



wwPDB EM Validation Summary Report ⓘ

Sep 21, 2024 – 10:28 am BST

PDB ID : 9F1B
EMDB ID : EMD-50124
Title : Mammalian ternary complex of a translating 80S ribosome, NAC and NatA/E
Authors : Yudin, D.; Scaiola, A.; Ban, N.
Deposited on : 2024-04-18
Resolution : 3.01 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.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 3.01 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

There are 97 unique types of molecules in this entry. The entry contains 234232 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BP	153	1242	777	241	215	9	0	0

- Molecule 2 is a protein called 40S ribosomal protein eS17.

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

- Molecule 3 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Bo	105	863	543	175	139	6	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 protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Cu	105	813	508	152	150	3	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	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 8 is a protein called Ribosomal_L23eN domain-containing protein.

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

- Molecule 9 is a protein called 60S ribosomal protein L37a.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL18.

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

- Molecule 11 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	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 12 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	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 13 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	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 14 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 15 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 16 is a protein called 60S ribosomal protein L7a.

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

- Molecule 17 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	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 18 is a protein called Ribosomal protein S15a.

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

- Molecule 19 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 20 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace	
20	Ct	115	Total	C	N	O	S	0	0
			895	561	163	167	4		

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
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 21 is a protein called 60S ribosomal protein L9.

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

- Molecule 22 is a protein called Ribosomal protein L23.

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

- Molecule 23 is a protein called 40S ribosomal protein S23.

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

- Molecule 24 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	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 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called 60S ribosomal protein L10.

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

- Molecule 28 is a protein called 40S ribosomal protein S24.

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

- Molecule 29 is a RNA chain called 5S rRNA.

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

- Molecule 30 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 31 is a protein called 60S ribosomal protein L11.

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

- Molecule 32 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 33 is a protein called 40S ribosomal protein S25.

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

- Molecule 34 is a RNA chain called 5.8S rRNA.

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

- Molecule 35 is a protein called Nascent chain.

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

- Molecule 36 is a protein called 40S ribosomal protein S3a.

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

- Molecule 37 is a protein called 60S ribosomal protein L41.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 39 is a protein called 60S ribosomal protein L12.

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

- Molecule 40 is a protein called 60S ribosomal protein L14.

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

- Molecule 41 is a protein called 40S ribosomal protein S2.

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

- Molecule 42 is a protein called Ribosomal protein L26.

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

- Molecule 43 is a protein called Ribosomal protein L3.

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

- Molecule 44 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 45 is a protein called 40S ribosomal protein S3.

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

- Molecule 46 is a protein called 60S ribosomal protein L27.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 48 is a protein called Ribosomal protein L15.

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

- Molecule 49 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	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 50 is a protein called 60S ribosomal protein L27a.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	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 52 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 53 is a protein called Ribosomal protein S5.

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

- Molecule 54 is a protein called 60S ribosomal protein L29.

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

- Molecule 55 is a protein called 60S ribosomal protein L6.

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

- Molecule 56 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		
56	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
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 57 is a protein called 40S ribosomal protein S6.

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

- Molecule 58 is a protein called 60S ribosomal protein L30.

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

- Molecule 59 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	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 60 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	DC	165	1339	844	242	242	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 S7.

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

- Molecule 62 is a protein called 60S ribosomal protein L31.

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

- Molecule 63 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
63	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 64 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	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 65 is a protein called Ribosomal protein L32.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Be	22	ARG	CYS	variant	UNP G1U6S0
Be	75	ARG	HIS	variant	UNP G1U6S0

- Molecule 66 is a protein called 40S ribosomal protein S27.

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

- Molecule 67 is a protein called 40S ribosomal protein S9.

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

- Molecule 68 is a protein called 60S ribosomal protein L35a.

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

- Molecule 69 is a protein called 40S ribosomal protein S28.

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

- Molecule 70 is a protein called S10_ plectin domain-containing protein.

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

- Molecule 71 is a protein called Large ribosomal subunit protein eL34.

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

- Molecule 72 is a protein called Ribosomal protein S27a.

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

- 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 60S ribosomal protein L35.

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

- Molecule 75 is a protein called 40S ribosomal protein S30.

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

- Molecule 76 is a protein called 40S ribosomal protein S12.

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

- Molecule 77 is a protein called 60S ribosomal protein L36.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 79 is a protein called 40S ribosomal protein S13.

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

- Molecule 80 is a protein called Ribosomal protein L37.

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

- Molecule 81 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 82 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 83 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	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	variant	UNP G1U001

- Molecule 84 is a protein called 40S ribosomal protein S29.

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

- Molecule 85 is a protein called 40S ribosomal protein uS19.

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

- Molecule 86 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 87 is a RNA chain called mRNA.

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

- Molecule 88 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 89 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

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

- Molecule 90 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	BP	1	Total 1	Mg 1	0
90	AT	3	Total 3	Mg 3	0
90	BR	1	Total 1	Mg 1	0
90	Ct	1	Total 1	Mg 1	0
90	BV	1	Total 1	Mg 1	0
90	B5	282	Total 282	Mg 282	0
90	BI	1	Total 1	Mg 1	0
90	B7	9	Total 9	Mg 9	0
90	B8	9	Total 9	Mg 9	0
90	Ba	1	Total 1	Mg 1	0
90	Af	1	Total 1	Mg 1	0
90	A2	108	Total 108	Mg 108	0
90	Bj	1	Total 1	Mg 1	0
90	An	1	Total 1	Mg 1	0

- Molecule 91 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	Bo	1	Total 1	Zn 1	0
91	Bp	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
91	Bg	1	Total 1	Zn 1	0
91	AC	1	Total 1	Zn 1	0
91	AE	1	Total 1	Zn 1	0
91	Bj	1	Total 1	Zn 1	0
91	AG	1	Total 1	Zn 1	0
91	Bm	1	Total 1	Zn 1	0

- Molecule 92 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

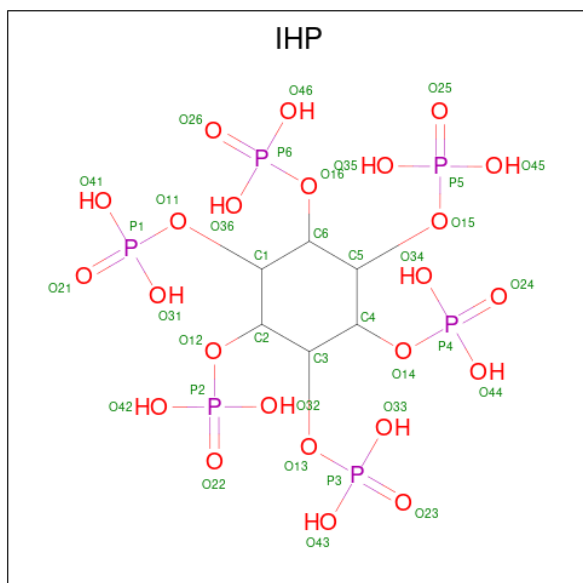
Mol	Chain	Residues	Atoms		AltConf
92	Bo	1	Total 1	X 1	0
92	AT	2	Total 2	X 2	0
92	Ar	1	Total 1	X 1	0
92	BL	1	Total 1	X 1	0
92	BQ	2	Total 2	X 2	0
92	BH	1	Total 1	X 1	0
92	B5	207	Total 207	X 207	0
92	BT	2	Total 2	X 2	0
92	BI	1	Total 1	X 1	0
92	B7	6	Total 6	X 6	0
92	B8	7	Total 7	X 7	0
92	BA	4	Total 4	X 4	0
92	BB	2	Total 2	X 2	0

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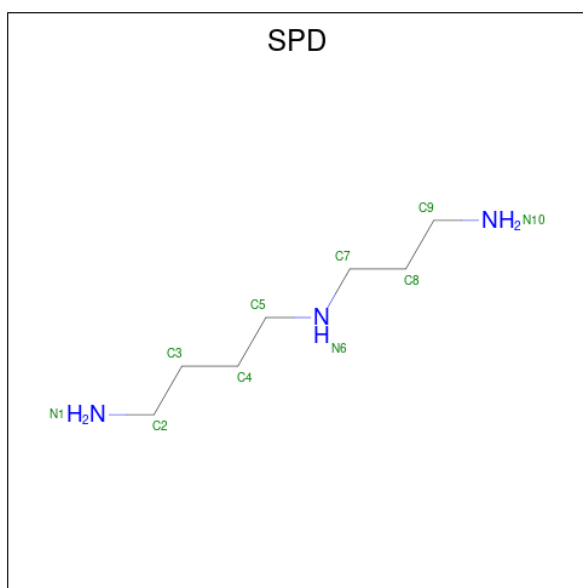
Mol	Chain	Residues	Atoms		AltConf
			Total	X	
92	BN	1	1	1	0
92	Ae	1	1	1	0
92	Bb	2	2	2	0
92	A2	57	57	57	0
92	Be	3	3	3	0
92	Bf	1	1	1	0
92	Ak	1	1	1	0
92	Bj	1	1	1	0
92	An	1	1	1	0
92	Bl	1	1	1	0

- Molecule 93 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

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



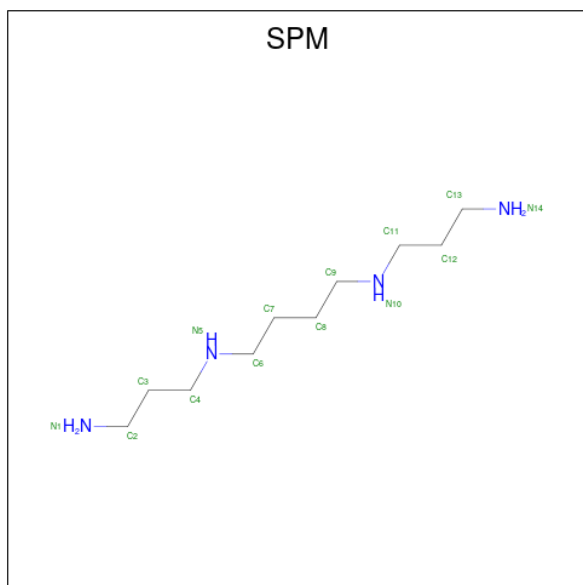
Mol	Chain	Residues	Atoms			AltConf
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N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

