



## wwPDB EM Validation Summary Report ⓘ

Sep 21, 2024 – 10:29 am BST

PDB ID : 9F1C  
EMDB ID : EMD-50125  
Title : Mammalian quaternary complex of a translating 80S ribosome, NAC, MetAP1 and NatA/E  
Authors : Yudin, D.; Scaiola, A.; Ban, N.  
Deposited on : 2024-04-18  
Resolution : 3.78 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev112  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

## 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 3.78 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 236684 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 mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	O	P		
1	AH	3	36	15	18	3	0	0

- Molecule 2 is a protein called 60S ribosomal protein L29.

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

- Molecule 3 is a RNA chain called 5S rRNA.

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

- Molecule 4 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	AT	76	939	393	11	459	76	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 6 is a RNA chain called 5.8S rRNA.

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

- Molecule 7 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	BU	102	831	531	146	152	2	0	0

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 8 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	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	variant	UNP G1TN62
As	142	ASN	LYS	variant	UNP G1TN62

- Molecule 9 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 10 is a protein called Ribosomal protein L23.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	At	104	822	514	156	148	4	0	0

- Molecule 12 is a protein called Ribosomal protein L3.

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

- Molecule 13 is a protein called Ribosomal\_L23eN domain-containing protein.

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

- Molecule 14 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 17 is a protein called 60S ribosomal protein L27.

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

- Molecule 18 is a protein called 40S ribosomal protein S23.

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

- Molecule 19 is a protein called 60S ribosomal protein L6.

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

- Molecule 20 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	B5	3706	79525	35447	14532	25840	3706	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 21 is a protein called Large ribosomal subunit protein eL18.

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

- Molecule 22 is a protein called 60S ribosomal protein L27a.

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

- Molecule 23 is a protein called 40S ribosomal protein S24.

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

- Molecule 24 is a protein called Ribosomal Protein uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	61	ARG	GLY	variant	UNP G1TUB1
BF	93	ARG	GLY	variant	UNP G1TUB1
BF	131	MET	VAL	variant	UNP G1TUB1
BF	153	ILE	VAL	variant	UNP G1TUB1

- Molecule 25 is a protein called Ribosomal protein L26.

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 28 is a protein called 40S ribosomal protein S25.

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

- Molecule 29 is a protein called 60S ribosomal protein L7a.

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

- Molecule 30 is a protein called Ribosomal protein S15a.

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

- Molecule 31 is a protein called Ribosomal protein L19.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	38	ARG	CYS	variant	UNP G1TJR3
BR	64	ARG	GLN	variant	UNP G1TJR3
BR	94	THR	LYS	variant	UNP G1TJR3

- Molecule 32 is a protein called 40S ribosomal protein S3a.

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

- Molecule 33 is a protein called 60S ribosomal protein L41.

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

- Molecule 34 is a protein called 60S ribosomal protein L9.

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

- Molecule 35 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS5.



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

- Molecule 37 is a protein called 60S ribosomal protein L30.

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

- Molecule 38 is a protein called 60S ribosomal protein L10.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	B	295	2398	1516	439	429	14	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	SER	GLY	variant	UNP G1SZF4
B	248	ARG	GLN	variant	UNP G1SZF4

- Molecule 40 is a protein called Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	EA	304	2445	1540	439	443	23	13	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EA	220	ASN	ASP	engineered mutation	UNP P53582

- Molecule 41 is a protein called 40S ribosomal protein S3.

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

- Molecule 42 is a protein called 60S ribosomal protein L31.

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

- Molecule 43 is a protein called 60S ribosomal protein L11.

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

- Molecule 44 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Ct	116	904	566	165	169	4	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ct	-22	MET	-	initiating methionine	UNP Q13765
Ct	-21	GLY	-	expression tag	UNP Q13765
Ct	-20	SER	-	expression tag	UNP Q13765
Ct	-19	SER	-	expression tag	UNP Q13765
Ct	-18	HIS	-	expression tag	UNP Q13765
Ct	-17	HIS	-	expression tag	UNP Q13765
Ct	-16	HIS	-	expression tag	UNP Q13765
Ct	-15	HIS	-	expression tag	UNP Q13765
Ct	-14	HIS	-	expression tag	UNP Q13765
Ct	-13	HIS	-	expression tag	UNP Q13765
Ct	-12	SER	-	expression tag	UNP Q13765
Ct	-11	SER	-	expression tag	UNP Q13765
Ct	-10	GLY	-	expression tag	UNP Q13765
Ct	-9	LEU	-	expression tag	UNP Q13765
Ct	-8	GLU	-	expression tag	UNP Q13765
Ct	-7	VAL	-	expression tag	UNP Q13765
Ct	-6	LEU	-	expression tag	UNP Q13765
Ct	-5	PHE	-	expression tag	UNP Q13765
Ct	-4	GLN	-	expression tag	UNP Q13765

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Chain	Residue	Modelled	Actual	Comment	Reference
Ct	-3	GLY	-	expression tag	UNP Q13765
Ct	-2	PRO	-	expression tag	UNP Q13765
Ct	-1	SER	-	expression tag	UNP Q13765
Ct	0	GLY	-	expression tag	UNP Q13765

- Molecule 45 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	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	variant	UNP G1TK17
Ad	51	ARG	LYS	variant	UNP G1TK17
Ad	78	THR	ALA	variant	UNP G1TK17
Ad	156	VAL	MET	variant	UNP G1TK17

- Molecule 46 is a protein called Ribosomal protein L32.

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

- Molecule 47 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	BK	32	160	96	32	32	0	0

- Molecule 48 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Cu	106	821	514	153	151	3	0	0

- Molecule 49 is a protein called Ribosomal protein S5.

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

- Molecule 50 is a protein called 60S ribosomal protein L35a.

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

- Molecule 51 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	BL	210	1702	1065	354	279	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 52 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,N-alpha-acetyltransferase 50.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	DA	155	1260	808	221	225	6	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	-15	GLY	-	linker	UNP P08515
DA	-14	SER	-	linker	UNP P08515
DA	-13	GLY	-	linker	UNP P08515
DA	-12	SER	-	linker	UNP P08515
DA	-11	GLY	-	linker	UNP P08515
DA	-10	SER	-	linker	UNP P08515
DA	-9	GLU	-	linker	UNP P08515
DA	-8	ASN	-	linker	UNP P08515
DA	-7	LEU	-	linker	UNP P08515
DA	-6	TYR	-	linker	UNP P08515
DA	-5	PHE	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	-4	GLN	-	linker	UNP P08515
DA	-3	GLY	-	linker	UNP P08515
DA	-2	ALA	-	linker	UNP P08515
DA	-1	MET	-	linker	UNP P08515
DA	0	VAL	-	linker	UNP P08515

- Molecule 53 is a protein called 40S ribosomal protein S6.

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

- Molecule 54 is a protein called 60S ribosomal protein L34.

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

- Molecule 55 is a protein called 60S ribosomal protein L14.

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

- Molecule 56 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	DB	837	6900	4391	1192	1276	41	0	0

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	-48	MET	-	initiating methionine	UNP Q9BXJ9
DB	-47	GLY	-	expression tag	UNP Q9BXJ9
DB	-46	SER	-	expression tag	UNP Q9BXJ9
DB	-45	SER	-	expression tag	UNP Q9BXJ9
DB	-44	HIS	-	expression tag	UNP Q9BXJ9
DB	-43	HIS	-	expression tag	UNP Q9BXJ9
DB	-42	HIS	-	expression tag	UNP Q9BXJ9
DB	-41	HIS	-	expression tag	UNP Q9BXJ9

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	-40	HIS	-	expression tag	UNP Q9BXJ9
DB	-39	HIS	-	expression tag	UNP Q9BXJ9
DB	-38	SER	-	expression tag	UNP Q9BXJ9
DB	-37	SER	-	expression tag	UNP Q9BXJ9
DB	-36	GLY	-	expression tag	UNP Q9BXJ9
DB	-35	LEU	-	expression tag	UNP Q9BXJ9
DB	-34	VAL	-	expression tag	UNP Q9BXJ9
DB	-33	PRO	-	expression tag	UNP Q9BXJ9
DB	-32	ARG	-	expression tag	UNP Q9BXJ9
DB	-31	GLY	-	expression tag	UNP Q9BXJ9
DB	-30	SER	-	expression tag	UNP Q9BXJ9
DB	-29	HIS	-	expression tag	UNP Q9BXJ9
DB	-28	MET	-	expression tag	UNP Q9BXJ9
DB	-27	ALA	-	expression tag	UNP Q9BXJ9
DB	-26	SER	-	expression tag	UNP Q9BXJ9
DB	-25	MET	-	expression tag	UNP Q9BXJ9
DB	-24	THR	-	expression tag	UNP Q9BXJ9
DB	-23	GLY	-	expression tag	UNP Q9BXJ9
DB	-22	GLY	-	expression tag	UNP Q9BXJ9
DB	-21	GLN	-	expression tag	UNP Q9BXJ9
DB	-20	GLN	-	expression tag	UNP Q9BXJ9
DB	-19	MET	-	expression tag	UNP Q9BXJ9
DB	-18	GLY	-	expression tag	UNP Q9BXJ9
DB	-17	ARG	-	expression tag	UNP Q9BXJ9
DB	-16	ALA	-	expression tag	UNP Q9BXJ9
DB	-15	ARG	-	expression tag	UNP Q9BXJ9
DB	-14	GLY	-	expression tag	UNP Q9BXJ9
DB	-13	ILE	-	expression tag	UNP Q9BXJ9
DB	-12	GLN	-	expression tag	UNP Q9BXJ9
DB	-11	ARG	-	expression tag	UNP Q9BXJ9
DB	-10	PRO	-	expression tag	UNP Q9BXJ9
DB	-9	THR	-	expression tag	UNP Q9BXJ9
DB	-8	SER	-	expression tag	UNP Q9BXJ9
DB	-7	THR	-	expression tag	UNP Q9BXJ9
DB	-6	SER	-	expression tag	UNP Q9BXJ9
DB	-5	SER	-	expression tag	UNP Q9BXJ9
DB	-4	LEU	-	expression tag	UNP Q9BXJ9
DB	-3	VAL	-	expression tag	UNP Q9BXJ9
DB	-2	ALA	-	expression tag	UNP Q9BXJ9
DB	-1	ALA	-	expression tag	UNP Q9BXJ9
DB	0	ALA	-	expression tag	UNP Q9BXJ9

- Molecule 57 is a protein called 40S ribosomal protein S7.

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

- Molecule 58 is a protein called 60S ribosomal protein L35.

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

- Molecule 59 is a protein called Ribosomal protein L15.

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

- Molecule 60 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	DC	160	1295	815	234	235	11	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	24	GLN	GLU	engineered mutation	UNP P41227
DC	26	PHE	TYR	engineered mutation	UNP P41227

- Molecule 61 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 62 is a protein called 60S ribosomal protein L36.

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

- Molecule 63 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 64 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
64	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 65 is a protein called 40S ribosomal protein S9.

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

- Molecule 66 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	Bj	86	705	434	155	111	5	0	0

- Molecule 67 is a protein called 40S ribosomal protein S27.

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

- Molecule 68 is a protein called S10\_ plectin domain-containing protein.



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

- Molecule 69 is a protein called 60S ribosomal protein L38.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 70 is a protein called 40S ribosomal protein S28.

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

- Molecule 71 is a protein called 40S ribosomal protein S11.

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

- Molecule 72 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 73 is a protein called Ribosomal protein S27a.

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

- 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 Large ribosomal subunit protein eL40.

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

- Molecule 76 is a protein called 40S ribosomal protein S30.

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

- Molecule 77 is a protein called 40S ribosomal protein S13.

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

- Molecule 78 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 79 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 80 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	An	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	IAS	ASP	conflict	UNP A0AAA9WYR1

- Molecule 81 is a protein called 60S ribosomal protein L37a.

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

- Molecule 82 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 83 is a protein called 40S ribosomal protein uS19.

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

- Molecule 84 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	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 85 is a protein called 40S ribosomal protein S29.

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

- Molecule 86 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 87 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 88 is a protein called 60S ribosomal protein L21.

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

- Molecule 89 is a protein called 40S ribosomal protein eS17.

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

- Molecule 90 is a protein called 60S ribosomal protein L12.

