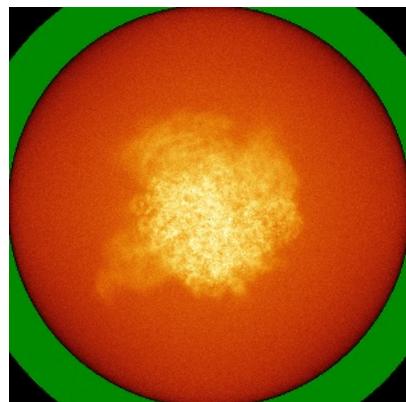


Y

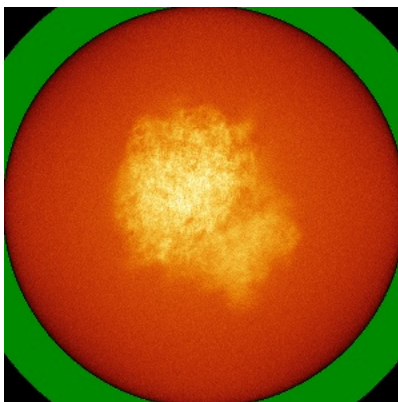


Z

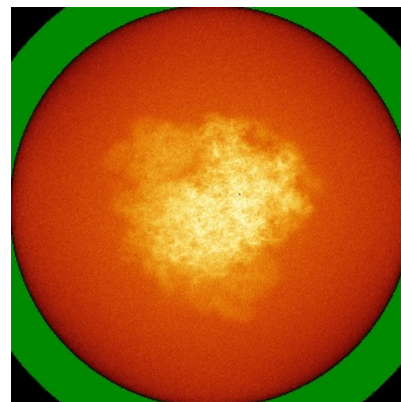
5.4.2 Raw map



X



Y

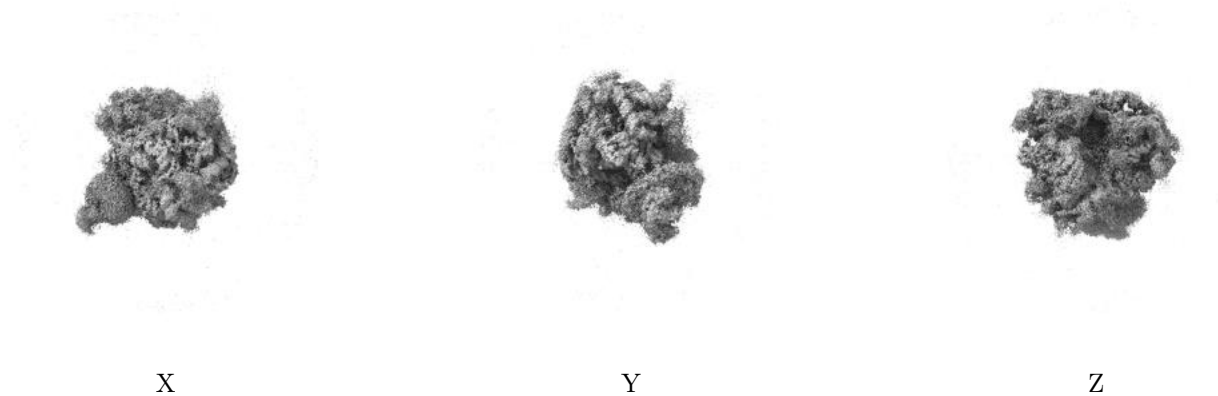


Z