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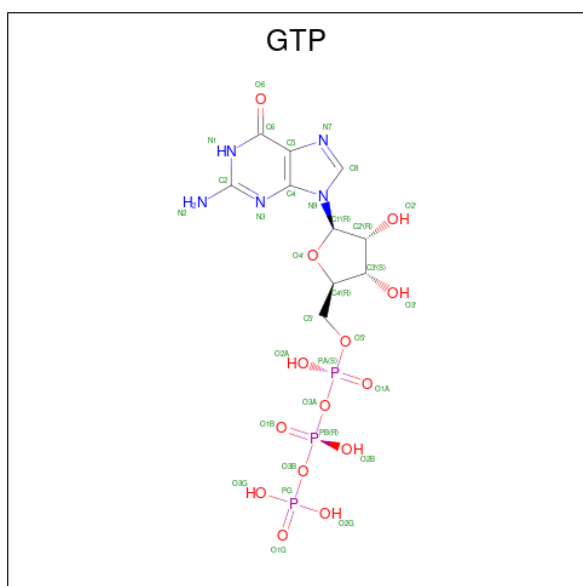
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	B5	1	10	7	3	0
94	A2	1	10	7	3	0
94	A2	1	10	7	3	0
94	A2	1	10	7	3	0
94	A2	1	10	7	3	0
94	A2	1	10	7	3	0
94	A2	1	10	7	3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

- Molecule 95 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



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 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 water.

Mol	Chain	Residues	Atoms		AltConf
97	BP	3	Total 3	O 3	0
97	Bo	1	Total 1	O 1	0
97	AT	13	Total 13	O 13	0
97	Ar	1	Total 1	O 1	0
97	BL	2	Total 2	O 2	0
97	BX	1	Total 1	O 1	0
97	As	3	Total 3	O 3	0
97	BR	5	Total 5	O 5	0
97	At	1	Total 1	O 1	0
97	Ct	1	Total 1	O 1	0
97	BH	2	Total 2	O 2	0
97	BV	2	Total 2	O 2	0
97	Aw	5	Total 5	O 5	0
97	B5	1383	Total 1383	O 1383	0
97	BI	3	Total 3	O 3	0
97	B7	43	Total 43	O 43	0
97	BJ	1	Total 1	O 1	0
97	B8	50	Total 50	O 50	0
97	Aa	2	Total 2	O 2	0

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Mol	Chain	Residues	Atoms		AltConf
97	BA	8	Total 8	O 8	0
97	BM	1	Total 1	O 1	0
97	BB	9	Total 9	O 9	0
97	BC	7	Total 7	O 7	0
97	BN	4	Total 4	O 4	0
97	Ba	8	Total 8	O 8	0
97	B	1	Total 1	O 1	0
97	BO	1	Total 1	O 1	0
97	Af	1	Total 1	O 1	0
97	BF	1	Total 1	O 1	0
97	Bd	1	Total 1	O 1	0
97	A2	526	Total 526	O 526	0
97	Be	5	Total 5	O 5	0
97	Bf	1	Total 1	O 1	0
97	Bg	2	Total 2	O 2	0
97	Ak	2	Total 2	O 2	0
97	AE	1	Total 1	O 1	0
97	Am	1	Total 1	O 1	0
97	Bj	3	Total 3	O 3	0
97	An	3	Total 3	O 3	0
97	Bl	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
97	AH	5	Total	O	0
			5	5	
97	Ap	2	Total	O	0
			2	2	