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

- Molecule 91 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
91	Bb	2	Total	X	0
			2	2	
91	B7	6	Total	X	0
			6	6	
91	AT	2	Total	X	0
			2	2	
91	Ar	1	Total	X	0
			1	1	
91	B8	6	Total	X	0
			6	6	
91	BA	3	Total	X	0
			3	3	
91	BB	1	Total	X	0
			1	1	
91	BP	1	Total	X	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
91	B5	186	Total 186	X 186	0
91	BQ	2	Total 2	X 2	0
91	BY	1	Total 1	X 1	0
91	BH	1	Total 1	X 1	0
91	BI	1	Total 1	X 1	0
91	Ad	1	Total 1	X 1	0
91	Be	4	Total 4	X 4	0
91	Bf	1	Total 1	X 1	0
91	BL	1	Total 1	X 1	0
91	BN	1	Total 1	X 1	0
91	A2	49	Total 49	X 49	0
91	Bj	1	Total 1	X 1	0
91	Ak	1	Total 1	X 1	0
91	Bo	1	Total 1	X 1	0
91	AE	1	Total 1	X 1	0
91	An	1	Total 1	X 1	0
91	BT	2	Total 2	X 2	0

- Molecule 92 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

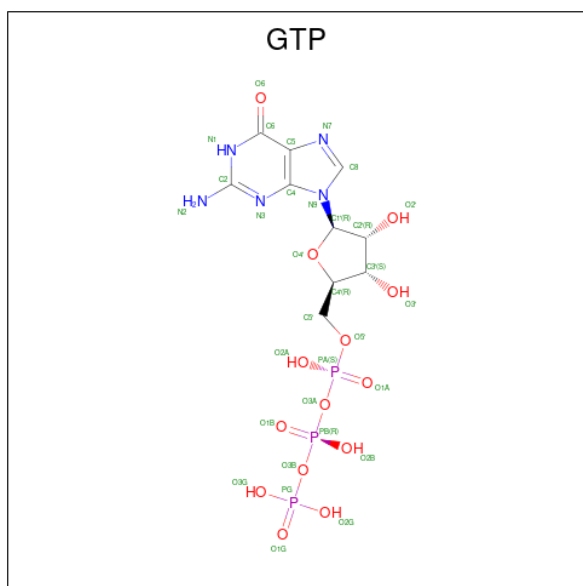
Mol	Chain	Residues	Atoms		AltConf
92	B7	9	Total 9	Mg 9	0
92	AT	2	Total 2	Mg 2	0

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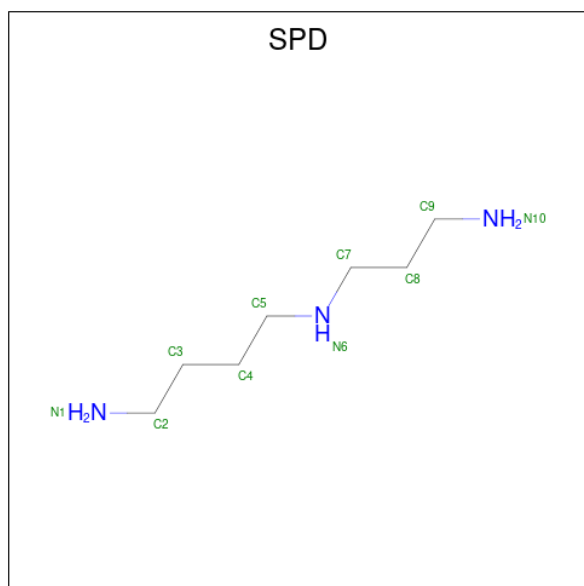
Mol	Chain	Residues	Atoms		AltConf
92	B8	8	Total 8	Mg 8	0
92	BV	1	Total 1	Mg 1	0
92	BB	1	Total 1	Mg 1	0
92	BP	1	Total 1	Mg 1	0
92	B5	282	Total 282	Mg 282	0
92	Ba	1	Total 1	Mg 1	0
92	BR	1	Total 1	Mg 1	0
92	BI	1	Total 1	Mg 1	0
92	Be	1	Total 1	Mg 1	0
92	A2	111	Total 111	Mg 111	0
92	Bj	1	Total 1	Mg 1	0

- Molecule 93 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	
93	B7	1	32	10	5	14	3	0

- Molecule 94 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



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

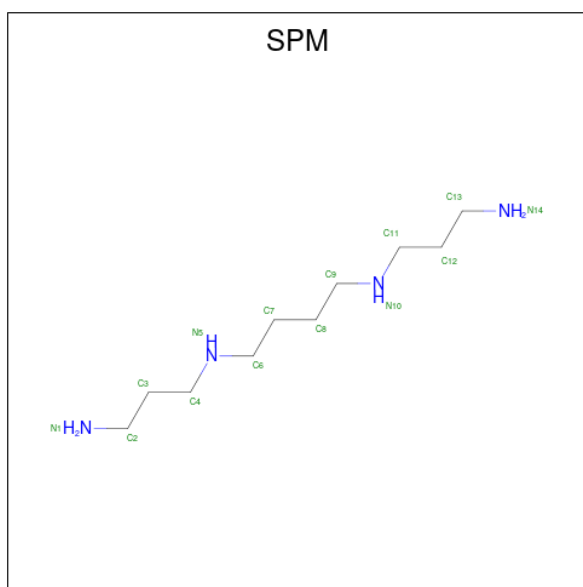
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7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

- Molecule 95 is SPERMINE (three-letter code: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).



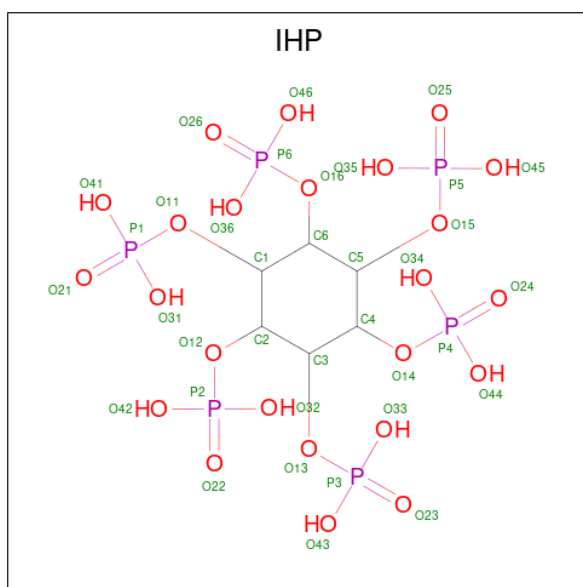


Mol	Chain	Residues	Atoms			AltConf
95	B5	1	Total	C	N	0
			14	10	4	
95	B5	1	Total	C	N	0
			14	10	4	
95	A2	1	Total	C	N	0
			14	10	4	

- Molecule 96 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 97 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
97	DB	1	36	6	24	6	0

- Molecule 98 is water.

Mol	Chain	Residues	Atoms		AltConf
98	AH	3	Total	O	0
			3	3	
98	Bb	1	Total	O	0
			1	1	
98	B7	44	Total	O	0
			44	44	
98	AT	12	Total	O	0
			12	12	
98	Ar	2	Total	O	0
			2	2	
98	B8	47	Total	O	0
			47	47	
98	As	2	Total	O	0
			2	2	
98	BA	5	Total	O	0
			5	5	
98	BV	2	Total	O	0
			2	2	
98	At	1	Total	O	0
			1	1	
98	BB	6	Total	O	0
			6	6	

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Mol	Chain	Residues	Atoms		AltConf
98	BX	2	Total 2	O 2	0
98	BC	7	Total 7	O 7	0
98	BP	3	Total 3	O 3	0
98	Aw	5	Total 5	O 5	0
98	B5	1398	Total 1398	O 1398	0
98	Ba	8	Total 8	O 8	0
98	BR	5	Total 5	O 5	0
98	Aa	3	Total 3	O 3	0
98	BH	1	Total 1	O 1	0
98	Ab	1	Total 1	O 1	0
98	BI	2	Total 2	O 2	0
98	B	1	Total 1	O 1	0
98	Bd	1	Total 1	O 1	0
98	Ct	1	Total 1	O 1	0
98	Ad	1	Total 1	O 1	0
98	Be	4	Total 4	O 4	0
98	BL	2	Total 2	O 2	0
98	Af	1	Total 1	O 1	0
98	Bg	1	Total 1	O 1	0
98	BN	5	Total 5	O 5	0
98	A2	527	Total 527	O 527	0

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Mol	Chain	Residues	Atoms		AltConf
98	Bj	5	Total 5	O 5	0
98	Ak	2	Total 2	O 2	0
98	Bl	2	Total 2	O 2	0
98	AE	1	Total 1	O 1	0
98	An	1	Total 1	O 1	0
98	Ap	2	Total 2	O 2	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	21864	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	0.906	Depositor
Minimum map value	-0.490	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.175	Depositor
Map size ( $\text{\AA}$ )	596.4, 596.4, 596.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.065, 1.065, 1.065	Depositor

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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