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

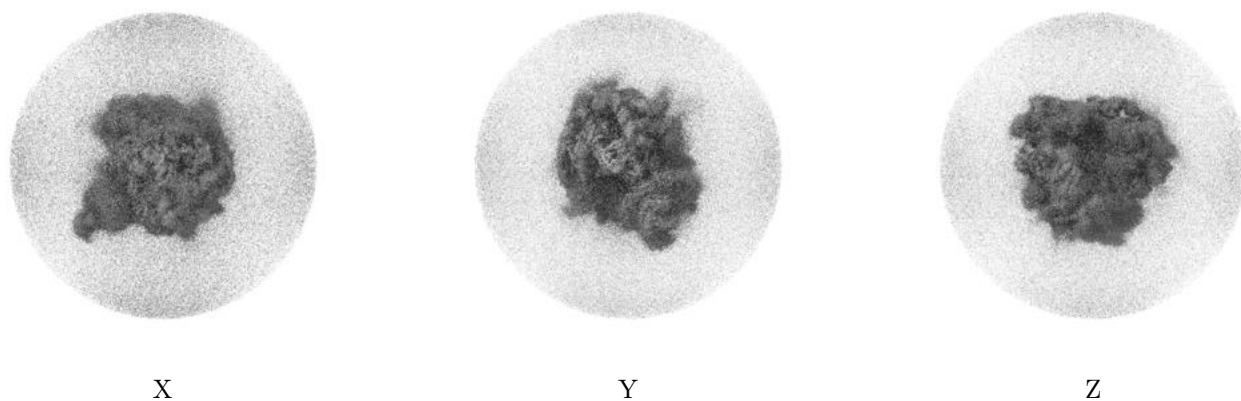
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

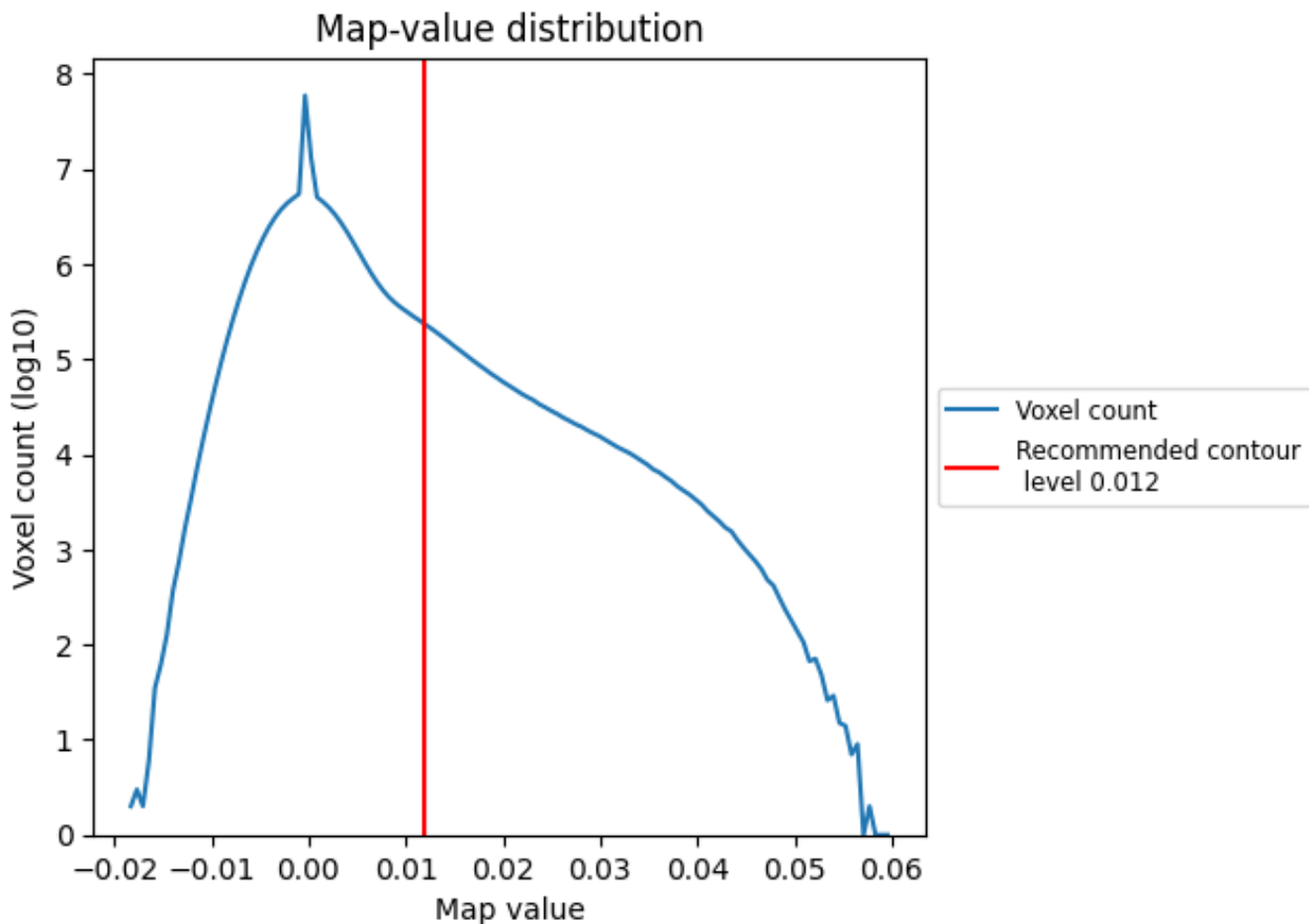
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