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	37182	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)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.360	Depositor
Minimum map value	-0.419	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.275	Depositor
Map size (\AA)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	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$
63	MA6	A2	1851	63	18,26,27	1.09	2 (11%)	19,38,41	2.02	3 (15%)
24	PSU	B5	1721	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
24	A2M	B5	3492	63,24	18,25,26	1.01	1 (5%)	18,36,39	1.38	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	OMC	B5	3540	24	19,22,23	0.82	0	26,31,34	0.81	0
63	PSU	A2	573	63	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
63	OMG	A2	510	63,90	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
63	PSU	A2	1693	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	A2M	A2	1384	63	18,25,26	1.04	1 (5%)	18,36,39	1.23	2 (11%)
63	A2M	A2	591	63	18,25,26	1.06	1 (5%)	18,36,39	1.23	2 (11%)
24	OMC	B5	2667	24	19,22,23	0.81	0	26,31,34	0.80	0
24	OMC	B5	4202	24	19,22,23	0.81	0	26,31,34	0.77	0
24	A2M	B5	3562	24	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
24	A2M	B5	2206	90,24	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
63	PSU	A2	34	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	610	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
63	OMG	A2	1448	63	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
24	OMC	B5	3573	24	19,22,23	0.81	0	26,31,34	0.91	1 (3%)
24	A2M	B5	4336	24	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
50	V5N	Ba	39	50	4,11,12	0.77	0	5,14,16	1.51	1 (20%)
63	PSU	A2	867	63	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
63	OMG	A2	437	63	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
63	PSU	A2	1046	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
63	PSU	A2	1175	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
63	OMG	A2	1491	63,90	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
34	OMG	B8	75	34	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
24	PSU	B5	1801	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4711	24	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
24	A2M	B5	3599	24	18,25,26	1.00	1 (5%)	18,36,39	1.24	2 (11%)
24	PSU	B5	3652	90,24	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	4325	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	UY1	B5	3550	24	19,22,23	1.39	3 (15%)	22,31,34	1.89	5 (22%)
24	OMG	B5	2207	24	18,26,27	0.91	1 (5%)	19,38,41	1.10	2 (10%)
63	OMC	A2	1392	63	19,22,23	0.82	0	26,31,34	0.83	0
24	PSU	B5	4278	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
24	PSU	B5	4419	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
63	OMG	A2	1329	63	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
24	PSU	B5	1638	24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	36	63	18,21,22	1.34	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
24	OMG	B5	4245	24	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
63	OMU	A2	116	63	19,22,23	1.18	2 (10%)	26,31,34	1.69	5 (19%)
24	OMC	B5	2647	24	19,22,23	0.81	0	26,31,34	0.82	0
24	PSU	B5	2351	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	1718	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	3466	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
63	A2M	A2	513	63	18,25,26	1.04	1 (5%)	18,36,39	1.20	2 (11%)
63	PSU	A2	1057	63	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4374	24	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
24	PSU	B5	3369	24	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
34	PSU	B8	69	34	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
24	PSU	B5	4749	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	1047	63	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
63	PSU	A2	815	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
54	MLZ	Bb	5	54	8,9,10	0.49	0	4,9,11	0.18	0
24	OMC	B5	4282	90,24	19,22,23	0.82	0	26,31,34	0.85	0
24	A2M	B5	3517	24	18,25,26	0.97	1 (5%)	18,36,39	1.33	2 (11%)
63	OMU	A2	172	63	19,22,23	1.20	2 (10%)	26,31,34	1.68	5 (19%)
24	OMG	B5	3942	4,24	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
63	OMU	A2	628	63	19,22,23	1.17	2 (10%)	26,31,34	1.69	5 (19%)
24	OMG	B5	4383	24	18,26,27	0.93	1 (5%)	19,38,41	1.11	2 (10%)
63	OMU	A2	1805	63	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
24	PSU	B5	3500	24	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	1720	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4322	24	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
63	A2M	A2	27	63,90	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
63	PSU	A2	1446	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	864	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	3494	24	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
24	PSU	B5	4045	24	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4217	24	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
47	AYA	BC	2	47	6,7,8	0.71	0	5,8,10	0.36	0
63	MA6	A2	1852	63	18,26,27	1.09	2 (11%)	19,38,41	1.93	3 (15%)
63	PSU	A2	816	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	3427	24	18,21,22	1.34	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
63	PSU	A2	1644	63,90	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
63	PSU	A2	1082	63	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
24	UR3	B5	4276	24	19,22,23	0.99	0	26,32,35	1.41	1 (3%)
63	OMU	A2	429	63	19,22,23	1.20	2 (10%)	26,31,34	1.69	4 (15%)
24	A2M	B5	400	24	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
24	A2M	B5	3456	24	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
24	OMG	B5	4240	24	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
63	PSU	A2	210	63	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
63	OMU	A2	1289	63	19,22,23	1.23	3 (15%)	26,31,34	1.68	5 (19%)
24	A2M	B5	398	24	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
24	OMU	B5	2258	24	19,22,23	1.22	3 (15%)	26,31,34	1.67	4 (15%)
34	PSU	B8	55	34	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
63	4AC	A2	1338	63	21,24,25	1.07	2 (9%)	29,34,37	1.21	3 (10%)
63	OMU	A2	355	63	19,22,23	1.23	2 (10%)	26,31,34	1.71	4 (15%)
24	A2M	B5	1489	90,24	18,25,26	1.00	1 (5%)	18,36,39	1.37	2 (11%)
63	PSU	A2	105	63	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
24	A2M	B5	2658	90,24	18,25,26	1.01	1 (5%)	18,36,39	1.21	2 (11%)
24	PSU	B5	4058	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
3	MLZ	B ₀	53	3	8,9,10	0.40	0	4,9,11	0.15	0
24	PSU	B5	3585	90,24	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
24	OMC	B5	3619	24	19,22,23	0.81	0	26,31,34	0.84	0
24	PSU	B5	4188	24	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
63	A2M	A2	1032	63	18,25,26	1.01	1 (5%)	18,36,39	1.22	2 (11%)
63	G7M	A2	1640	63	20,26,27	3.00	7 (35%)	17,39,42	0.96	1 (5%)
12	SAC	Br	2	12	7,8,9	0.52	0	8,9,11	0.83	1 (12%)
63	6MZ	A2	1833	63,90	18,25,26	0.92	1 (5%)	16,36,39	1.89	4 (25%)
24	OMC	B5	1284	24	19,22,23	0.81	0	26,31,34	0.79	0
24	PSU	B5	4740	24	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
24	OMU	B5	3973	24	19,22,23	1.22	3 (15%)	26,31,34	1.70	4 (15%)
63	PSU	A2	407	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
63	4AC	A2	1843	63	21,24,25	1.11	2 (9%)	29,34,37	1.27	3 (10%)
24	PSU	B5	3502	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
24	A2M	B5	2630	90,24	18,25,26	0.99	1 (5%)	18,36,39	1.31	2 (11%)
24	PSU	B5	3496	24	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
24	OMU	B5	4052	24	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
63	PSU	A2	93	63	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	OMG	B5	4369	24	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
24	OMG	B5	2267	24	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
24	OMC	B5	2704	24	19,22,23	0.81	0	26,31,34	0.83	0
24	PSU	B5	1683	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4169	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
24	5MC	B5	4193	24	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
24	A2M	B5	3450	24	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
24	OMG	B5	3676	24	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
24	OMG	B5	4138	24	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
24	6MZ	B5	3966	24	18,25,26	0.88	1 (5%)	16,36,39	2.00	4 (25%)
5	SAC	Ar	2	5	7,8,9	0.54	0	8,9,11	0.90	1 (12%)
63	B8N	A2	1249	63	24,29,30	1.31	3 (12%)	29,42,45	1.30	3 (10%)
24	OMG	B5	1260	24	18,26,27	0.94	1 (5%)	19,38,41	1.12	2 (10%)
24	PSU	B5	2475	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
23	HY3	Aw	62	23	6,8,9	2.06	1 (16%)	5,10,12	1.12	1 (20%)
63	OMC	A2	174	63,90	19,22,23	0.81	0	26,31,34	0.82	0
24	OMG	B5	1580	24	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
24	PSU	B5	1799	24	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
24	5MC	B5	3514	90,24	18,22,23	0.95	2 (11%)	26,32,35	1.14	3 (11%)
63	OMG	A2	645	63	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
24	A2M	B5	3557	24	18,25,26	1.01	1 (5%)	18,36,39	1.20	2 (11%)
63	A2M	A2	1679	63	18,25,26	1.00	1 (5%)	18,36,39	1.32	2 (11%)
24	PSU	B5	4267	90,24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	OMG	A2	602	63	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
63	PSU	A2	119	63	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
63	PSU	A2	802	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
63	PSU	A2	682	63	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	3554	24	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4107	24	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
30	AME	Au	1	30	9,10,11	0.48	0	9,11,13	0.86	1 (11%)
24	OMG	B5	3974	24	18,26,27	0.91	1 (5%)	19,38,41	1.12	2 (10%)
24	A2M	B5	1479	24	18,25,26	1.01	1 (5%)	18,36,39	1.25	2 (11%)
24	PSU	B5	3490	24	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
11	NMM	As	67	11	9,11,12	0.60	0	6,12,14	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	PSU	A2	1239	63	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	4246	24	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
24	PSU	B5	4099	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	1491	24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	OMU	A2	1327	63,90	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
24	OMC	B5	3601	24	19,22,23	0.81	0	26,31,34	0.80	0
24	PSU	B5	4149	24	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
24	PSU	B5	4039	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	OMG	B5	3631	24	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
32	SAC	AZ	2	32	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
24	PSU	B5	1731	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	2194	90,24	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
24	PSU	B5	3462	24	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
63	OMC	A2	1704	63	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
24	A2M	B5	4317	24	18,25,26	1.02	1 (5%)	18,36,39	1.25	2 (11%)
82	IAS	An	138	82	6,7,8	0.97	0	6,8,10	1.38	1 (16%)
63	PSU	A2	967	63	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4203	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
24	PSU	B5	1632	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
24	OMG	B5	1477	24	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
24	OMU	B5	2680	24	19,22,23	1.21	2 (10%)	26,31,34	1.72	4 (15%)
24	OMG	B5	2719	24	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
63	A2M	A2	99	63,90	18,25,26	1.04	1 (5%)	18,36,39	1.19	2 (11%)
63	PSU	A2	652	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
24	OMG	B5	4116	24	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
63	OMG	A2	868	63	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
63	PSU	A2	650	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
24	1MA	B5	1266	90,24	16,25,26	1.58	2 (12%)	18,37,40	1.05	3 (16%)
24	OMC	B5	2265	90,24	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
24	PSU	B5	4042	24	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
24	PSU	B5	4177	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
63	A2M	A2	669	63,90	18,25,26	0.99	1 (5%)	18,36,39	1.34	2 (11%)
63	A2M	A2	469	63	18,25,26	1.04	1 (5%)	18,36,39	1.23	2 (11%)
63	PSU	A2	1348	63	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	687	63	18,21,22	1.34	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
24	OMG	B5	3476	24	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
63	A2M	A2	485	63	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
63	PSU	A2	1245	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
24	PSU	B5	3583	24	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
24	OMG	B5	3524	24	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
24	PSU	B5	3616	24	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
63	PSU	A2	823	63	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	218	63	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	4166	24	18,21,22	1.37	2 (11%)	22,30,33	1.81	3 (13%)
24	OMG	B5	3359	24	18,26,27	0.93	1 (5%)	19,38,41	1.11	2 (10%)
24	OMG	B5	4364	24	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
24	OMU	B5	4366	24	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
24	PSU	B5	4298	24	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
63	OMC	A2	463	63	19,22,23	0.81	0	26,31,34	0.86	1 (3%)
63	OMU	A2	121	63	19,22,23	1.21	3 (15%)	26,31,34	1.66	4 (15%)
89	M3L	Bm	98	89	10,11,12	0.83	0	9,14,16	0.53	0
24	OMC	B5	3433	24	19,22,23	0.79	0	26,31,34	0.75	0
24	OMU	B5	3657	24	19,22,23	1.23	2 (10%)	26,31,34	1.71	4 (15%)
63	PSU	A2	109	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
24	OMC	B5	1820	90,24	19,22,23	0.80	0	26,31,34	0.79	0
38	V5N	BA	216	38	4,11,12	0.79	0	5,14,16	1.56	1 (20%)
63	PSU	A2	1178	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	A2M	B5	2244	90,24	18,25,26	1.02	1 (5%)	18,36,39	1.20	2 (11%)
63	OMU	A2	1443	63,90	19,22,23	1.24	3 (15%)	26,31,34	1.69	5 (19%)
63	PSU	A2	1626	63	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
24	A2M	B5	4269	90,24	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
24	A2M	B5	1270	24	18,25,26	0.99	1 (5%)	18,36,39	1.24	2 (11%)
63	PSU	A2	1233	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	OMC	A2	518	63	19,22,23	0.82	0	26,31,34	0.81	0
24	PSU	B5	3371	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
63	A2M	A2	166	63	18,25,26	1.05	1 (5%)	18,36,39	1.26	2 (11%)
63	OMG	A2	684	63	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
63	PSU	A2	1368	63	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
24	OMC	B5	2208	90,24	19,22,23	0.81	0	26,31,34	0.83	0
63	PSU	A2	1005	63	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
24	PSU	B5	4435	24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	HIC	BB	245	43	8,11,12	0.87	0	6,14,16	0.83	0
63	A2M	A2	577	63	18,25,26	1.02	1 (5%)	18,36,39	1.21	2 (11%)
63	A2M	A2	159	63	18,25,26	1.01	1 (5%)	18,36,39	1.26	2 (11%)
24	PSU	B5	4382	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	3576	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	1537	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	A2M	B5	1810	90,24	18,25,26	1.03	1 (5%)	18,36,39	1.25	2 (11%)
24	OMU	B5	4244	24	19,22,23	1.21	2 (10%)	26,31,34	1.70	5 (19%)
24	PSU	B5	3447	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)