### 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](#)

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

#### 4.3.2 Protein sidechains [i](#)

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

#### 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](#)

223 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	$\# Z  > 2$
6	PSU	B8	69	6	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	OMC	B5	2265	20,92	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
20	A2M	B5	3456	20	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PSU	B5	4711	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
2	MLZ	Bb	5	2	8,9,10	0.49	0	4,9,11	0.14	0
64	OMU	A2	1805	64	19,22,23	1.22	3 (15%)	26,31,34	1.69	5 (19%)
64	OMG	A2	602	64	18,26,27	0.92	1 (5%)	19,38,41	1.06	2 (10%)
20	OMC	B5	2208	20,92	19,22,23	0.81	0	26,31,34	0.84	0
64	A2M	A2	669	92,64	18,25,26	1.00	1 (5%)	18,36,39	1.37	2 (11%)
6	OMG	B8	75	6	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
64	PSU	A2	802	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	3616	20	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
20	PSU	B5	4169	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
20	OMG	B5	4245	20	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
20	OMG	B5	3476	20	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
64	MA6	A2	1851	64	18,26,27	1.08	2 (11%)	19,38,41	2.01	3 (15%)
64	OMU	A2	429	64	19,22,23	1.21	3 (15%)	26,31,34	1.67	4 (15%)
20	PSU	B5	3500	20	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
64	PSU	A2	1693	64	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	5MC	B5	4193	20	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
20	OMG	B5	2267	20	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
64	PSU	A2	815	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
64	PSU	A2	867	64	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
64	PSU	A2	864	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	OMG	B5	3631	20	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
64	PSU	A2	816	64	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
64	A2M	A2	1032	64	18,25,26	1.02	1 (5%)	18,36,39	1.21	2 (11%)
64	PSU	A2	1348	64	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
20	OMC	B5	4202	20	19,22,23	0.82	0	26,31,34	0.81	0
20	PSU	B5	3369	20	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
64	4AC	A2	1338	64	21,24,25	1.07	1 (4%)	29,34,37	1.15	3 (10%)
20	OMG	B5	1580	20	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
20	PSU	B5	2351	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
64	OMU	A2	355	64	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
20	PSU	B5	4325	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
64	OMC	A2	518	64	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
20	PSU	B5	1720	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	OMC	B5	3540	20	19,22,23	0.82	0	26,31,34	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PSU	B5	4039	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	OMU	B5	3657	20	19,22,23	1.21	2 (10%)	26,31,34	1.71	5 (19%)
20	OMG	B5	1260	20	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
20	A2M	B5	2658	20,92	18,25,26	1.02	1 (5%)	18,36,39	1.20	2 (11%)
64	OMG	A2	868	64	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
20	A2M	B5	1489	20,92	18,25,26	0.99	1 (5%)	18,36,39	1.32	2 (11%)
64	PSU	A2	1005	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	3554	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
9	V5N	BA	216	9	4,11,12	0.78	0	5,14,16	1.53	1 (20%)
20	OMU	B5	2680	20	19,22,23	1.20	2 (10%)	26,31,34	1.70	5 (19%)
64	OMU	A2	172	64	19,22,23	1.20	3 (15%)	26,31,34	1.70	4 (15%)
20	PSU	B5	3652	20,92	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4278	20	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4435	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
64	OMG	A2	684	64	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
20	A2M	B5	398	20	18,25,26	1.01	1 (5%)	18,36,39	1.24	2 (11%)
20	OMG	B5	4364	20	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
64	A2M	A2	166	64	18,25,26	1.05	1 (5%)	18,36,39	1.23	2 (11%)
20	OMC	B5	1820	20,92	19,22,23	0.80	0	26,31,34	0.79	0
20	PSU	B5	4322	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
64	A2M	A2	469	64	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
20	6MZ	B5	3966	20	18,25,26	0.89	1 (5%)	16,36,39	2.01	4 (25%)
64	OMC	A2	174	92,64	19,22,23	0.81	0	26,31,34	0.80	0
20	A2M	B5	3557	20	18,25,26	1.01	1 (5%)	18,36,39	1.21	2 (11%)
64	B8N	A2	1249	64	24,29,30	1.33	3 (12%)	29,42,45	1.30	3 (10%)
20	OMG	B5	1477	20	18,26,27	0.95	1 (5%)	19,38,41	1.06	2 (10%)
18	HY3	Aw	62	18	6,8,9	1.99	1 (16%)	5,10,12	1.10	1 (20%)
64	PSU	A2	1082	64	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
64	OMG	A2	510	92,64	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
20	PSU	B5	4267	20,92	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
64	PSU	A2	105	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	A2M	B5	2630	20,92	18,25,26	1.00	1 (5%)	18,36,39	1.36	2 (11%)
20	PSU	B5	2475	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	4419	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	OMU	B5	4052	20	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	SAC	Br	2	84	7,8,9	0.53	0	8,9,11	0.83	1 (12%)
20	PSU	B5	4045	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	1638	20	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
78	MLZ	Bo	53	78	8,9,10	0.49	0	4,9,11	0.13	0
64	A2M	A2	1679	64	18,25,26	0.99	1 (5%)	18,36,39	1.36	2 (11%)
64	PSU	A2	210	64	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
20	A2M	B5	1810	20,92	18,25,26	1.03	1 (5%)	18,36,39	1.24	2 (11%)
20	PSU	B5	4382	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	4740	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
64	A2M	A2	1384	64	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
20	PSU	B5	1801	20	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
20	PSU	B5	3466	20	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	OMU	B5	3973	20	19,22,23	1.21	2 (10%)	26,31,34	1.69	4 (15%)
20	OMC	B5	1284	20	19,22,23	0.82	0	26,31,34	0.82	0
20	PSU	B5	4149	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4177	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	A2M	B5	4269	20,92	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
20	PSU	B5	4203	20	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
64	PSU	A2	1178	64	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
20	OMC	B5	2667	20	19,22,23	0.81	0	26,31,34	0.82	0
64	OMG	A2	645	64	18,26,27	0.95	1 (5%)	19,38,41	1.09	2 (10%)
20	PSU	B5	3462	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	OMG	B5	4240	20	18,26,27	0.95	1 (5%)	19,38,41	1.09	2 (10%)
64	4AC	A2	1843	64	21,24,25	1.09	2 (9%)	29,34,37	1.23	3 (10%)
64	A2M	A2	577	64	18,25,26	1.02	1 (5%)	18,36,39	1.21	2 (11%)
20	PSU	B5	3490	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4298	20	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	PSU	B5	4188	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	3583	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	4374	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	1537	20	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
20	A2M	B5	1479	20	18,25,26	1.02	1 (5%)	18,36,39	1.27	2 (11%)
6	PSU	B8	55	6	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
20	PSU	B5	3576	20	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
64	PSU	A2	1368	64	18,21,22	1.35	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
64	PSU	A2	610	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
64	PSU	A2	1175	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
64	PSU	A2	1057	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
20	1MA	B5	1266	20,92	16,25,26	1.60	2 (12%)	18,37,40	1.04	2 (11%)
20	OMG	B5	3359	20	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
20	OMG	B5	3974	20	18,26,27	0.92	1 (5%)	19,38,41	1.11	2 (10%)
64	OMU	A2	121	64	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
64	OMU	A2	1327	92,64	19,22,23	1.19	2 (10%)	26,31,34	1.71	5 (19%)
20	OMG	B5	4369	20	18,26,27	0.95	1 (5%)	19,38,41	1.08	2 (10%)
64	A2M	A2	159	64	18,25,26	1.02	1 (5%)	18,36,39	1.28	2 (11%)
20	PSU	B5	3502	20	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
20	OMU	B5	4244	20	19,22,23	1.20	2 (10%)	26,31,34	1.68	5 (19%)
20	UR3	B5	4276	20	19,22,23	0.99	0	26,32,35	1.42	1 (3%)
64	PSU	A2	1245	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
20	OMC	B5	4282	20,92	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
64	PSU	A2	119	64	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
64	A2M	A2	591	64	18,25,26	1.05	1 (5%)	18,36,39	1.28	2 (11%)
8	NMM	As	67	8	9,11,12	0.59	0	6,12,14	0.45	0
64	A2M	A2	513	64	18,25,26	1.01	1 (5%)	18,36,39	1.25	2 (11%)
20	A2M	B5	400	20	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
20	A2M	B5	2206	20,92	18,25,26	1.03	1 (5%)	18,36,39	1.18	2 (11%)
20	A2M	B5	3562	20	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
64	PSU	A2	1239	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	OMC	B5	2194	20,92	19,22,23	0.82	0	26,31,34	0.85	0
64	OMG	A2	1448	64	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
64	PSU	A2	682	64	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
20	5MC	B5	3514	20,92	18,22,23	0.97	2 (11%)	26,32,35	1.15	3 (11%)
64	PSU	A2	1626	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
22	V5N	Ba	39	22	4,11,12	0.77	0	5,14,16	1.49	1 (20%)
64	PSU	A2	109	64	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
64	OMG	A2	1491	92,64	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
64	PSU	A2	650	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	A2M	B5	4317	20	18,25,26	1.01	1 (5%)	18,36,39	1.28	2 (11%)
20	OMC	B5	2647	20	19,22,23	0.83	0	26,31,34	0.84	0
20	OMG	B5	3524	20	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SAC	Ar	2	5	7,8,9	0.52	0	8,9,11	0.90	1 (12%)
20	PSU	B5	4058	20	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
64	OMC	A2	1392	64	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
20	OMC	B5	3433	20	19,22,23	0.79	0	26,31,34	0.75	0
64	OMG	A2	1329	64	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
64	A2M	A2	485	64	18,25,26	1.02	1 (5%)	18,36,39	1.24	2 (11%)
64	A2M	A2	27	92,64	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
64	PSU	A2	1047	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
64	OMG	A2	437	64	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
20	PSU	B5	3494	20	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
64	PSU	A2	1233	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	3427	20	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	4099	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	OMG	B5	4116	20	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
20	OMG	B5	4383	20	18,26,27	0.94	1 (5%)	19,38,41	1.10	2 (10%)
20	OMG	B5	2719	20	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
20	OMG	B5	4138	20	18,26,27	0.92	1 (5%)	19,38,41	1.06	2 (10%)
64	6MZ	A2	1833	92,64	18,25,26	0.91	1 (5%)	16,36,39	1.91	4 (25%)
20	PSU	B5	3447	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
20	OMC	B5	2704	20	19,22,23	0.82	0	26,31,34	0.82	0
20	PSU	B5	4107	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	A2M	B5	3450	20	18,25,26	1.03	1 (5%)	18,36,39	1.18	2 (11%)
64	PSU	A2	1644	92,64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
64	PSU	A2	573	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
64	OMC	A2	463	64	19,22,23	0.83	0	26,31,34	0.88	1 (3%)
20	A2M	B5	3492	20,64	18,25,26	1.01	1 (5%)	18,36,39	1.37	2 (11%)
64	OMU	A2	1443	92,64	19,22,23	1.23	3 (15%)	26,31,34	1.69	5 (19%)
64	PSU	A2	652	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
64	PSU	A2	687	64	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
64	OMC	A2	1704	64	19,22,23	0.80	0	26,31,34	0.79	0
20	PSU	B5	4749	20	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	3585	20,92	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
64	OMU	A2	116	64	19,22,23	1.20	2 (10%)	26,31,34	1.70	4 (15%)
64	MA6	A2	1852	64	18,26,27	1.08	2 (11%)	19,38,41	1.93	4 (21%)
20	PSU	B5	4166	20	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PSU	B5	4217	20	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
20	PSU	B5	1718	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
14	AME	Au	1	14	9,10,11	0.47	0	9,11,13	0.87	1 (11%)
64	OMU	A2	1289	64	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
20	PSU	B5	1491	20	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
20	OMC	B5	3619	20	19,22,23	0.81	0	26,31,34	0.84	0
20	PSU	B5	1799	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
64	PSU	A2	34	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	1731	20	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
20	OMC	B5	3573	20	19,22,23	0.81	0	26,31,34	0.87	1 (3%)
12	HIC	BB	245	12	8,11,12	0.88	0	6,14,16	0.84	0
20	OMG	B5	3942	20,4	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
20	OMU	B5	4366	20	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
64	PSU	A2	967	64	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
20	OMG	B5	2207	20	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
20	A2M	B5	1270	20	18,25,26	0.99	1 (5%)	18,36,39	1.25	2 (11%)
64	PSU	A2	407	64	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
15	AYA	BC	2	15	6,7,8	0.70	0	5,8,10	0.39	0
64	PSU	A2	1446	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
64	G7M	A2	1640	64	20,26,27	3.00	7 (35%)	17,39,42	0.96	1 (5%)
75	M3L	Bm	98	75	10,11,12	0.83	0	9,14,16	0.52	0
80	IAS	An	138	80	6,7,8	1.07	0	6,8,10	1.33	1 (16%)
20	OMU	B5	2258	20	19,22,23	1.21	2 (10%)	26,31,34	1.67	4 (15%)
20	OMC	B5	3601	20	19,22,23	0.81	0	26,31,34	0.81	0
20	A2M	B5	3517	20	18,25,26	0.97	1 (5%)	18,36,39	1.32	2 (11%)
20	PSU	B5	4042	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	1683	20	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
64	PSU	A2	218	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
20	UY1	B5	3550	20	19,22,23	1.40	3 (15%)	22,31,34	1.85	5 (22%)
64	PSU	A2	93	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	3496	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
64	OMU	A2	628	64	19,22,23	1.18	2 (10%)	26,31,34	1.73	5 (19%)
27	SAC	AZ	2	27	7,8,9	0.54	0	8,9,11	0.87	1 (12%)
20	A2M	B5	3599	20	18,25,26	1.00	1 (5%)	18,36,39	1.30	2 (11%)
64	PSU	A2	1046	64	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4246	20	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	OMG	B5	3676	20	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
20	PSU	B5	1721	20	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
20	A2M	B5	2244	20,92	18,25,26	1.01	1 (5%)	18,36,39	1.22	2 (11%)
20	PSU	B5	1632	20	18,21,22	1.36	2 (11%)	22,30,33	1.85	4 (18%)
64	PSU	A2	823	64	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	3371	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
64	PSU	A2	36	64	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
64	A2M	A2	99	92,64	18,25,26	1.03	1 (5%)	18,36,39	1.18	2 (11%)
20	A2M	B5	4336	20	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)