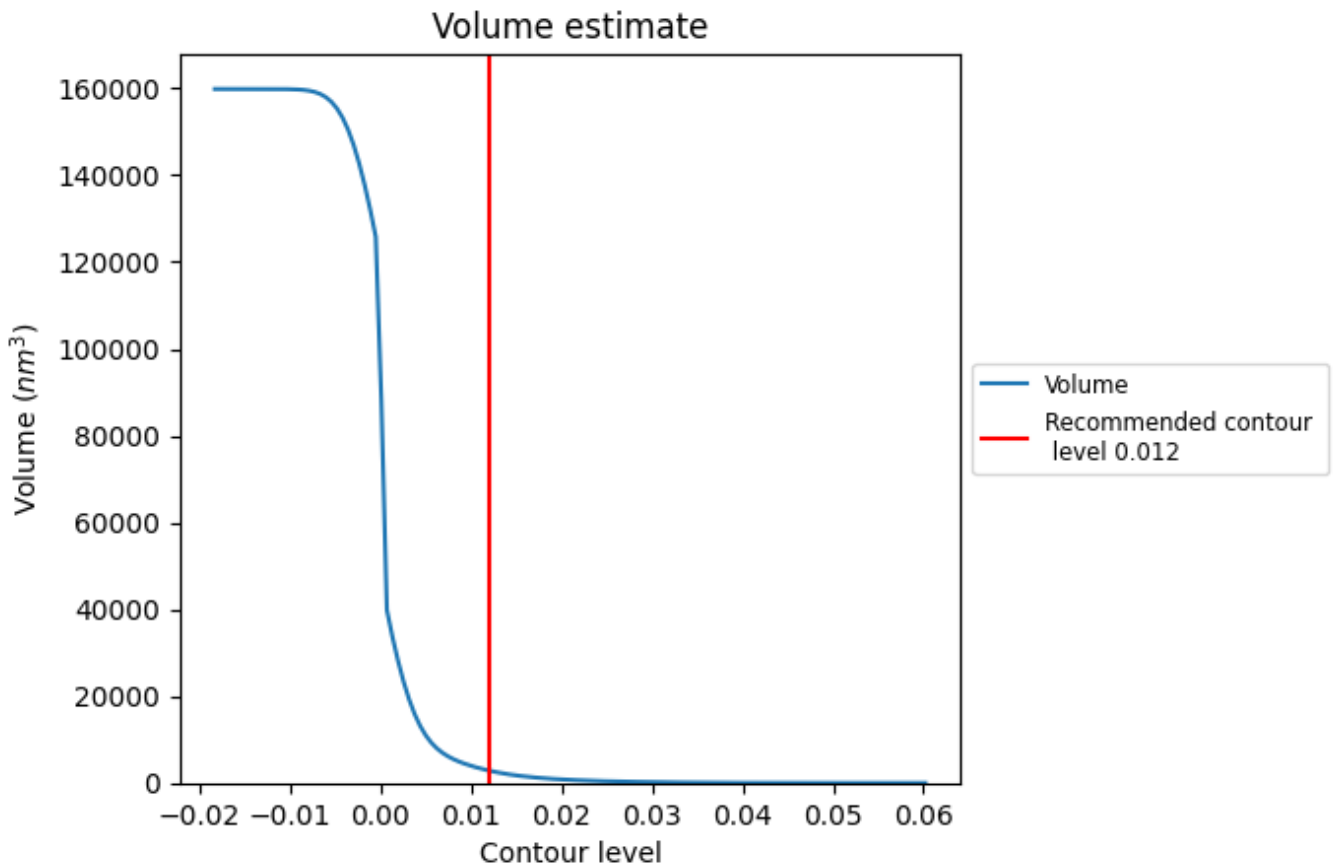
This section contains the results of statistical analysis of the map.