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
63	MA6	A2	1851	63	-	0/7/29/30	0/3/3/3
24	PSU	B5	1721	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	3492	63,24	-	1/5/27/28	0/3/3/3
24	OMC	B5	3540	24	-	0/9/27/28	0/2/2/2
63	PSU	A2	573	63	-	0/7/25/26	0/2/2/2
63	OMG	A2	510	63,90	-	2/5/27/28	0/3/3/3
63	PSU	A2	1693	63	-	0/7/25/26	0/2/2/2
63	A2M	A2	1384	63	-	0/5/27/28	0/3/3/3
63	A2M	A2	591	63	-	1/5/27/28	0/3/3/3
24	OMC	B5	2667	24	-	1/9/27/28	0/2/2/2
24	OMC	B5	4202	24	-	0/9/27/28	0/2/2/2
24	A2M	B5	3562	24	-	0/5/27/28	0/3/3/3
24	A2M	B5	2206	90,24	-	0/5/27/28	0/3/3/3
63	PSU	A2	34	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	610	63	-	0/7/25/26	0/2/2/2
63	OMG	A2	1448	63	-	3/5/27/28	0/3/3/3
24	OMC	B5	3573	24	-	0/9/27/28	0/2/2/2
24	A2M	B5	4336	24	-	1/5/27/28	0/3/3/3
50	V5N	Ba	39	50	-	0/5/10/12	0/1/1/1
63	PSU	A2	867	63	-	0/7/25/26	0/2/2/2
63	OMG	A2	437	63	-	0/5/27/28	0/3/3/3
63	PSU	A2	1046	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1175	63	-	0/7/25/26	0/2/2/2
63	OMG	A2	1491	63,90	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	OMG	B8	75	34	-	0/5/27/28	0/3/3/3
24	PSU	B5	1801	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4711	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	3599	24	-	0/5/27/28	0/3/3/3
24	PSU	B5	3652	90,24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4325	24	-	0/7/25/26	0/2/2/2
24	UY1	B5	3550	24	-	1/9/27/28	0/2/2/2
24	OMG	B5	2207	24	-	3/5/27/28	0/3/3/3
63	OMC	A2	1392	63	-	0/9/27/28	0/2/2/2
24	PSU	B5	4278	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4419	24	-	0/7/25/26	0/2/2/2
63	OMG	A2	1329	63	-	0/5/27/28	0/3/3/3
24	PSU	B5	1638	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	36	63	-	0/7/25/26	0/2/2/2
24	OMG	B5	4245	24	-	0/5/27/28	0/3/3/3
63	OMU	A2	116	63	-	0/9/27/28	0/2/2/2
24	OMC	B5	2647	24	-	0/9/27/28	0/2/2/2
24	PSU	B5	2351	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1718	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	3466	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	513	63	-	2/5/27/28	0/3/3/3
63	PSU	A2	1057	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	4374	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	3369	24	-	0/7/25/26	0/2/2/2
34	PSU	B8	69	34	-	0/7/25/26	0/2/2/2
24	PSU	B5	4749	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	1047	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	815	63	-	0/7/25/26	0/2/2/2
54	MLZ	Bb	5	54	-	2/7/8/10	-
24	OMC	B5	4282	90,24	-	1/9/27/28	0/2/2/2
24	A2M	B5	3517	24	-	2/5/27/28	0/3/3/3
63	OMU	A2	172	63	-	0/9/27/28	0/2/2/2
24	OMG	B5	3942	4,24	-	0/5/27/28	0/3/3/3
63	OMU	A2	628	63	-	4/9/27/28	0/2/2/2
24	OMG	B5	4383	24	-	1/5/27/28	0/3/3/3
63	OMU	A2	1805	63	-	0/9/27/28	0/2/2/2
24	PSU	B5	3500	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1720	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4322	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	27	63,90	-	1/5/27/28	0/3/3/3
63	PSU	A2	1446	63	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PSU	A2	864	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	3494	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4045	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4217	24	-	0/7/25/26	0/2/2/2
47	AYA	BC	2	47	-	3/4/6/8	-
63	MA6	A2	1852	63	-	2/7/29/30	0/3/3/3
63	PSU	A2	816	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	3427	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	1644	63,90	-	0/7/25/26	0/2/2/2
63	PSU	A2	1082	63	-	0/7/25/26	0/2/2/2
24	UR3	B5	4276	24	-	0/7/25/26	0/2/2/2
63	OMU	A2	429	63	-	6/9/27/28	0/2/2/2
24	A2M	B5	400	24	-	0/5/27/28	0/3/3/3
24	A2M	B5	3456	24	-	0/5/27/28	0/3/3/3
24	OMG	B5	4240	24	-	0/5/27/28	0/3/3/3
63	PSU	A2	210	63	-	0/7/25/26	0/2/2/2
63	OMU	A2	1289	63	-	0/9/27/28	0/2/2/2
24	A2M	B5	398	24	-	4/5/27/28	0/3/3/3
24	OMU	B5	2258	24	-	0/9/27/28	0/2/2/2
34	PSU	B8	55	34	-	0/7/25/26	0/2/2/2
63	4AC	A2	1338	63	-	3/11/29/30	0/2/2/2
63	OMU	A2	355	63	-	1/9/27/28	0/2/2/2
24	A2M	B5	1489	90,24	-	2/5/27/28	0/3/3/3
63	PSU	A2	105	63	-	0/7/25/26	0/2/2/2
24	A2M	B5	2658	90,24	-	0/5/27/28	0/3/3/3
24	PSU	B5	4058	24	-	0/7/25/26	0/2/2/2
3	MLZ	B _o	53	3	-	1/7/8/10	-
24	PSU	B5	3585	90,24	-	0/7/25/26	0/2/2/2
24	OMC	B5	3619	24	-	3/9/27/28	0/2/2/2
24	PSU	B5	4188	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	1032	63	-	0/5/27/28	0/3/3/3
63	G7M	A2	1640	63	-	2/3/25/26	0/3/3/3
12	SAC	Br	2	12	-	0/7/8/10	-
63	6MZ	A2	1833	63,90	-	0/5/27/28	0/3/3/3
24	OMC	B5	1284	24	-	1/9/27/28	0/2/2/2
24	PSU	B5	4740	24	-	0/7/25/26	0/2/2/2
24	OMU	B5	3973	24	-	0/9/27/28	0/2/2/2
63	PSU	A2	407	63	-	0/7/25/26	0/2/2/2
63	4AC	A2	1843	63	-	4/11/29/30	0/2/2/2
24	PSU	B5	3502	24	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	A2M	B5	2630	90,24	-	0/5/27/28	0/3/3/3
24	PSU	B5	3496	24	-	0/7/25/26	0/2/2/2
24	OMU	B5	4052	24	-	0/9/27/28	0/2/2/2
63	PSU	A2	93	63	-	0/7/25/26	0/2/2/2
24	OMG	B5	4369	24	-	0/5/27/28	0/3/3/3
24	OMG	B5	2267	24	-	0/5/27/28	0/3/3/3
24	OMC	B5	2704	24	-	1/9/27/28	0/2/2/2
24	PSU	B5	1683	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4169	24	-	0/7/25/26	0/2/2/2
24	5MC	B5	4193	24	-	4/7/25/26	0/2/2/2
24	A2M	B5	3450	24	-	0/5/27/28	0/3/3/3
24	OMG	B5	3676	24	-	2/5/27/28	0/3/3/3
24	OMG	B5	4138	24	-	1/5/27/28	0/3/3/3
24	6MZ	B5	3966	24	-	0/5/27/28	0/3/3/3
5	SAC	Ar	2	5	-	0/7/8/10	-
63	B8N	A2	1249	63	-	4/16/34/35	0/2/2/2
24	OMG	B5	1260	24	-	1/5/27/28	0/3/3/3
24	PSU	B5	2475	24	-	0/7/25/26	0/2/2/2
23	HY3	Aw	62	23	-	1/1/12/14	0/1/1/1
63	OMC	A2	174	63,90	-	0/9/27/28	0/2/2/2
24	OMG	B5	1580	24	-	0/5/27/28	0/3/3/3
24	PSU	B5	1799	24	-	0/7/25/26	0/2/2/2
24	5MC	B5	3514	90,24	-	0/7/25/26	0/2/2/2
63	OMG	A2	645	63	-	3/5/27/28	0/3/3/3
24	A2M	B5	3557	24	-	1/5/27/28	0/3/3/3
63	A2M	A2	1679	63	-	0/5/27/28	0/3/3/3
24	PSU	B5	4267	90,24	-	0/7/25/26	0/2/2/2
63	OMG	A2	602	63	-	0/5/27/28	0/3/3/3
63	PSU	A2	119	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	802	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	682	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	3554	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4107	24	-	0/7/25/26	0/2/2/2
30	AME	Au	1	30	-	2/9/10/12	-
24	OMG	B5	3974	24	-	0/5/27/28	0/3/3/3
24	A2M	B5	1479	24	-	0/5/27/28	0/3/3/3
24	PSU	B5	3490	24	-	0/7/25/26	0/2/2/2
11	NMM	As	67	11	-	0/9/11/13	-
63	PSU	A2	1239	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	4246	24	-	1/7/25/26	0/2/2/2
24	PSU	B5	4099	24	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	B5	1491	24	-	0/7/25/26	0/2/2/2
63	OMU	A2	1327	63,90	-	0/9/27/28	0/2/2/2
24	OMC	B5	3601	24	-	0/9/27/28	0/2/2/2
24	PSU	B5	4149	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4039	24	-	0/7/25/26	0/2/2/2
24	OMG	B5	3631	24	-	1/5/27/28	0/3/3/3
32	SAC	AZ	2	32	-	2/7/8/10	-
24	PSU	B5	1731	24	-	0/7/25/26	0/2/2/2
24	OMC	B5	2194	90,24	-	2/9/27/28	0/2/2/2
24	PSU	B5	3462	24	-	0/7/25/26	0/2/2/2
63	OMC	A2	1704	63	-	1/9/27/28	0/2/2/2
24	A2M	B5	4317	24	-	0/5/27/28	0/3/3/3
82	IAS	An	138	82	-	2/7/7/8	-
63	PSU	A2	967	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	4203	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1632	24	-	0/7/25/26	0/2/2/2
24	OMG	B5	1477	24	-	0/5/27/28	0/3/3/3
24	OMU	B5	2680	24	-	1/9/27/28	0/2/2/2
24	OMG	B5	2719	24	-	0/5/27/28	0/3/3/3
63	A2M	A2	99	63,90	-	2/5/27/28	0/3/3/3
63	PSU	A2	652	63	-	0/7/25/26	0/2/2/2
24	OMG	B5	4116	24	-	0/5/27/28	0/3/3/3
63	OMG	A2	868	63	-	2/5/27/28	0/3/3/3
63	PSU	A2	650	63	-	0/7/25/26	0/2/2/2
24	1MA	B5	1266	90,24	-	0/3/25/26	0/3/3/3
24	OMC	B5	2265	90,24	-	1/9/27/28	0/2/2/2
24	PSU	B5	4042	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4177	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	669	63,90	-	2/5/27/28	0/3/3/3
63	A2M	A2	469	63	-	0/5/27/28	0/3/3/3
63	PSU	A2	1348	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	687	63	-	0/7/25/26	0/2/2/2
24	OMG	B5	3476	24	-	1/5/27/28	0/3/3/3
63	A2M	A2	485	63	-	0/5/27/28	0/3/3/3
63	PSU	A2	1245	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	3583	24	-	0/7/25/26	0/2/2/2
24	OMG	B5	3524	24	-	0/5/27/28	0/3/3/3
24	PSU	B5	3616	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	823	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	218	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	4166	24	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	OMG	B5	3359	24	-	0/5/27/28	0/3/3/3
24	OMG	B5	4364	24	-	0/5/27/28	0/3/3/3
24	OMU	B5	4366	24	-	0/9/27/28	0/2/2/2
24	PSU	B5	4298	24	-	0/7/25/26	0/2/2/2
63	OMC	A2	463	63	-	0/9/27/28	0/2/2/2
63	OMU	A2	121	63	-	0/9/27/28	0/2/2/2
89	M3L	Bm	98	89	-	0/9/10/12	-
24	OMC	B5	3433	24	-	4/9/27/28	0/2/2/2
24	OMU	B5	3657	24	-	0/9/27/28	0/2/2/2
63	PSU	A2	109	63	-	0/7/25/26	0/2/2/2
24	OMC	B5	1820	90,24	-	1/9/27/28	0/2/2/2
38	V5N	BA	216	38	-	1/5/10/12	0/1/1/1
63	PSU	A2	1178	63	-	0/7/25/26	0/2/2/2
24	A2M	B5	2244	90,24	-	0/5/27/28	0/3/3/3
63	OMU	A2	1443	63,90	-	0/9/27/28	0/2/2/2
63	PSU	A2	1626	63	-	0/7/25/26	0/2/2/2
24	A2M	B5	4269	90,24	-	0/5/27/28	0/3/3/3
24	A2M	B5	1270	24	-	0/5/27/28	0/3/3/3
63	PSU	A2	1233	63	-	0/7/25/26	0/2/2/2
63	OMC	A2	518	63	-	0/9/27/28	0/2/2/2
24	PSU	B5	3371	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	166	63	-	0/5/27/28	0/3/3/3
63	OMG	A2	684	63	-	1/5/27/28	0/3/3/3
63	PSU	A2	1368	63	-	0/7/25/26	0/2/2/2
24	OMC	B5	2208	90,24	-	0/9/27/28	0/2/2/2
63	PSU	A2	1005	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	4435	24	-	0/7/25/26	0/2/2/2
43	HIC	BB	245	43	-	2/5/6/8	0/1/1/1
63	A2M	A2	577	63	-	2/5/27/28	0/3/3/3
63	A2M	A2	159	63	-	0/5/27/28	0/3/3/3
24	PSU	B5	4382	24	-	4/7/25/26	0/2/2/2
24	PSU	B5	3576	24	-	1/7/25/26	0/2/2/2
24	PSU	B5	1537	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	1810	90,24	-	1/5/27/28	0/3/3/3
24	OMU	B5	4244	24	-	0/9/27/28	0/2/2/2
24	PSU	B5	3447	24	-	0/7/25/26	0/2/2/2