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
6	PSU	B8	69	6	-	0/7/25/26	0/2/2/2
20	OMC	B5	2265	20,92	-	0/9/27/28	0/2/2/2
20	A2M	B5	3456	20	-	0/5/27/28	0/3/3/3
20	PSU	B5	4711	20	-	0/7/25/26	0/2/2/2
2	MLZ	Bb	5	2	-	2/7/8/10	-
64	OMU	A2	1805	64	-	0/9/27/28	0/2/2/2
64	OMG	A2	602	64	-	0/5/27/28	0/3/3/3
20	OMC	B5	2208	20,92	-	0/9/27/28	0/2/2/2
64	A2M	A2	669	92,64	-	2/5/27/28	0/3/3/3
6	OMG	B8	75	6	-	0/5/27/28	0/3/3/3
64	PSU	A2	802	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	3616	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4169	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	4245	20	-	0/5/27/28	0/3/3/3
20	OMG	B5	3476	20	-	1/5/27/28	0/3/3/3
64	MA6	A2	1851	64	-	3/7/29/30	0/3/3/3
64	OMU	A2	429	64	-	4/9/27/28	0/2/2/2
20	PSU	B5	3500	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	1693	64	-	0/7/25/26	0/2/2/2
20	5MC	B5	4193	20	-	4/7/25/26	0/2/2/2
20	OMG	B5	2267	20	-	0/5/27/28	0/3/3/3
64	PSU	A2	815	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	867	64	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	PSU	A2	864	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	3631	20	-	1/5/27/28	0/3/3/3
64	PSU	A2	816	64	-	0/7/25/26	0/2/2/2
64	A2M	A2	1032	64	-	0/5/27/28	0/3/3/3
64	PSU	A2	1348	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	4202	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	3369	20	-	0/7/25/26	0/2/2/2
64	4AC	A2	1338	64	-	3/11/29/30	0/2/2/2
20	OMG	B5	1580	20	-	0/5/27/28	0/3/3/3
20	PSU	B5	2351	20	-	0/7/25/26	0/2/2/2
64	OMU	A2	355	64	-	0/9/27/28	0/2/2/2
20	PSU	B5	4325	20	-	0/7/25/26	0/2/2/2
64	OMC	A2	518	64	-	0/9/27/28	0/2/2/2
20	PSU	B5	1720	20	-	0/7/25/26	0/2/2/2
20	OMC	B5	3540	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	4039	20	-	0/7/25/26	0/2/2/2
20	OMU	B5	3657	20	-	1/9/27/28	0/2/2/2
20	OMG	B5	1260	20	-	0/5/27/28	0/3/3/3
20	A2M	B5	2658	20,92	-	0/5/27/28	0/3/3/3
64	OMG	A2	868	64	-	1/5/27/28	0/3/3/3
20	A2M	B5	1489	20,92	-	2/5/27/28	0/3/3/3
64	PSU	A2	1005	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	3554	20	-	0/7/25/26	0/2/2/2
9	V5N	BA	216	9	-	1/5/10/12	0/1/1/1
20	OMU	B5	2680	20	-	1/9/27/28	0/2/2/2
64	OMU	A2	172	64	-	0/9/27/28	0/2/2/2
20	PSU	B5	3652	20,92	-	0/7/25/26	0/2/2/2
20	PSU	B5	4278	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4435	20	-	0/7/25/26	0/2/2/2
64	OMG	A2	684	64	-	0/5/27/28	0/3/3/3
20	A2M	B5	398	20	-	2/5/27/28	0/3/3/3
20	OMG	B5	4364	20	-	1/5/27/28	0/3/3/3
64	A2M	A2	166	64	-	0/5/27/28	0/3/3/3
20	OMC	B5	1820	20,92	-	0/9/27/28	0/2/2/2
20	PSU	B5	4322	20	-	0/7/25/26	0/2/2/2
64	A2M	A2	469	64	-	2/5/27/28	0/3/3/3
20	6MZ	B5	3966	20	-	0/5/27/28	0/3/3/3
64	OMC	A2	174	92,64	-	0/9/27/28	0/2/2/2
20	A2M	B5	3557	20	-	0/5/27/28	0/3/3/3
64	B8N	A2	1249	64	-	4/16/34/35	0/2/2/2
20	OMG	B5	1477	20	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	HY3	Aw	62	18	-	1/1/12/14	0/1/1/1
64	PSU	A2	1082	64	-	0/7/25/26	0/2/2/2
64	OMG	A2	510	92,64	-	1/5/27/28	0/3/3/3
20	PSU	B5	4267	20,92	-	0/7/25/26	0/2/2/2
64	PSU	A2	105	64	-	0/7/25/26	0/2/2/2
20	A2M	B5	2630	20,92	-	0/5/27/28	0/3/3/3
20	PSU	B5	2475	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4419	20	-	0/7/25/26	0/2/2/2
20	OMU	B5	4052	20	-	1/9/27/28	0/2/2/2
84	SAC	Br	2	84	-	1/7/8/10	-
20	PSU	B5	4045	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1638	20	-	0/7/25/26	0/2/2/2
78	MLZ	Bo	53	78	-	1/7/8/10	-
64	A2M	A2	1679	64	-	1/5/27/28	0/3/3/3
64	PSU	A2	210	64	-	0/7/25/26	0/2/2/2
20	A2M	B5	1810	20,92	-	0/5/27/28	0/3/3/3
20	PSU	B5	4382	20	-	4/7/25/26	0/2/2/2
20	PSU	B5	4740	20	-	0/7/25/26	0/2/2/2
64	A2M	A2	1384	64	-	0/5/27/28	0/3/3/3
20	PSU	B5	1801	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3466	20	-	0/7/25/26	0/2/2/2
20	OMU	B5	3973	20	-	0/9/27/28	0/2/2/2
20	OMC	B5	1284	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	4149	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4177	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	4269	20,92	-	0/5/27/28	0/3/3/3
20	PSU	B5	4203	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	1178	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	2667	20	-	1/9/27/28	0/2/2/2
64	OMG	A2	645	64	-	3/5/27/28	0/3/3/3
20	PSU	B5	3462	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	4240	20	-	0/5/27/28	0/3/3/3
64	4AC	A2	1843	64	-	4/11/29/30	0/2/2/2
64	A2M	A2	577	64	-	2/5/27/28	0/3/3/3
20	PSU	B5	3490	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4298	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4188	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3583	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4374	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1537	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	1479	20	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	B8	55	6	-	0/7/25/26	0/2/2/2
20	PSU	B5	3576	20	-	1/7/25/26	0/2/2/2
64	PSU	A2	1368	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	610	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	1175	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	1057	64	-	0/7/25/26	0/2/2/2
20	1MA	B5	1266	20,92	-	0/3/25/26	0/3/3/3
20	OMG	B5	3359	20	-	0/5/27/28	0/3/3/3
20	OMG	B5	3974	20	-	0/5/27/28	0/3/3/3
64	OMU	A2	121	64	-	0/9/27/28	0/2/2/2
64	OMU	A2	1327	92,64	-	0/9/27/28	0/2/2/2
20	OMG	B5	4369	20	-	0/5/27/28	0/3/3/3
64	A2M	A2	159	64	-	0/5/27/28	0/3/3/3
20	PSU	B5	3502	20	-	0/7/25/26	0/2/2/2
20	OMU	B5	4244	20	-	0/9/27/28	0/2/2/2
20	UR3	B5	4276	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	1245	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	4282	20,92	-	0/9/27/28	0/2/2/2
64	PSU	A2	119	64	-	0/7/25/26	0/2/2/2
64	A2M	A2	591	64	-	1/5/27/28	0/3/3/3
8	NMM	As	67	8	-	0/9/11/13	-
64	A2M	A2	513	64	-	2/5/27/28	0/3/3/3
20	A2M	B5	400	20	-	0/5/27/28	0/3/3/3
20	A2M	B5	2206	20,92	-	0/5/27/28	0/3/3/3
20	A2M	B5	3562	20	-	0/5/27/28	0/3/3/3
64	PSU	A2	1239	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	2194	20,92	-	1/9/27/28	0/2/2/2
64	OMG	A2	1448	64	-	3/5/27/28	0/3/3/3
64	PSU	A2	682	64	-	0/7/25/26	0/2/2/2
20	5MC	B5	3514	20,92	-	0/7/25/26	0/2/2/2
64	PSU	A2	1626	64	-	0/7/25/26	0/2/2/2
22	V5N	Ba	39	22	-	0/5/10/12	0/1/1/1
64	PSU	A2	109	64	-	0/7/25/26	0/2/2/2
64	OMG	A2	1491	92,64	-	0/5/27/28	0/3/3/3
64	PSU	A2	650	64	-	0/7/25/26	0/2/2/2
20	A2M	B5	4317	20	-	0/5/27/28	0/3/3/3
20	OMC	B5	2647	20	-	0/9/27/28	0/2/2/2
20	OMG	B5	3524	20	-	0/5/27/28	0/3/3/3
5	SAC	Ar	2	5	-	0/7/8/10	-
20	PSU	B5	4058	20	-	0/7/25/26	0/2/2/2
64	OMC	A2	1392	64	-	0/9/27/28	0/2/2/2
20	OMC	B5	3433	20	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	OMG	A2	1329	64	-	0/5/27/28	0/3/3/3
64	A2M	A2	485	64	-	0/5/27/28	0/3/3/3
64	A2M	A2	27	92,64	-	3/5/27/28	0/3/3/3
64	PSU	A2	1047	64	-	0/7/25/26	0/2/2/2
64	OMG	A2	437	64	-	0/5/27/28	0/3/3/3
20	PSU	B5	3494	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	1233	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	3427	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4099	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	4116	20	-	0/5/27/28	0/3/3/3
20	OMG	B5	4383	20	-	1/5/27/28	0/3/3/3
20	OMG	B5	2719	20	-	0/5/27/28	0/3/3/3
20	OMG	B5	4138	20	-	0/5/27/28	0/3/3/3
64	6MZ	A2	1833	92,64	-	0/5/27/28	0/3/3/3
20	PSU	B5	3447	20	-	0/7/25/26	0/2/2/2
20	OMC	B5	2704	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	4107	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	3450	20	-	0/5/27/28	0/3/3/3
64	PSU	A2	1644	92,64	-	0/7/25/26	0/2/2/2
64	PSU	A2	573	64	-	0/7/25/26	0/2/2/2
64	OMC	A2	463	64	-	0/9/27/28	0/2/2/2
20	A2M	B5	3492	20,64	-	1/5/27/28	0/3/3/3
64	OMU	A2	1443	92,64	-	0/9/27/28	0/2/2/2
64	PSU	A2	652	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	687	64	-	0/7/25/26	0/2/2/2
64	OMC	A2	1704	64	-	1/9/27/28	0/2/2/2
20	PSU	B5	4749	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3585	20,92	-	0/7/25/26	0/2/2/2
64	OMU	A2	116	64	-	0/9/27/28	0/2/2/2
64	MA6	A2	1852	64	-	4/7/29/30	0/3/3/3
20	PSU	B5	4166	20	-	3/7/25/26	0/2/2/2
20	PSU	B5	4217	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1718	20	-	0/7/25/26	0/2/2/2
14	AME	Au	1	14	-	2/9/10/12	-
64	OMU	A2	1289	64	-	0/9/27/28	0/2/2/2
20	PSU	B5	1491	20	-	0/7/25/26	0/2/2/2
20	OMC	B5	3619	20	-	2/9/27/28	0/2/2/2
20	PSU	B5	1799	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	34	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	1731	20	-	0/7/25/26	0/2/2/2
20	OMC	B5	3573	20	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HIC	BB	245	12	-	2/5/6/8	0/1/1/1
20	OMG	B5	3942	20,4	-	0/5/27/28	0/3/3/3
20	OMU	B5	4366	20	-	0/9/27/28	0/2/2/2
64	PSU	A2	967	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	2207	20	-	2/5/27/28	0/3/3/3
20	A2M	B5	1270	20	-	0/5/27/28	0/3/3/3
64	PSU	A2	407	64	-	0/7/25/26	0/2/2/2
15	AYA	BC	2	15	-	3/4/6/8	-
64	PSU	A2	1446	64	-	0/7/25/26	0/2/2/2
64	G7M	A2	1640	64	-	2/3/25/26	0/3/3/3
75	M3L	Bm	98	75	-	0/9/10/12	-
80	IAS	An	138	80	-	2/7/7/8	-
20	OMU	B5	2258	20	-	0/9/27/28	0/2/2/2
20	OMC	B5	3601	20	-	0/9/27/28	0/2/2/2
20	A2M	B5	3517	20	-	2/5/27/28	0/3/3/3
20	PSU	B5	4042	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1683	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	218	64	-	0/7/25/26	0/2/2/2
20	UY1	B5	3550	20	-	1/9/27/28	0/2/2/2
64	PSU	A2	93	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	3496	20	-	0/7/25/26	0/2/2/2
64	OMU	A2	628	64	-	4/9/27/28	0/2/2/2
27	SAC	AZ	2	27	-	2/7/8/10	-
20	A2M	B5	3599	20	-	1/5/27/28	0/3/3/3
64	PSU	A2	1046	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	4246	20	-	2/7/25/26	0/2/2/2
20	OMG	B5	3676	20	-	0/5/27/28	0/3/3/3
20	PSU	B5	1721	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	2244	20,92	-	0/5/27/28	0/3/3/3
20	PSU	B5	1632	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	823	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	3371	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	36	64	-	0/7/25/26	0/2/2/2
64	A2M	A2	99	92,64	-	1/5/27/28	0/3/3/3
20	A2M	B5	4336	20	-	1/5/27/28	0/3/3/3

The worst 5 of 327 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	A2	1640	G7M	C5-C4	7.45	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	A2	1640	G7M	O6-C6	7.28	1.38	1.23
20	B5	1266	1MA	C2-N3	5.00	1.35	1.29
18	Aw	62	HY3	C3-CA	-4.49	1.50	1.55
64	A2	1640	G7M	C2-N2	4.48	1.44	1.34

The worst 5 of 546 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	4246	PSU	N1-C2-N3	6.09	122.03	115.13
20	B5	3494	PSU	N1-C2-N3	6.04	121.97	115.13
64	A2	682	PSU	N1-C2-N3	6.03	121.97	115.13
64	A2	1178	PSU	N1-C2-N3	6.01	121.94	115.13
20	B5	4267	PSU	N1-C2-N3	6.00	121.93	115.13

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	BA	216	V5N	O-C-CA-CB
12	BB	245	HIC	CA-CB-CG-ND1
15	BC	2	AYA	C-CA-N-CT
20	B5	3433	OMC	C2'-C1'-N1-C2
20	B5	3433	OMC	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

## 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 4.6 Ligand geometry [i](#)

Of 740 ligands modelled in this entry, 277 are unknown and 428 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	$\# Z  > 2$
94	SPD	B5	5276	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5066	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	A2	1928	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5359	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPD	B5	5122	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5257	-	9,9,9	0.16	0	8,8,8	0.17	0
97	IHP	DB	901	-	36,36,36	1.55	6 (16%)	54,60,60	1.13	4 (7%)
94	SPD	B5	5237	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	5046	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5101	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	5140	-	9,9,9	0.16	0	8,8,8	0.18	0
95	SPM	A2	1939	-	13,13,13	0.14	0	12,12,12	0.17	0
95	SPM	B5	4947	-	13,13,13	0.15	0	12,12,12	0.19	0
94	SPD	B5	5010	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	5027	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	2056	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5318	-	9,9,9	0.16	0	8,8,8	0.17	0
94	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.19	0
95	SPM	B5	5203	-	13,13,13	0.15	0	12,12,12	0.14	0
94	SPD	B5	5216	-	9,9,9	0.15	0	8,8,8	0.15	0
94	SPD	A2	2063	-	9,9,9	0.16	0	8,8,8	0.17	0
94	SPD	B5	4989	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPD	B5	4905	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5297	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	A2	1921	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	1935	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5159	-	9,9,9	0.15	0	8,8,8	0.16	0
93	GTP	B7	212	3	26,34,34	0.94	2 (7%)	32,54,54	0.76	0
94	SPD	A2	1908	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	4926	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	4968	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	A2	1915	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	5377	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	5338	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5084	-	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
94	SPD	B5	5276	-	-	0/7/7/7	-
94	SPD	B5	5066	-	-	0/7/7/7	-
94	SPD	A2	1928	-	-	1/7/7/7	-
94	SPD	B5	5359	-	-	0/7/7/7	-
94	SPD	B5	5122	-	-	1/7/7/7	-
94	SPD	B5	5257	-	-	1/7/7/7	-
97	IHP	DB	901	-	-	8/30/54/54	0/1/1/1
94	SPD	B5	5237	-	-	1/7/7/7	-
94	SPD	B5	5046	-	-	0/7/7/7	-
94	SPD	B5	5101	-	-	0/7/7/7	-
94	SPD	B5	5140	-	-	0/7/7/7	-
95	SPM	A2	1939	-	-	1/11/11/11	-
95	SPM	B5	4947	-	-	1/11/11/11	-
94	SPD	B5	5010	-	-	0/7/7/7	-
94	SPD	B5	5027	-	-	0/7/7/7	-
94	SPD	A2	2056	-	-	1/7/7/7	-
94	SPD	B5	5318	-	-	1/7/7/7	-
94	SPD	A2	1901	-	-	0/7/7/7	-
95	SPM	B5	5203	-	-	0/11/11/11	-
94	SPD	B5	5216	-	-	1/7/7/7	-
94	SPD	A2	2063	-	-	0/7/7/7	-
94	SPD	B5	4989	-	-	0/7/7/7	-
94	SPD	B5	4905	-	-	1/7/7/7	-
94	SPD	B5	5297	-	-	1/7/7/7	-
94	SPD	A2	1921	-	-	0/7/7/7	-
94	SPD	A2	1935	-	-	0/7/7/7	-
94	SPD	B5	5159	-	-	1/7/7/7	-
93	GTP	B7	212	3	-	0/18/38/38	0/3/3/3
94	SPD	A2	1908	-	-	0/7/7/7	-
94	SPD	B5	4926	-	-	0/7/7/7	-
94	SPD	B5	4968	-	-	0/7/7/7	-
94	SPD	A2	1915	-	-	0/7/7/7	-
94	SPD	B5	5377	-	-	0/7/7/7	-
94	SPD	B5	5338	-	-	0/7/7/7	-
94	SPD	B5	5084	-	-	0/7/7/7	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	DB	901	IHP	P2-O12	3.53	1.66	1.59
97	DB	901	IHP	P5-O15	3.45	1.65	1.59
97	DB	901	IHP	P1-O11	3.25	1.65	1.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	DB	901	IHP	P6-O16	3.22	1.65	1.59
97	DB	901	IHP	P3-O13	3.20	1.65	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	DB	901	IHP	C6-C5-C4	4.29	119.80	110.41
97	DB	901	IHP	C5-C4-C3	3.60	118.29	110.41
97	DB	901	IHP	C5-C6-C1	3.58	118.24	110.41
97	DB	901	IHP	C4-C3-C2	2.22	115.27	110.41

There are no chirality outliers.