6.1 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.

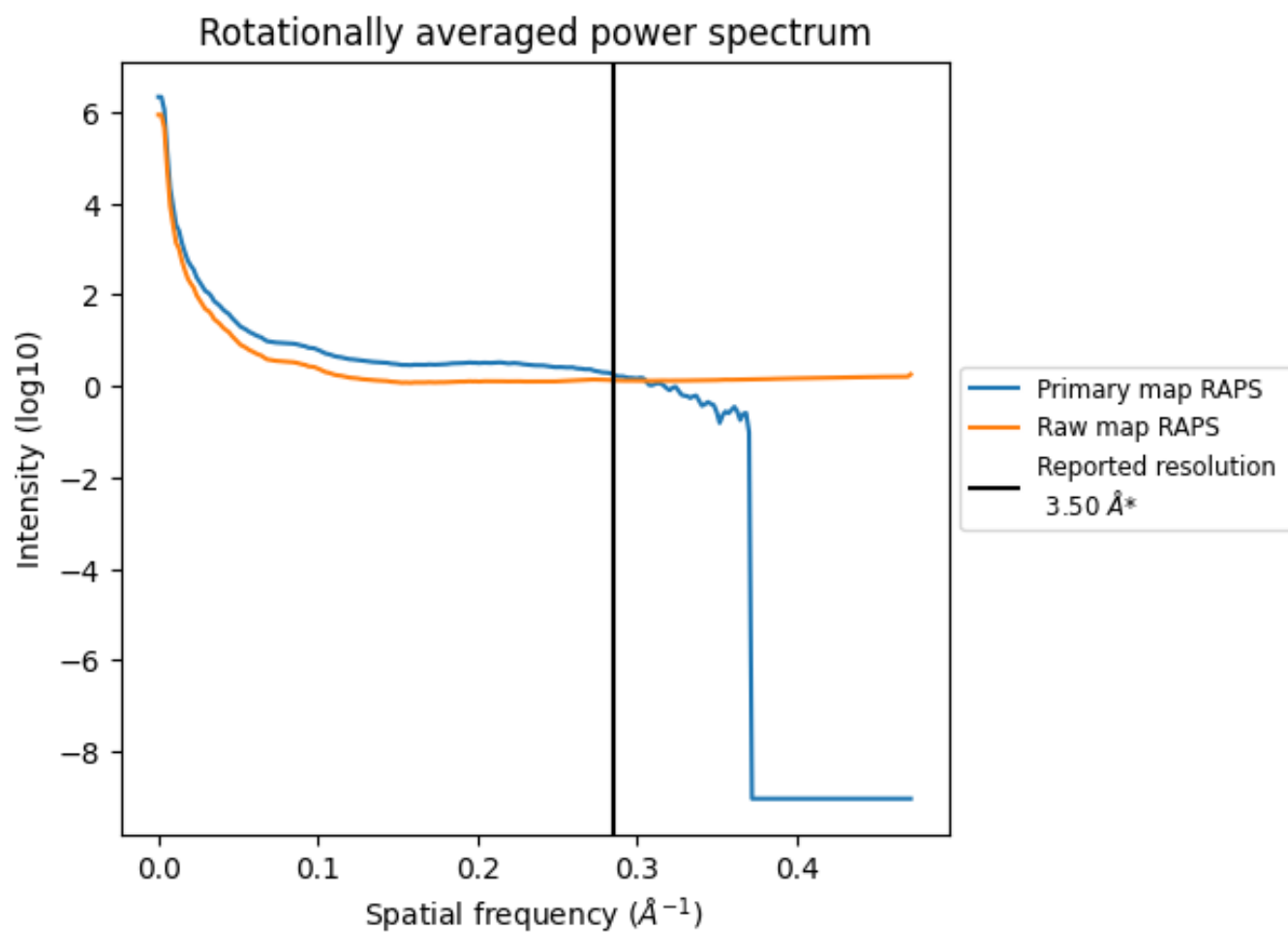
6.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 28520 nm³; this corresponds to an approximate mass of 2576 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.