The worst 5 of 326 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	A2	1640	G7M	C5-C4	7.42	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	A2	1640	G7M	O6-C6	7.33	1.38	1.23
24	B5	1266	1MA	C2-N3	4.83	1.34	1.29
23	Aw	62	HY3	C3-CA	-4.68	1.50	1.55
63	A2	1640	G7M	C2-N2	4.47	1.44	1.34

The worst 5 of 541 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	3494	PSU	N1-C2-N3	6.11	122.06	115.13
24	B5	4149	PSU	N1-C2-N3	6.09	122.03	115.13
24	B5	3616	PSU	N1-C2-N3	6.07	122.01	115.13
34	B8	69	PSU	N1-C2-N3	6.06	122.00	115.13
24	B5	3369	PSU	N1-C2-N3	6.06	122.00	115.13

There are no chirality outliers.

5 of 115 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Bo	53	MLZ	O-C-CA-CB
24	B5	3433	OMC	C2'-C1'-N1-C2
24	B5	3433	OMC	C2'-C1'-N1-C6
24	B5	3517	A2M	O4'-C4'-C5'-O5'
24	B5	4166	PSU	C2'-C1'-C5-C4

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 769 ligands modelled in this entry, 428 are monoatomic and 306 are unknown - 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	5224	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	A2	1985	-	9,9,9	0.16	0	8,8,8	0.17	0
94	SPD	B5	4954	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	1943	-	9,9,9	0.15	0	8,8,8	0.17	0
95	SPM	B5	5018	-	13,13,13	0.15	0	12,12,12	0.22	0
94	SPD	B5	5244	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	1950	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	4912	-	9,9,9	0.16	0	8,8,8	0.17	0
94	SPD	B5	5302	-	9,9,9	0.15	0	8,8,8	0.15	0
94	SPD	B5	5144	-	9,9,9	0.15	0	8,8,8	0.22	0
93	IHP	DB	901	-	36,36,36	1.55	6 (16%)	54,60,60	1.09	3 (5%)
94	SPD	B5	4945	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	4933	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	4997	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	4975	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	A2	1971	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5103	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	5405	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	A2	1957	-	9,9,9	0.15	0	8,8,8	0.19	0
96	GTP	B7	216	29	26,34,34	0.95	2 (7%)	32,54,54	0.78	0
94	SPD	B5	5385	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5165	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	5082	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	5041	-	9,9,9	0.14	0	8,8,8	0.20	0
94	SPD	B5	5363	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	5205	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	1964	-	9,9,9	0.15	0	8,8,8	0.17	0
95	SPM	A2	1994	-	13,13,13	0.15	0	12,12,12	0.16	0
94	SPD	A2	1986	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	A2	1978	-	9,9,9	0.15	0	8,8,8	0.20	0
95	SPM	B5	5061	-	13,13,13	0.15	0	12,12,12	0.14	0
94	SPD	B5	5322	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5343	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	5263	-	9,9,9	0.16	0	8,8,8	0.15	0
94	SPD	B5	5123	-	9,9,9	0.15	0	8,8,8	0.18	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	5224	-	-	1/7/7/7	-
94	SPD	A2	1985	-	-	1/7/7/7	-
94	SPD	B5	4954	-	-	0/7/7/7	-
94	SPD	A2	1943	-	-	0/7/7/7	-
95	SPM	B5	5018	-	-	1/11/11/11	-
94	SPD	B5	5244	-	-	0/7/7/7	-
94	SPD	A2	1950	-	-	0/7/7/7	-
94	SPD	B5	4912	-	-	0/7/7/7	-
94	SPD	B5	5302	-	-	1/7/7/7	-
94	SPD	B5	5144	-	-	0/7/7/7	-
93	IHP	DB	901	-	-	8/30/54/54	0/1/1/1
94	SPD	B5	4945	-	-	0/7/7/7	-
94	SPD	B5	4933	-	-	0/7/7/7	-
94	SPD	B5	4997	-	-	0/7/7/7	-
94	SPD	B5	4975	-	-	2/7/7/7	-
94	SPD	A2	1971	-	-	0/7/7/7	-
94	SPD	B5	5103	-	-	0/7/7/7	-
94	SPD	B5	5405	-	-	1/7/7/7	-
94	SPD	A2	1957	-	-	0/7/7/7	-
96	GTP	B7	216	29	-	0/18/38/38	0/3/3/3
94	SPD	B5	5385	-	-	1/7/7/7	-
94	SPD	B5	5165	-	-	1/7/7/7	-
94	SPD	B5	5082	-	-	0/7/7/7	-
94	SPD	B5	5041	-	-	0/7/7/7	-
94	SPD	B5	5363	-	-	0/7/7/7	-
94	SPD	B5	5205	-	-	0/7/7/7	-
94	SPD	A2	1964	-	-	0/7/7/7	-
95	SPM	A2	1994	-	-	2/11/11/11	-
94	SPD	A2	1986	-	-	0/7/7/7	-
94	SPD	A2	1978	-	-	1/7/7/7	-
95	SPM	B5	5061	-	-	0/11/11/11	-
94	SPD	B5	5322	-	-	1/7/7/7	-
94	SPD	B5	5343	-	-	1/7/7/7	-
94	SPD	B5	5263	-	-	1/7/7/7	-
94	SPD	B5	5123	-	-	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)
93	DB	901	IHP	P2-O12	3.53	1.66	1.59
93	DB	901	IHP	P5-O15	3.43	1.65	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
93	DB	901	IHP	P1-O11	3.25	1.65	1.59
93	DB	901	IHP	P6-O16	3.24	1.65	1.59
93	DB	901	IHP	P4-O14	3.18	1.65	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	DB	901	IHP	C6-C5-C4	4.26	119.74	110.41
93	DB	901	IHP	C5-C4-C3	3.49	118.05	110.41
93	DB	901	IHP	C5-C6-C1	3.40	117.86	110.41

There are no chirality outliers.

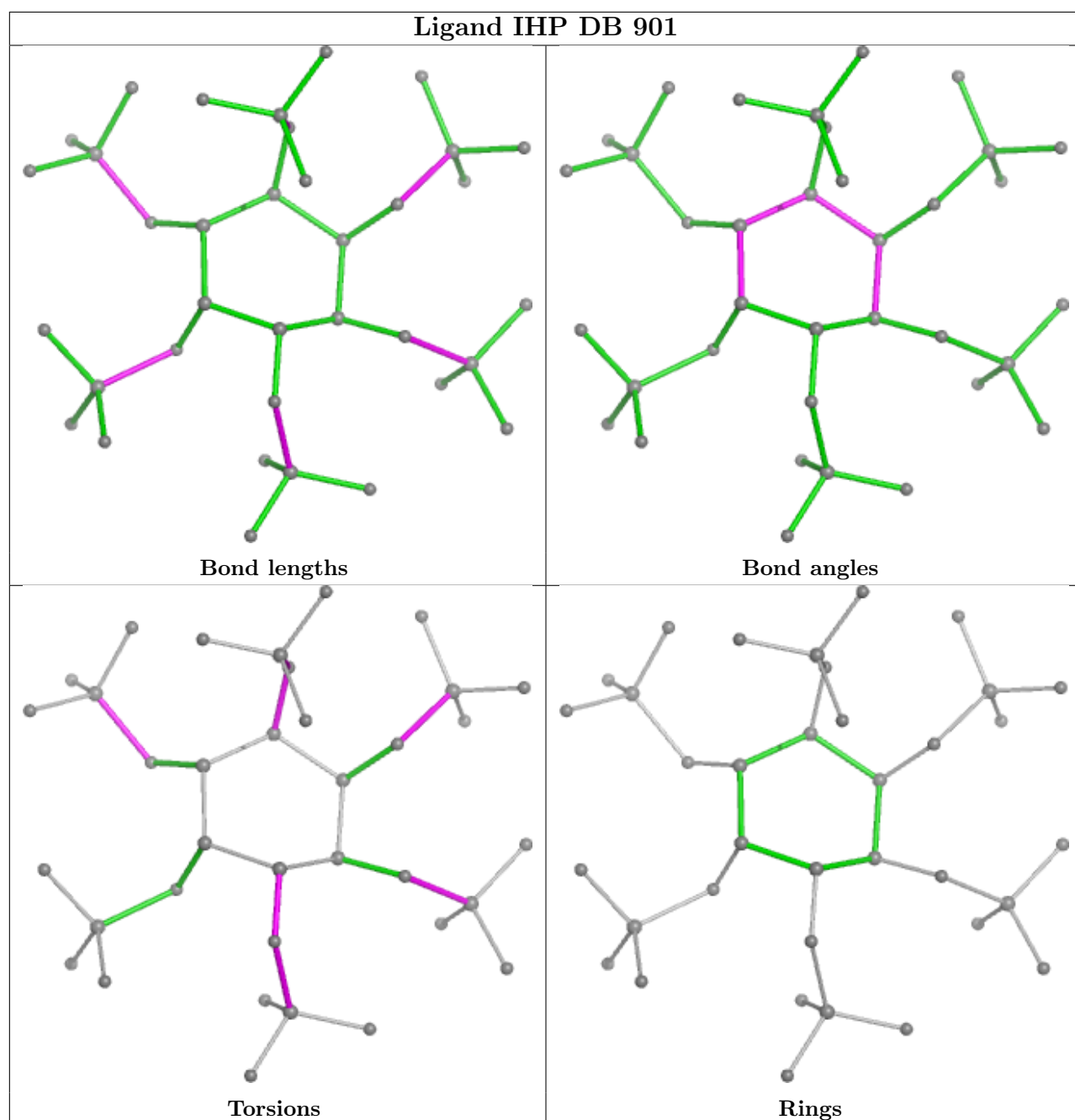
5 of 23 torsion outliers are listed below:

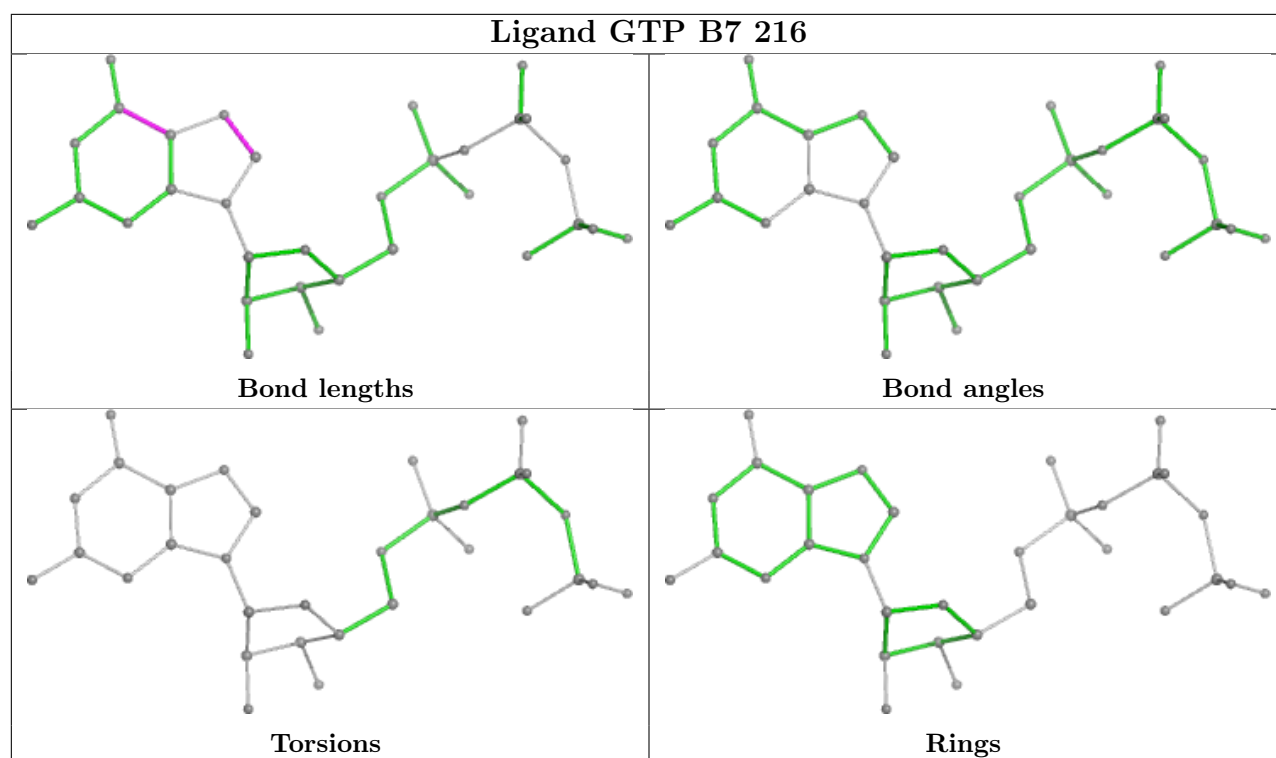
Mol	Chain	Res	Type	Atoms
93	DB	901	IHP	C1-C2-O12-P2
93	DB	901	IHP	C4-C5-O15-P5
93	DB	901	IHP	C4-O14-P4-O24
95	A2	1994	SPM	C8-C9-N10-C11
93	DB	901	IHP	C2-O12-P2-O32

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.

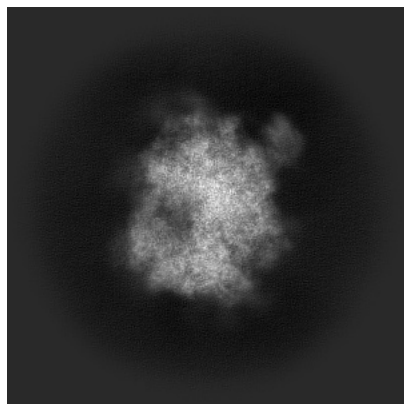
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50124. These allow visual inspection of the internal detail of the map and identification of artifacts.

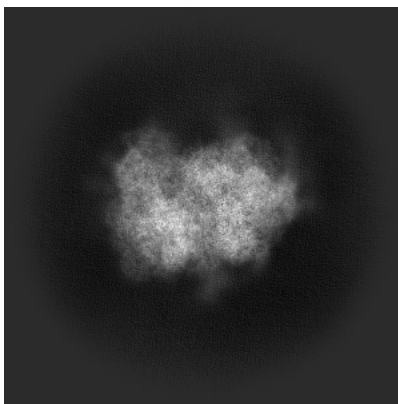
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

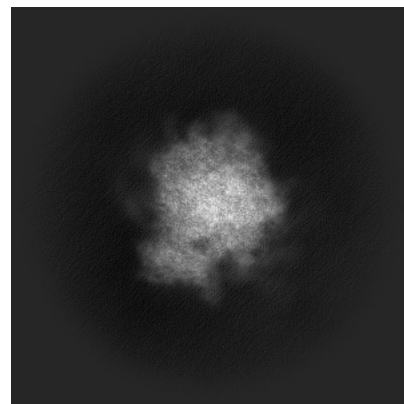
5.1.1 Primary map



X

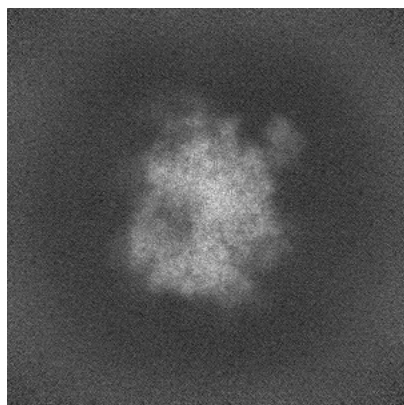


Y

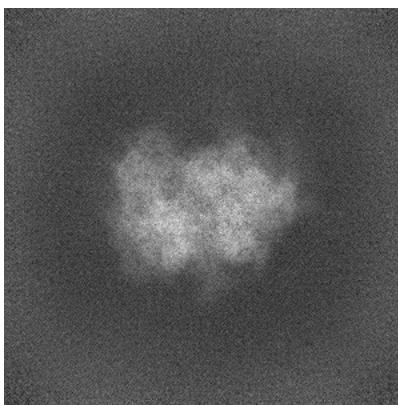


Z

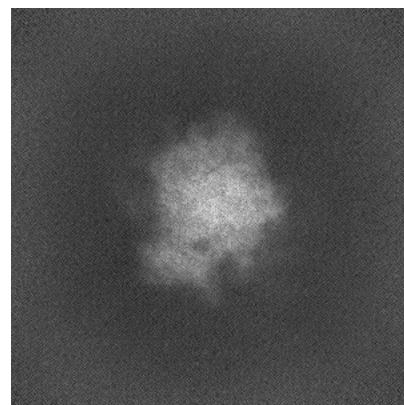
5.1.2 Raw map



X



Y

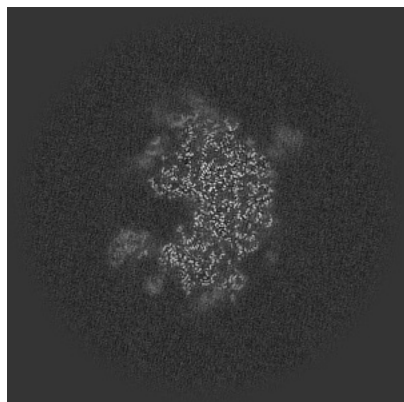


Z

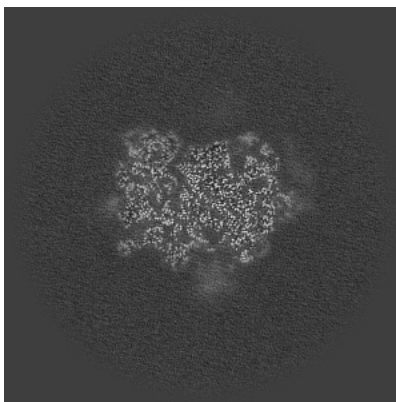
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