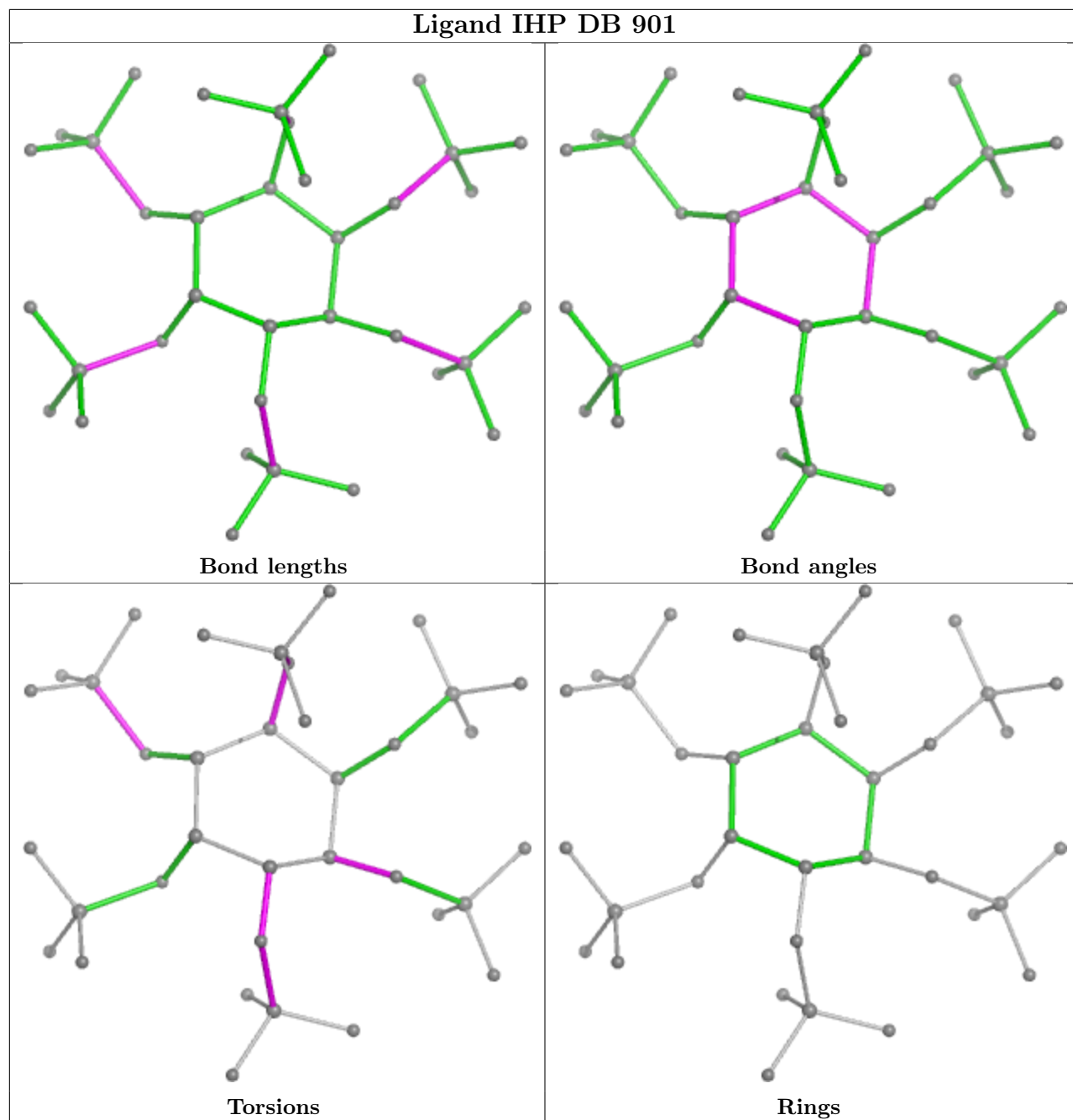
5 of 20 torsion outliers are listed below:

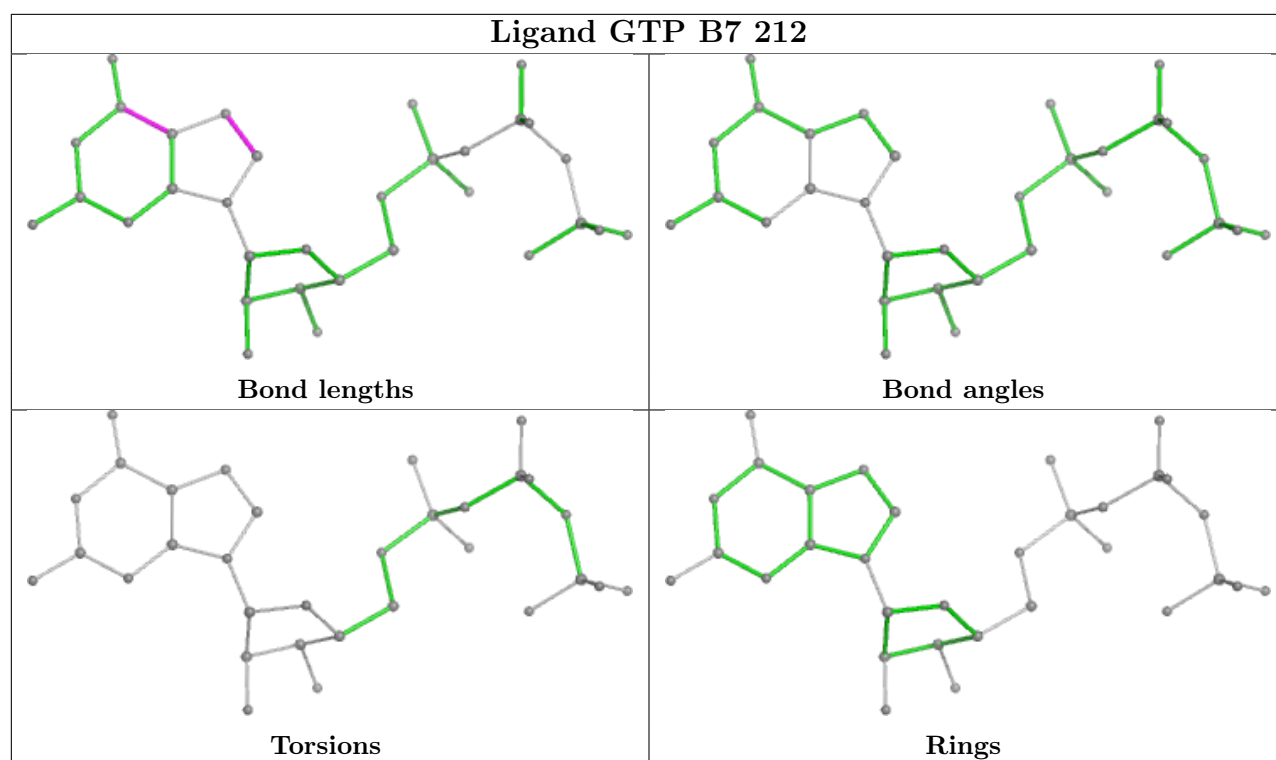
Mol	Chain	Res	Type	Atoms
97	DB	901	IHP	C1-C2-O12-P2
97	DB	901	IHP	C4-C5-O15-P5
97	DB	901	IHP	C4-O14-P4-O34
95	A2	1939	SPM	C8-C9-N10-C11
97	DB	901	IHP	C4-O14-P4-O24

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.



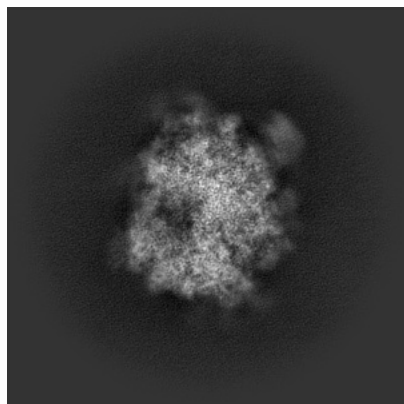
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50125. These allow visual inspection of the internal detail of the map and identification of artifacts.

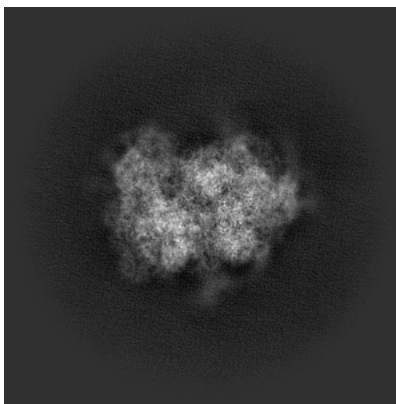
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 5.1 Orthogonal projections [i](#)

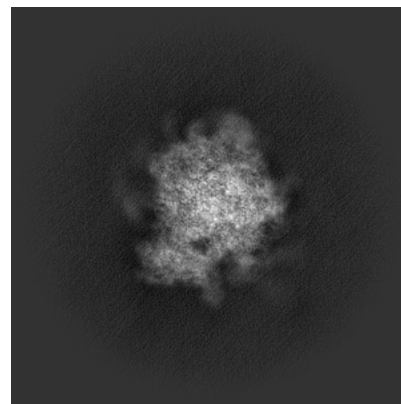
#### 5.1.1 Primary map



X

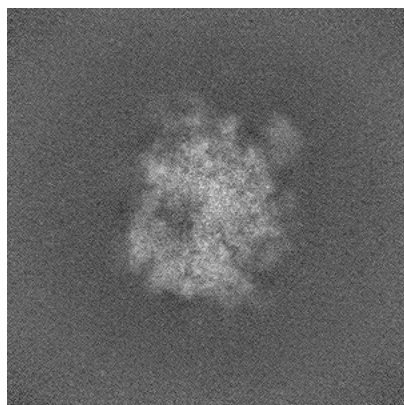


Y

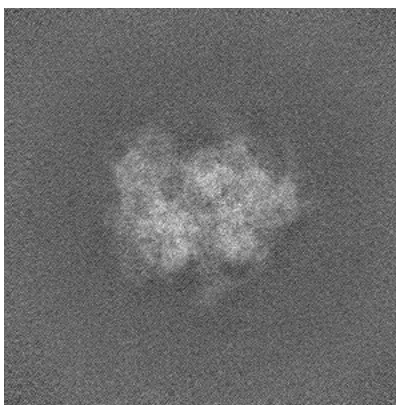


Z

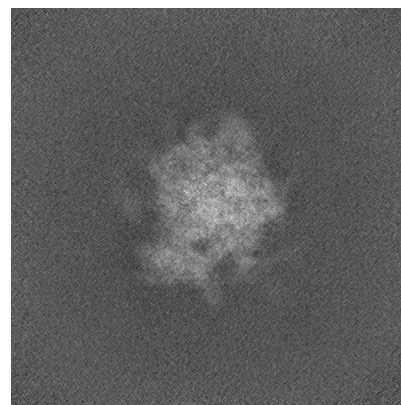
#### 5.1.2 Raw map



X



Y

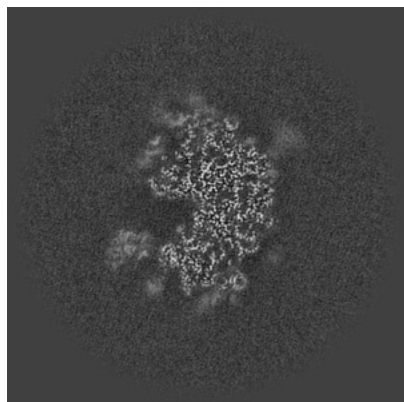


Z

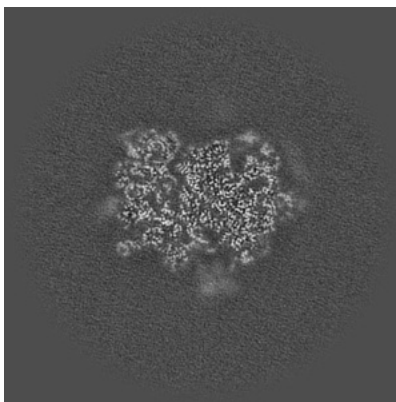
The images above show the map projected in three orthogonal directions.

## 5.2 Central slices [i](#)

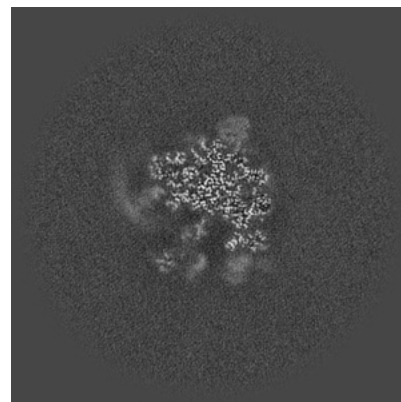
### 5.2.1 Primary map



X Index: 280

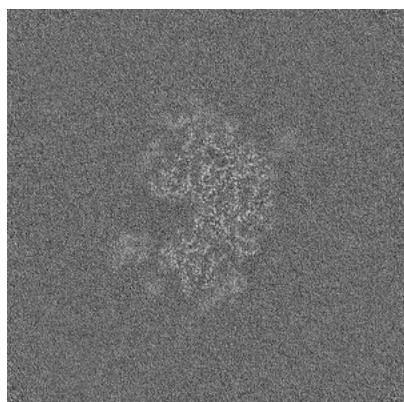


Y Index: 280

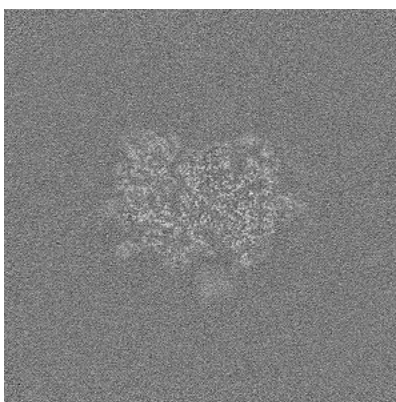


Z Index: 280

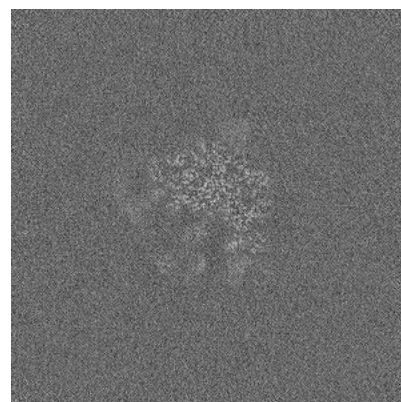
### 5.2.2 Raw map



X Index: 280



Y Index: 280

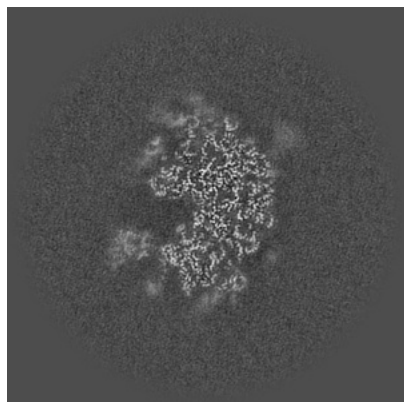


Z Index: 280

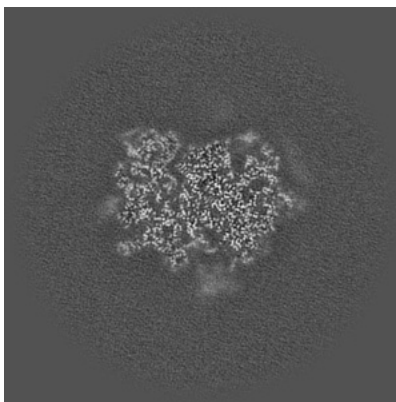
The images above show central slices of the map in three orthogonal directions.