6.3 Rotationally averaged power spectrum [i](#)

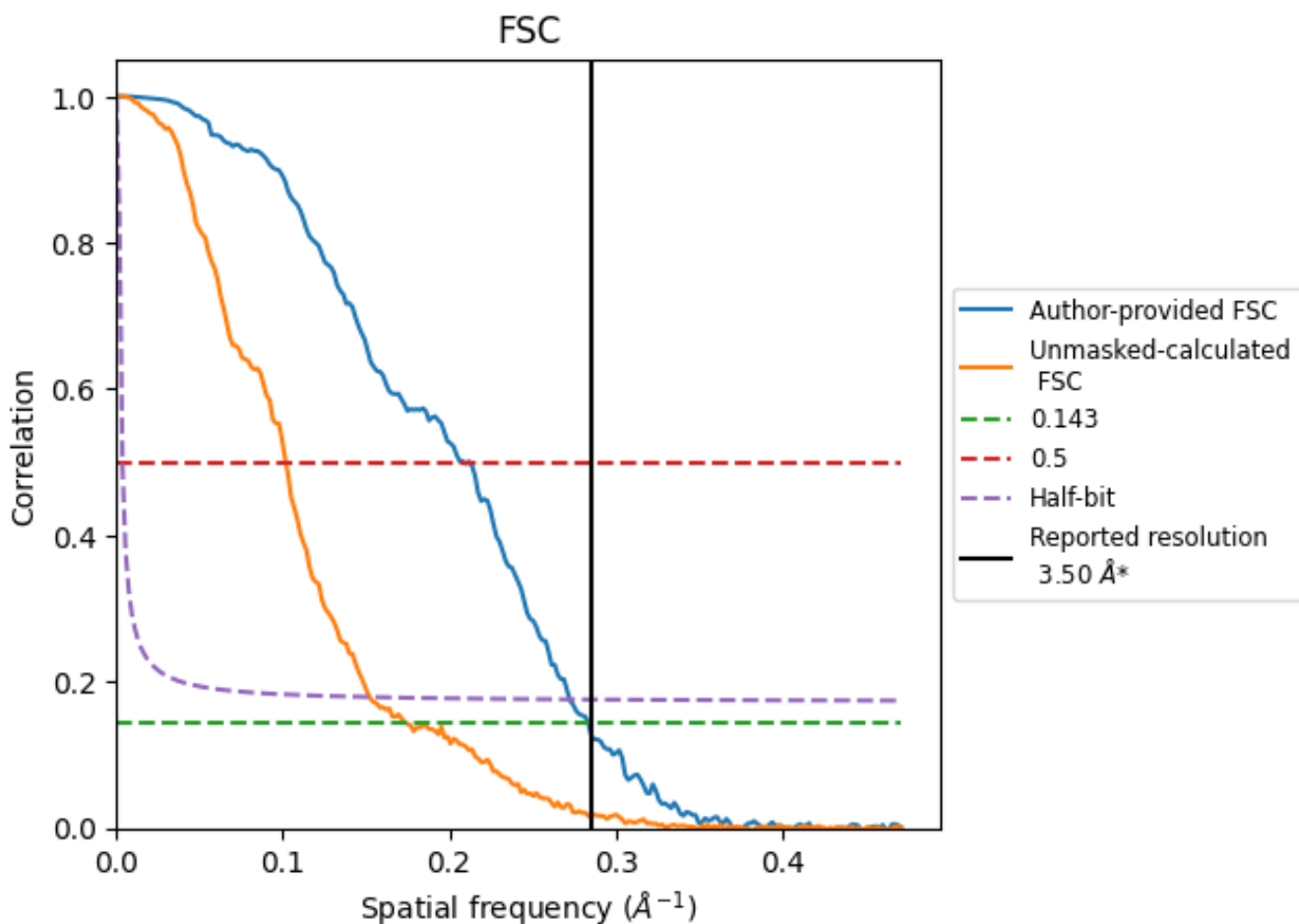


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

7.2 Resolution estimates [i](#)

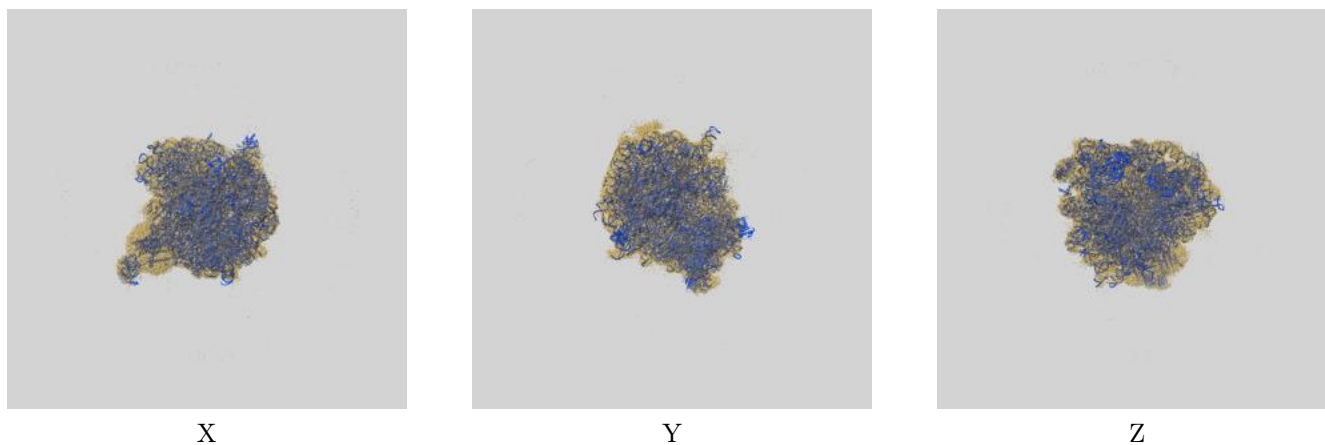
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.53	4.79	3.67
Unmasked-calculated*	5.74	9.82	6.57