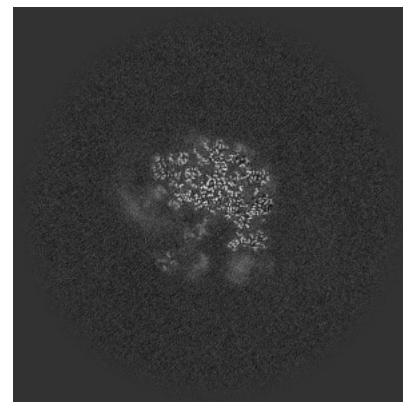
5.2.1 Primary map



X Index: 280

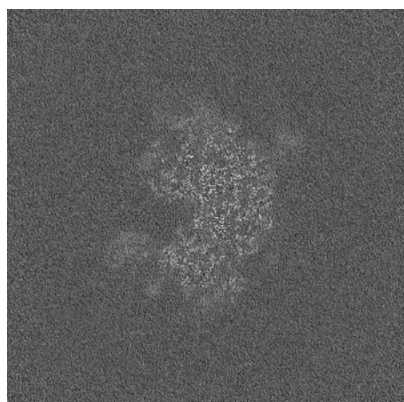


Y Index: 280

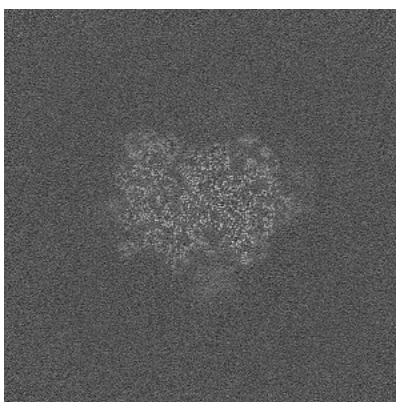


Z Index: 280

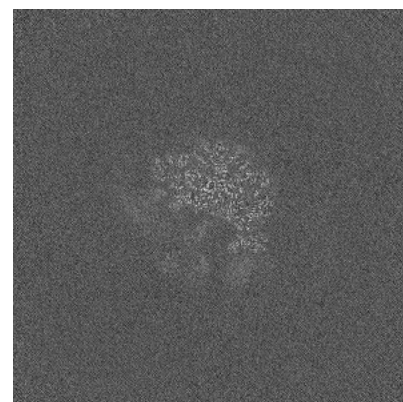
5.2.2 Raw map



X Index: 280



Y Index: 280

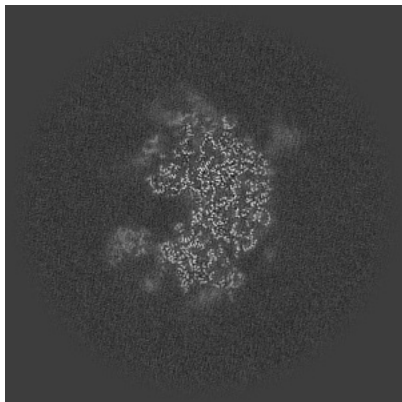


Z Index: 280

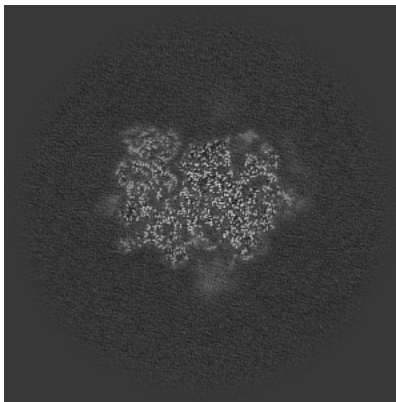
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

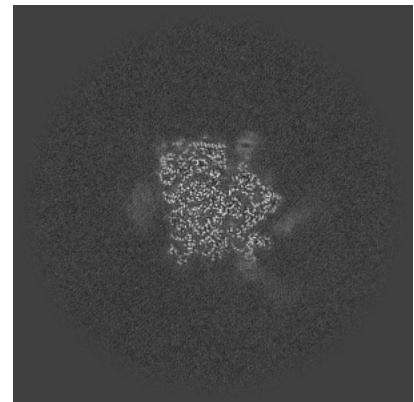
5.3.1 Primary map



X Index: 279

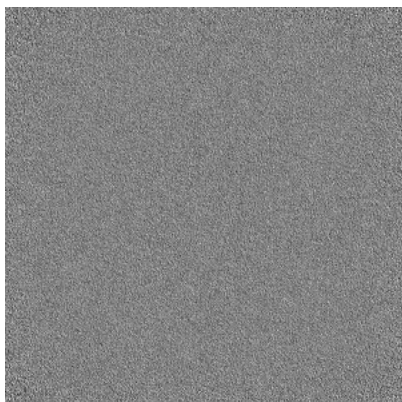


Y Index: 281

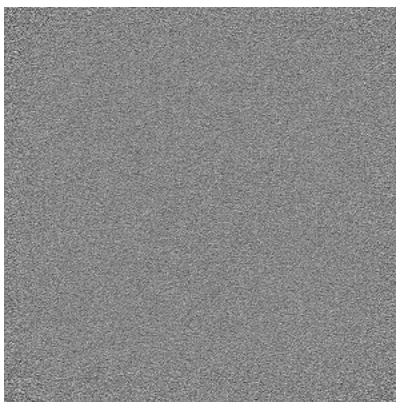


Z Index: 309

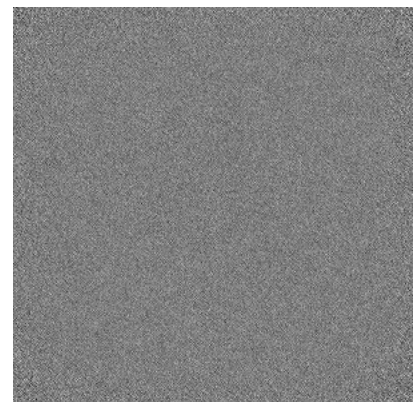
5.3.2 Raw map



X Index: 0



Y Index: 0

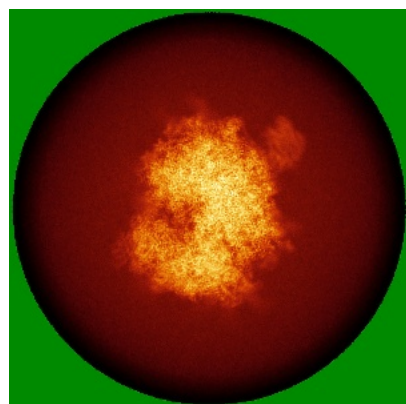


Z Index: 0

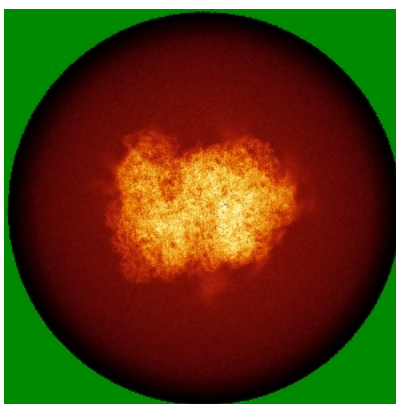
The images above show the largest variance slices of the map in three orthogonal directions.

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

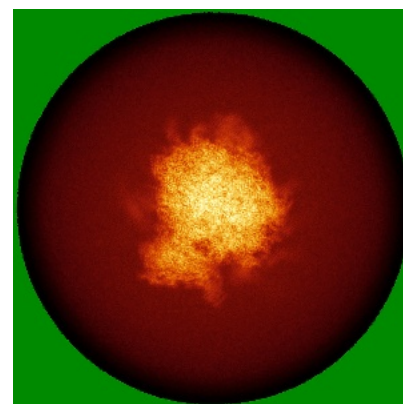
5.4.1 Primary map



X

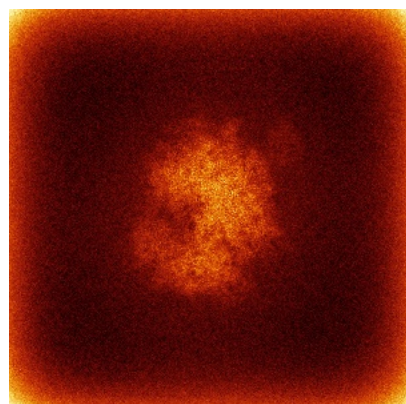


Y

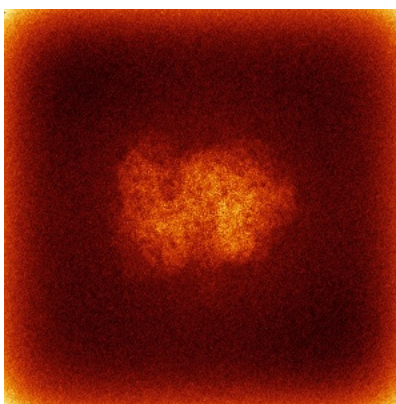


Z

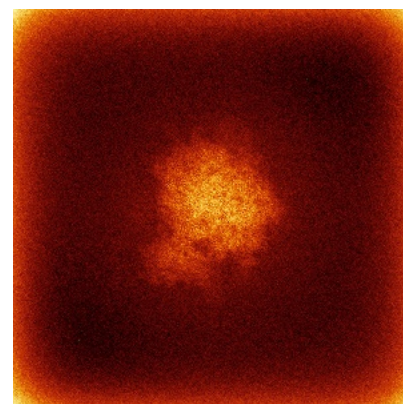
5.4.2 Raw map



X



Y

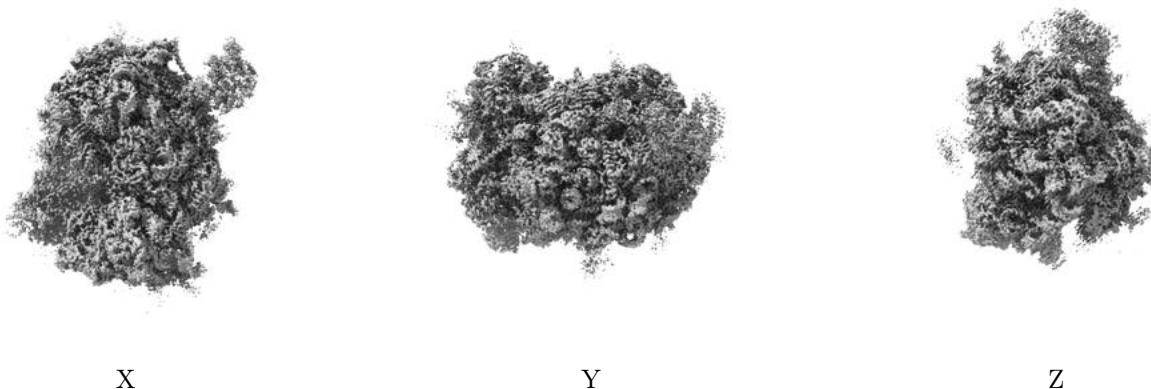


Z

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.