## 5.3 Largest variance slices [i](#)

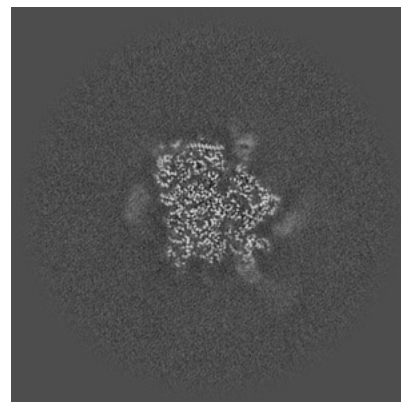
### 5.3.1 Primary map



X Index: 279

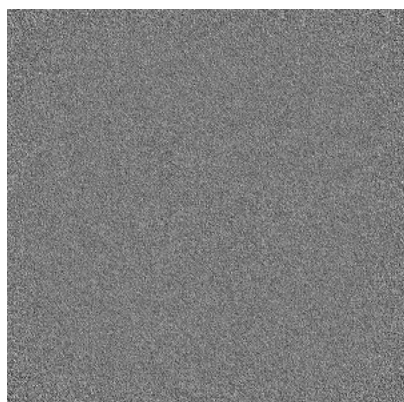


Y Index: 281

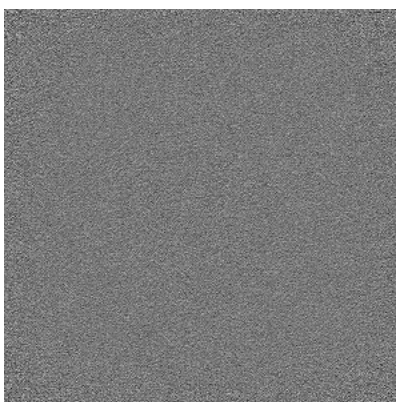


Z Index: 309

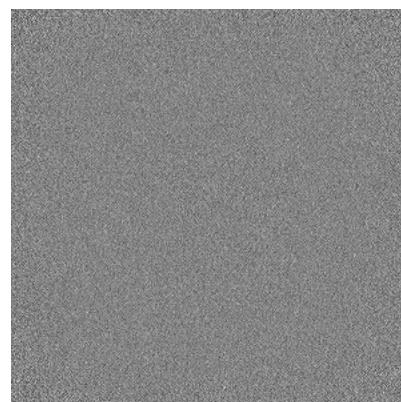
### 5.3.2 Raw map



X Index: 0



Y Index: 0



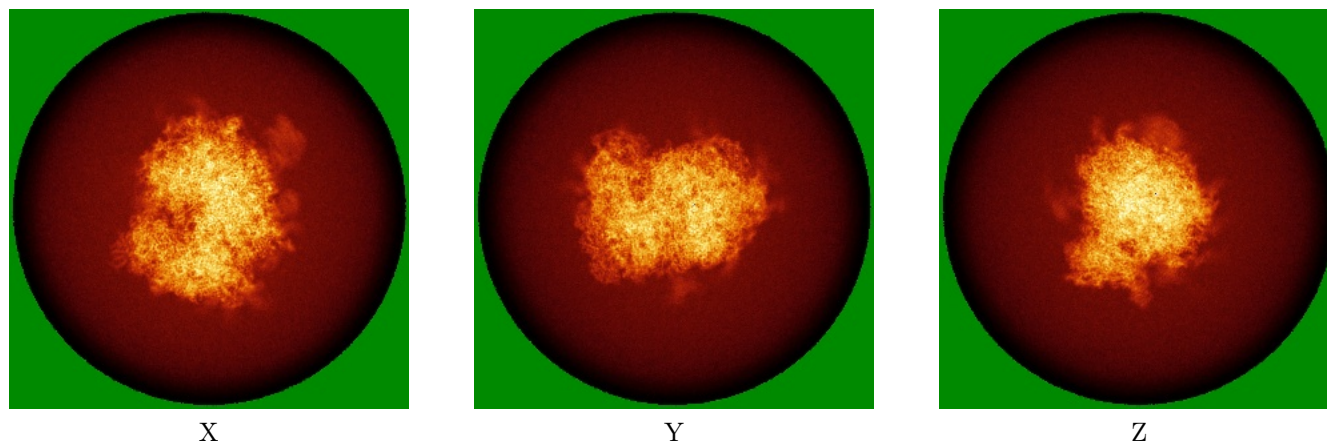
Z Index: 0

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

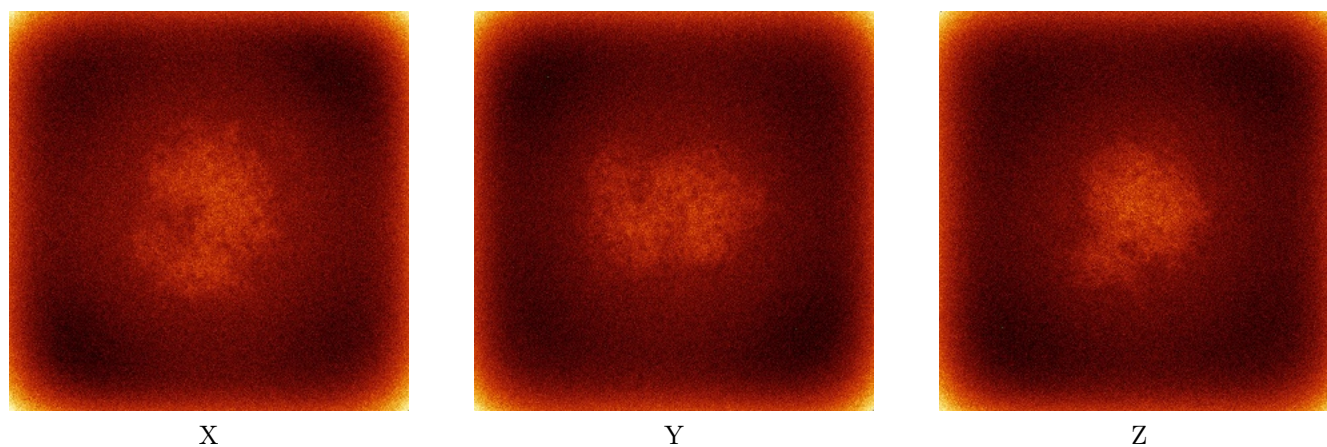


## 5.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 5.4.1 Primary map



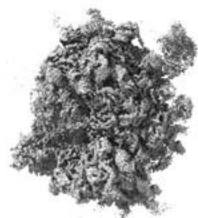
### 5.4.2 Raw map



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

## 5.5 Orthogonal surface views [i](#)

### 5.5.1 Primary map



X



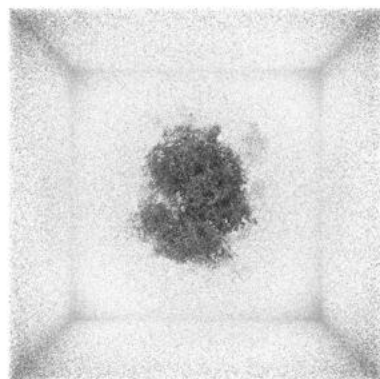
Y



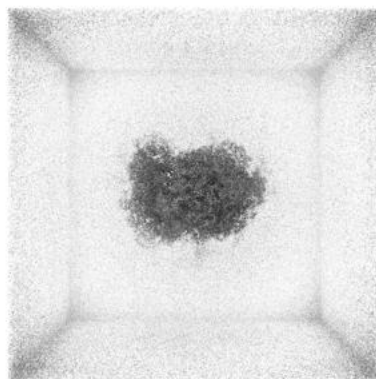
Z

The images above show the 3D surface view of the map at the recommended contour level 0.175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

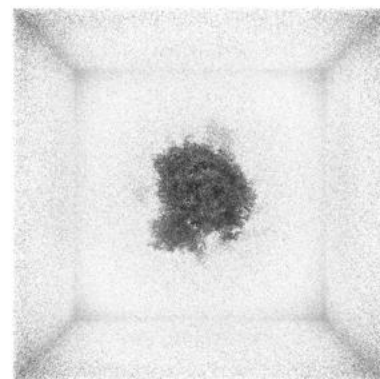
### 5.5.2 Raw map



X



Y



Z

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

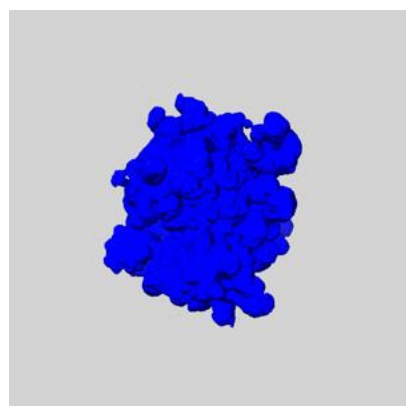
## 5.6 Mask visualisation [i](#)

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

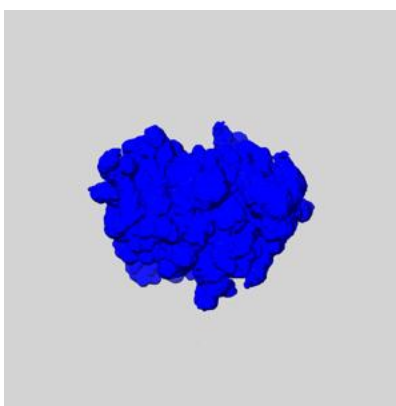
A mask typically either:

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

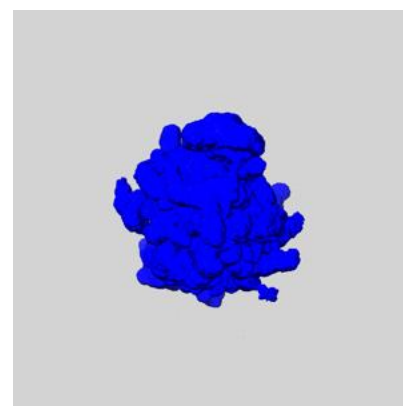
### 5.6.1 emd\_50125\_msk\_1.map [i](#)



X

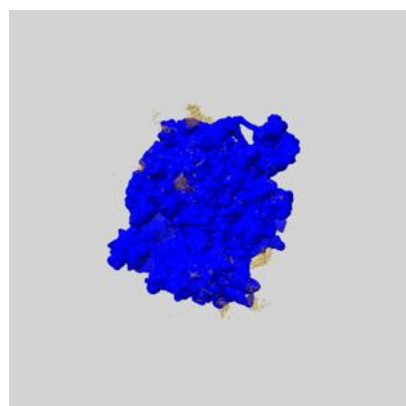


Y

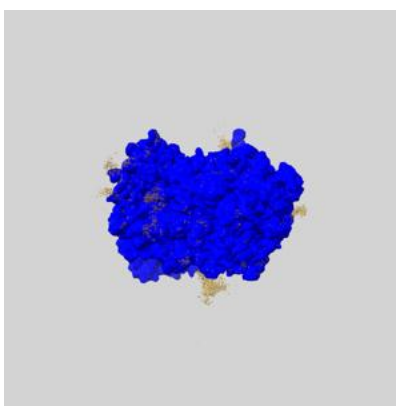


Z

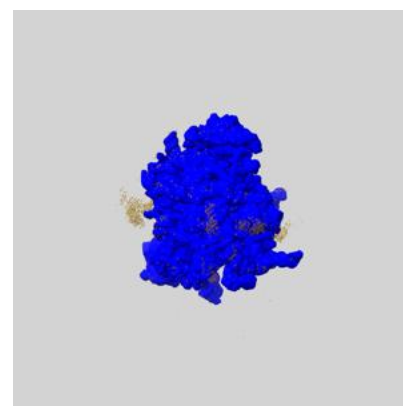
### 5.6.2 emd\_50125\_msk\_2.map [i](#)