*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 5.74 differs from the reported value 3.5 by more than 10 %

8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16232 and PDB model 8BTK. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

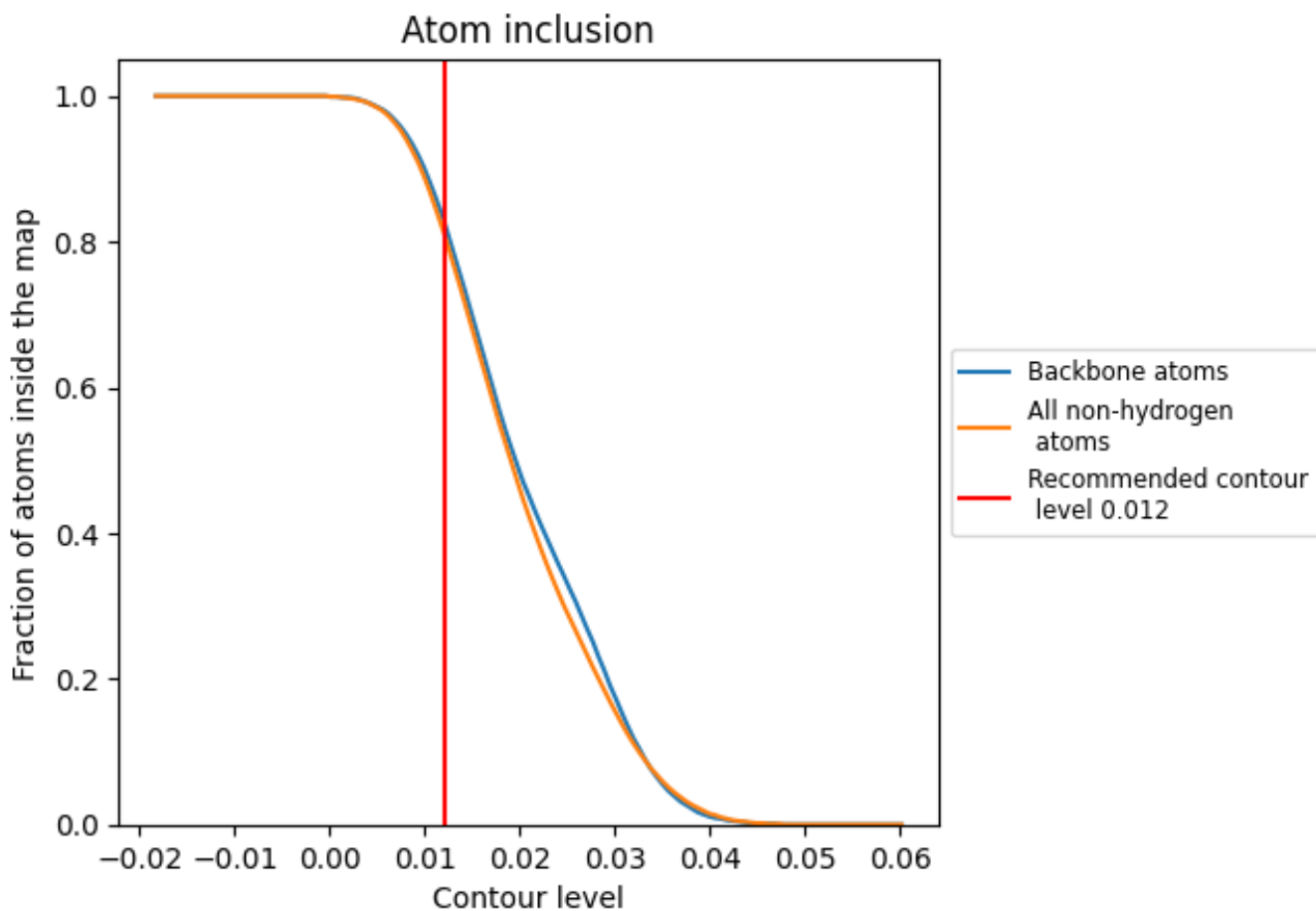
8.2 Q-score mapped to coordinate model [i](#)