X



Y

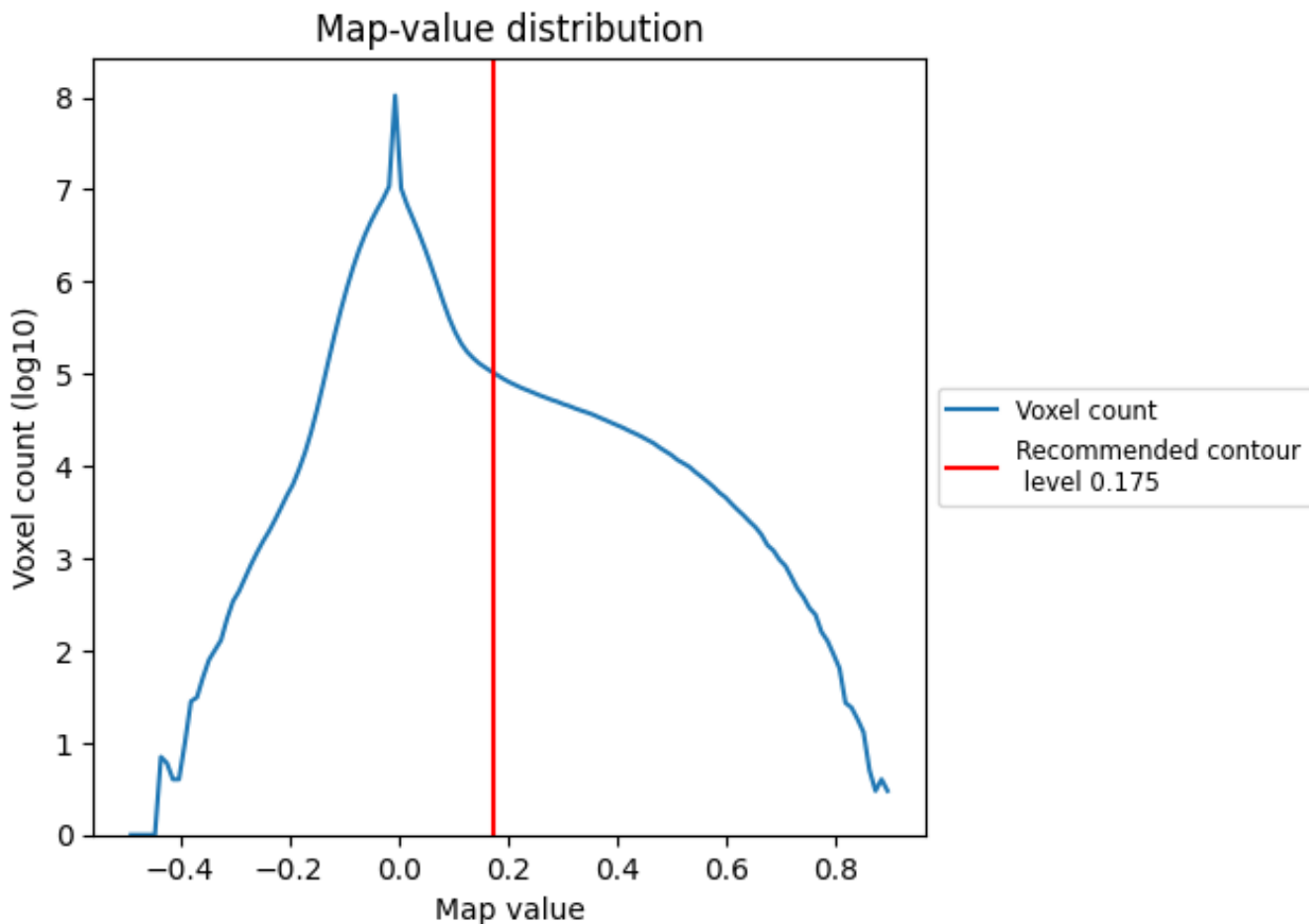


Z

## 6 Map analysis [i](#)

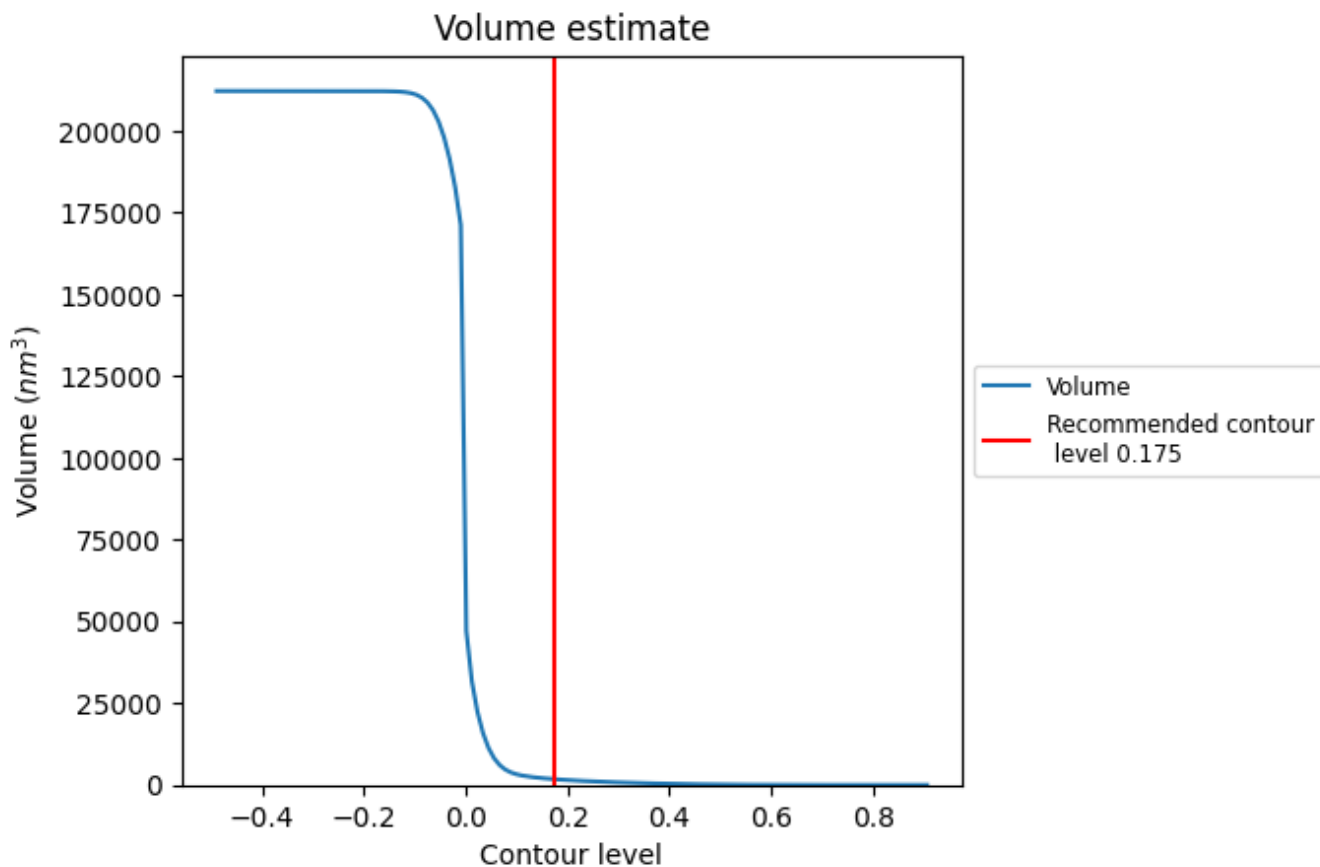
This section contains the results of statistical analysis of the map.

### 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](#)

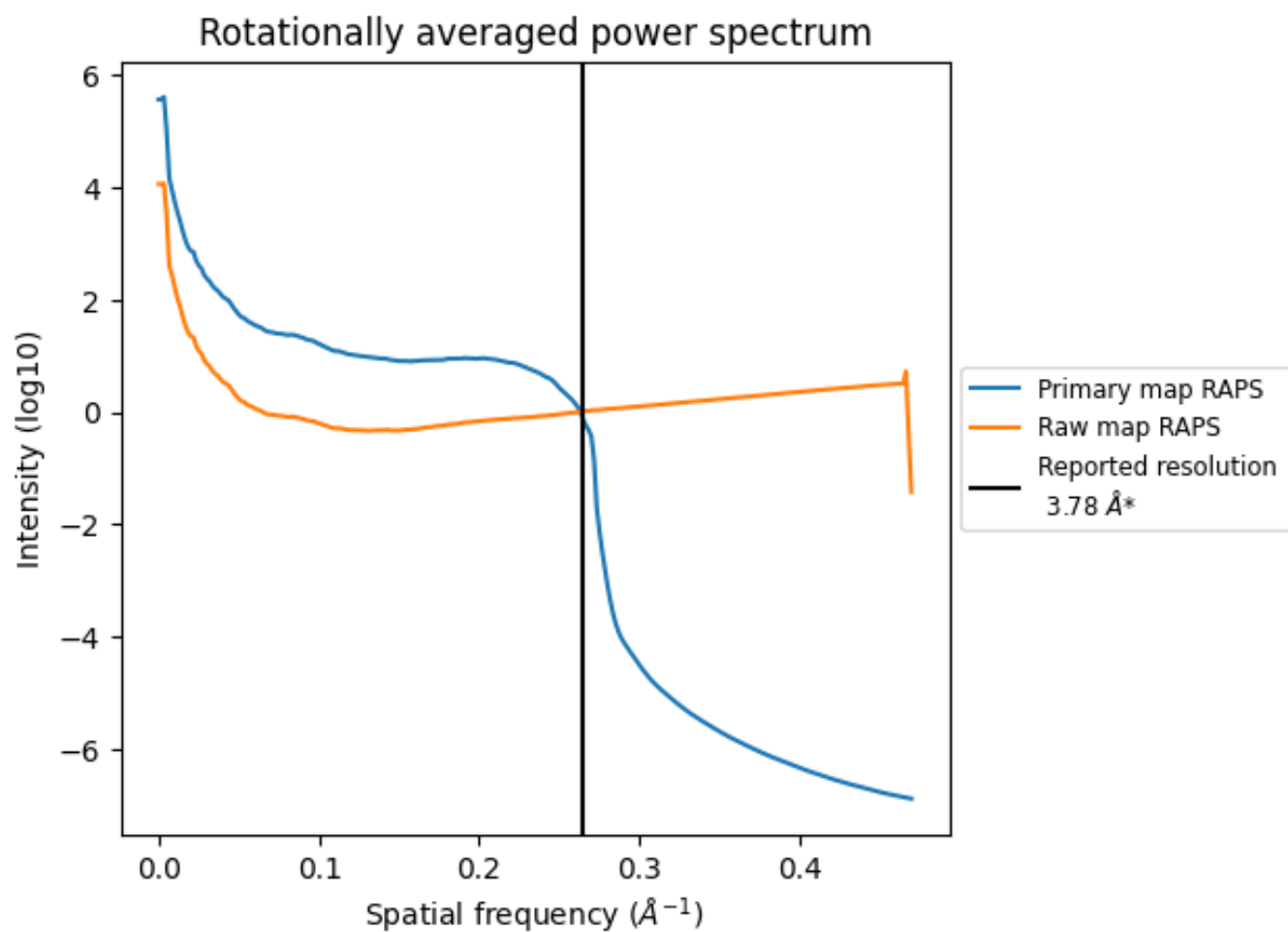


The volume at the recommended contour level is 1752  $\text{nm}^3$ ; this corresponds to an approximate mass of 1582 kDa.

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

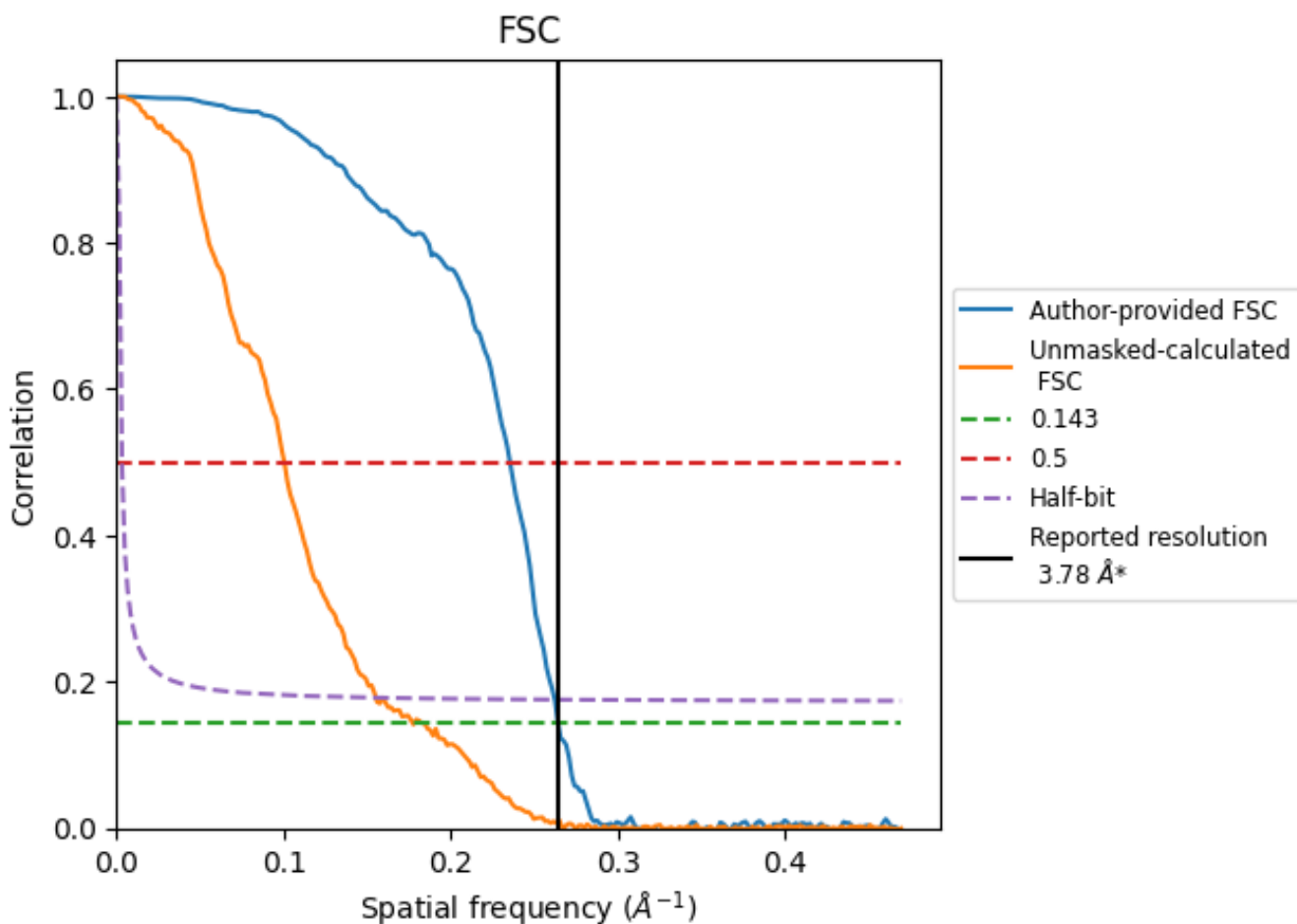


\*Reported resolution corresponds to spatial frequency of 0.265 Å<sup>-1</sup>

## 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 0.265 Å<sup>-1</sup>

## 7.2 Resolution estimates [i](#)

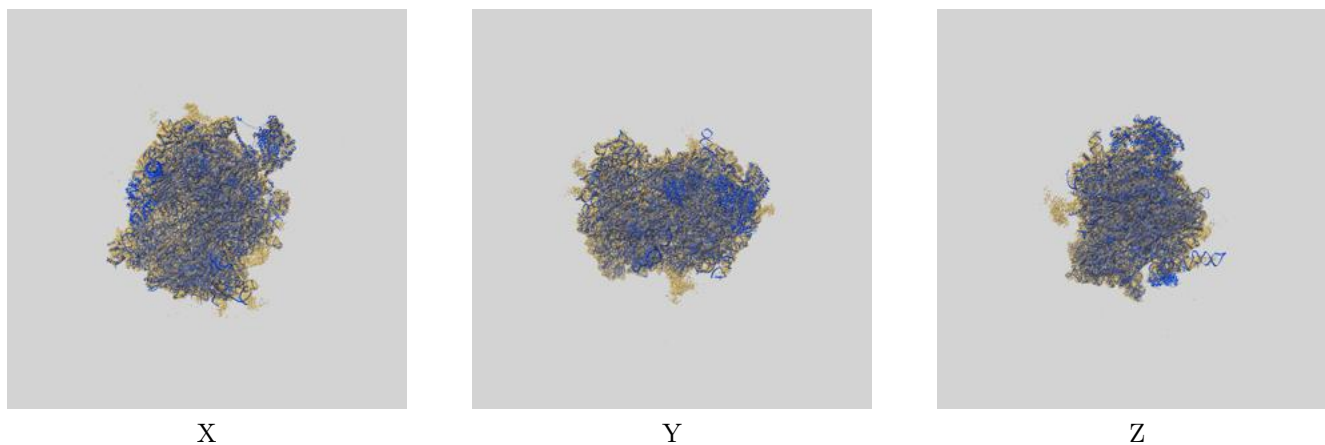
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.78	-	-
Author-provided FSC curve	3.79	4.25	3.81
Unmasked-calculated*	5.64	9.95	6.44

\*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 5.64 differs from the reported value 3.78 by more than 10 %

## 8 Map-model fit [i](#)

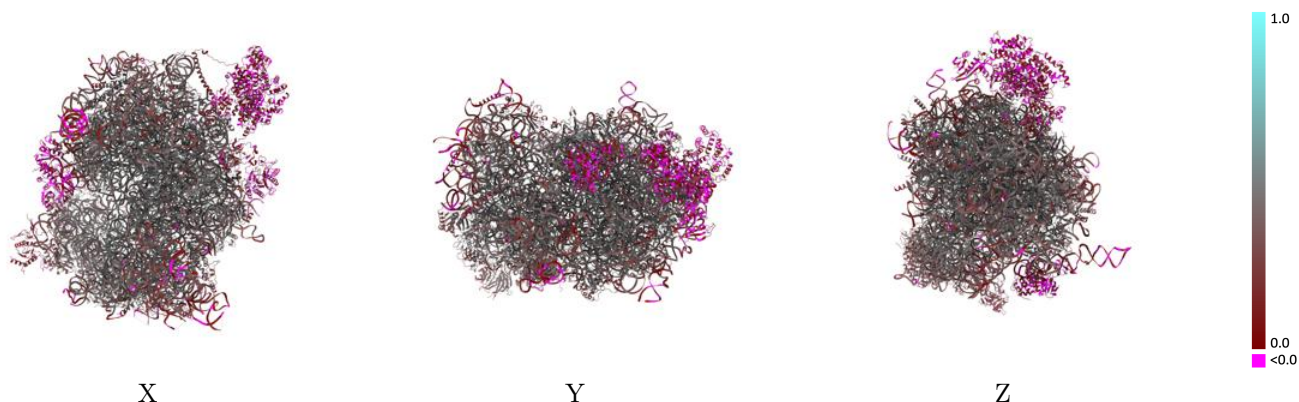
This section contains information regarding the fit between EMDB map EMD-50125 and PDB model 9F1C. Per-residue inclusion information can be found in section ?? on page ??.

### 8.1 Map-model overlay [i](#)



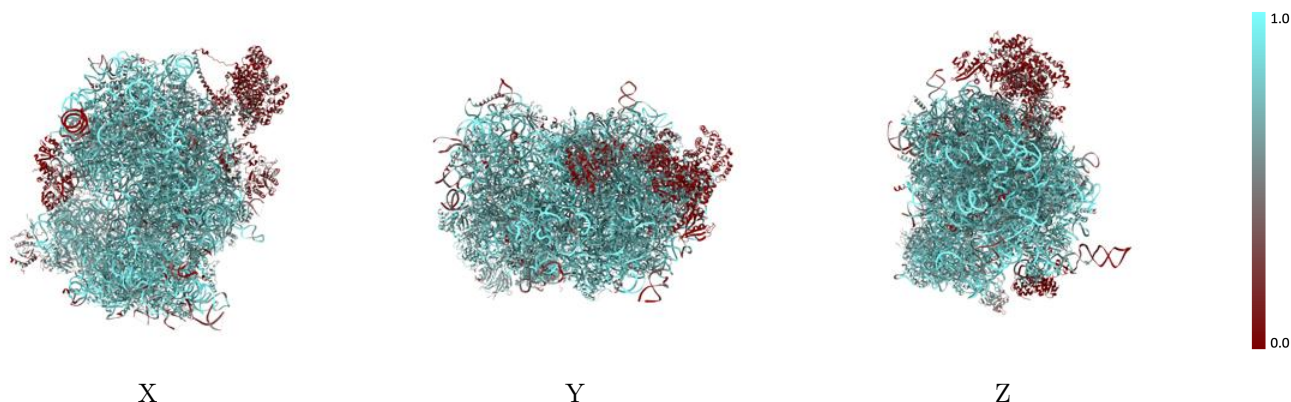
The images above show the 3D surface view of the map at the recommended contour level 0.175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



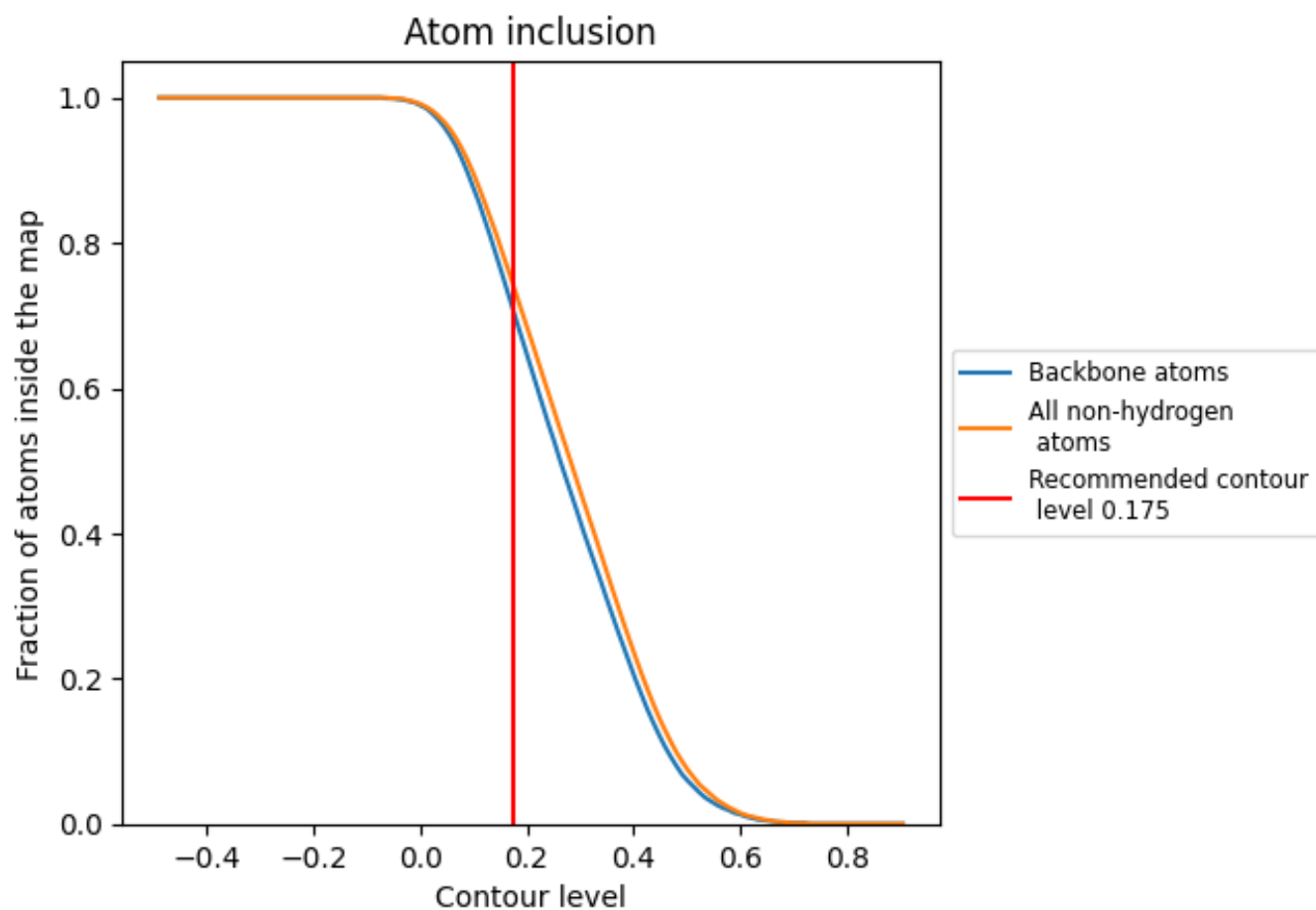
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.175).







































































## 8.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 74% 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 (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.3710
A2	 0.8600	 0.3810
AA	 0.6760	 0.4110
AB	 0.6600	 0.3880
AC	 0.3940	 0.1490
AD	 0.5930	 0.3680
AE	 0.7560	 0.4390
AF	 0.6470	 0.3060
AG	 0.7510	 0.4020
AH	 0.0280	 0.3250
AT	 0.6350	 0.3910
AZ	 0.7240	 0.4020
Aa	 0.6740	 0.3990
Ab	 0.7340	 0.4300
Ac	 0.6500	 0.3710
Ad	 0.7290	 0.4210
Ae	 0.6520	 0.3620
Af	 0.6510	 0.3130
Ag	 0.6710	 0.3600
Ah	 0.7170	 0.4040
Ai	 0.7510	 0.4030
Aj	 0.6900	 0.3310
Ak	 0.6670	 0.4120
Al	 0.3330	 0.1440
Am	 0.7160	 0.4190
An	 0.7180	 0.4140
Ao	 0.6340	 0.3030
Ap	 0.6990	 0.3720
Aq	 0.6880	 0.3610
Ar	 0.6410	 0.3170
As	 0.6820	 0.3330
At	 0.6270	 0.3340
Au	 0.7240	 0.4110
Av	 0.6950	 0.4460
Aw	 0.7440	 0.4470



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

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Chain	Atom inclusion	Q-score
Ax	 0.7400	 0.3790
Ay	 0.5380	 0.2820
Az	 0.6060	 0.4180
B	 0.7560	 0.3920
B5	 0.8520	 0.3890
B7	 0.9210	 0.4170
B8	 0.8800	 0.4080
BA	 0.7300	 0.4580
BB	 0.7510	 0.4410
BC	 0.7560	 0.4440
BE	 0.6790	 0.3760
BF	 0.7450	 0.4340
BG	 0.7050	 0.3870
BH	 0.7190	 0.4120
BI	 0.7360	 0.4420
BJ	 0.7080	 0.3880
BK	 0.2060	 0.4310
BL	 0.7220	 0.4110
BM	 0.7450	 0.4020
BN	 0.7720	 0.4610
BO	 0.7430	 0.4370
BP	 0.7280	 0.4460
BQ	 0.7530	 0.4590
BR	 0.7160	 0.3890
BS	 0.7550	 0.4500
BT	 0.7140	 0.4400
BU	 0.7220	 0.4260
BV	 0.7000	 0.4500
BW	 0.5760	 0.3170
BX	 0.7130	 0.4280
BY	 0.7160	 0.4270
BZ	 0.7470	 0.3990
Ba	 0.7950	 0.4520
Bb	 0.6600	 0.3700
Bc	 0.6290	 0.3620
Bd	 0.7350	 0.4430
Be	 0.7580	 0.4550
Bf	 0.7740	 0.4620
Bg	 0.7120	 0.4330
Bh	 0.7340	 0.4130
Bi	 0.7240	 0.4000
Bj	 0.8250	 0.4710

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Chain	Atom inclusion	Q-score
Bk	 0.6340	 0.3640
Bl	 0.7260	 0.4500
Bm	 0.7280	 0.4220
Bo	 0.7080	 0.4360
Bp	 0.7130	 0.4270
Br	 0.7430	 0.4560
Bs	 0.0440	 0.0350
Bt	 0.0450	 0.0550
Ct	 0.1950	 0.1080
Cu	 0.3250	 0.2200
DA	 0.0350	 0.0460
DB	 0.1690	 0.0860
DC	 0.1490	 0.0510
EA	 0.1620	 0.0470