This section was not generated.

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

This section was not generated.




































8.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.8130
A2	 0.8260
AA	 0.6120
AB	 0.4950
AC	 0.1480
AD	 0.5960
AE	 0.7810
AF	 0.3110
AG	 0.6240
AH	 0.1940
AT	 0.4880
AZ	 0.6640
Aa	 0.6470
Ab	 0.7530
Ac	 0.4050
Ad	 0.7170
Ae	 0.5430
Af	 0.5790
Ag	 0.4930
Ah	 0.6090
Ai	 0.6870
Aj	 0.3700
Ak	 0.6280
Al	 0.0140
Am	 0.7240
An	 0.6940
Ao	 0.5050
Ap	 0.6240
Aq	 0.5170
Ar	 0.5520
As	 0.5560
At	 0.5550
Au	 0.6760
Av	 0.7850
Aw	 0.7720



















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Chain	Atom inclusion
Ax	0.5930
Ay	0.4210
Az	0.8530
B5	0.9300
B7	0.9940
B8	0.9850
BA	0.9370
BB	0.9340
BC	0.9580
BD	0.9010
BE	0.8570
BF	0.9400
BG	0.8680
BH	0.8950
BI	0.8900
BJ	0.8390
BK	0.9170
BL	0.8980
BM	0.8980
BN	0.9720
BO	0.9470
BP	0.9230
BQ	0.9660
BR	0.8590
BS	0.9550
BT	0.9190
BU	0.8520
BV	0.9090
BW	0.5920
BX	0.9110
BY	0.9090
BZ	0.9080
Ba	0.9610
Bb	0.8180
Bc	0.8330
Bd	0.9050
Be	0.9530
Bf	0.9500
Bg	0.9150
Bh	0.9000
Bi	0.9070
Bj	0.9620

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Chain	Atom inclusion
Bk	 0.7900
Bl	 0.9490
Bm	 0.8160
Bo	 0.8840
Bp	 0.9200
Br	 0.9480
Bs	 0.3620
Bt	 0.1570
Bv	 0.0600
SX	 0.5620
SY	 0.6650
SZ	 0.2760
TA	 0.3920
TB	 0.3550
TC	 0.3960
TD	 0.2000