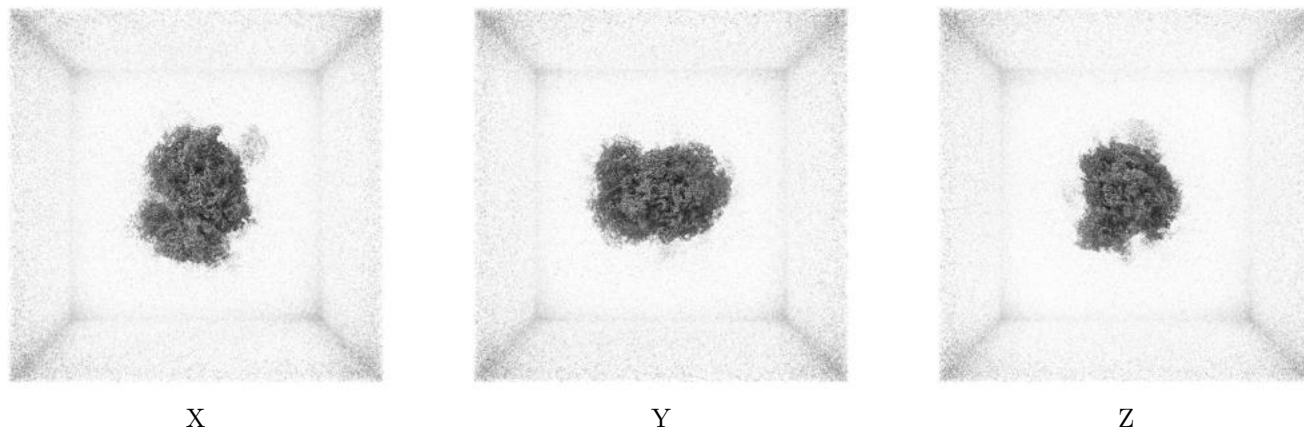
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.275. 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.

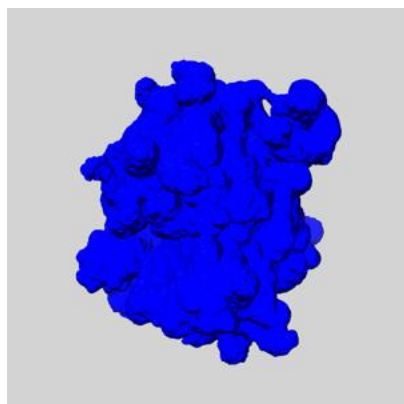
5.6 Mask visualisation [i](#)

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

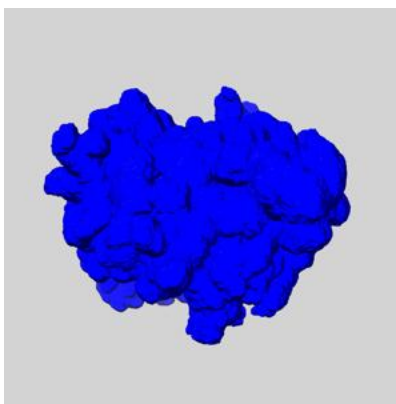
A mask typically either:

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

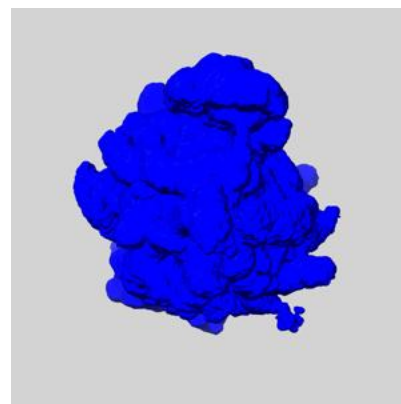
5.6.1 emd_50124_msk_1.map [i](#)



X

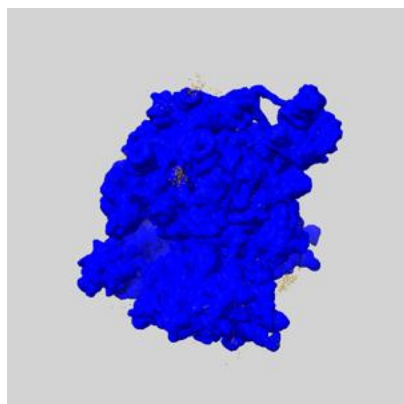


Y

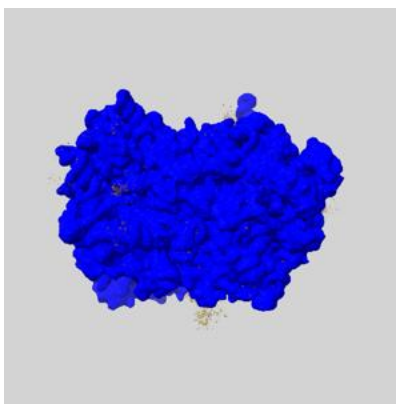


Z

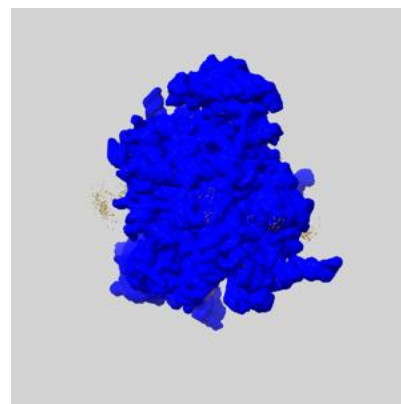
5.6.2 emd_50124_msk_2.map [i](#)



X



Y

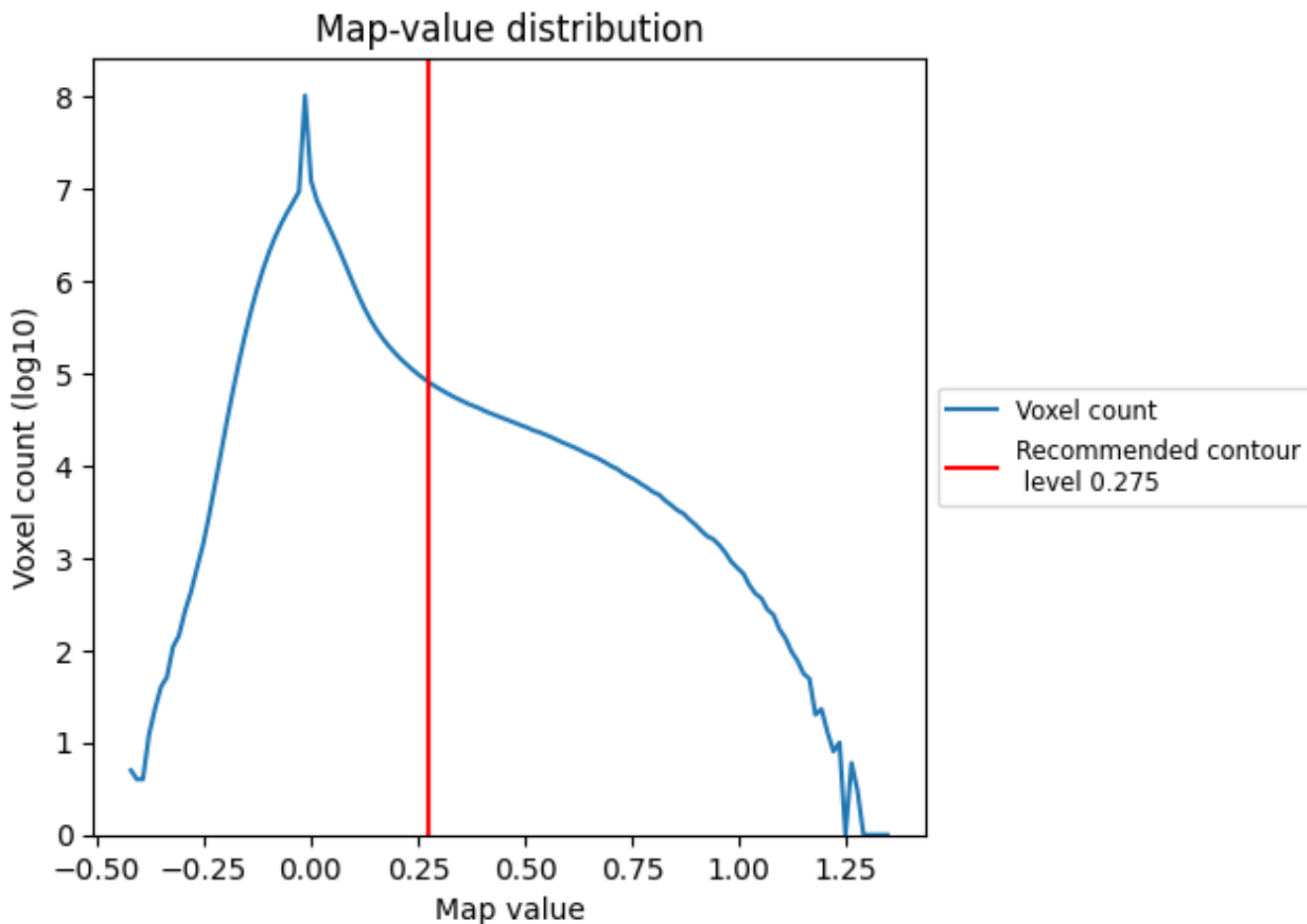


Z

6 Map analysis [i](#)

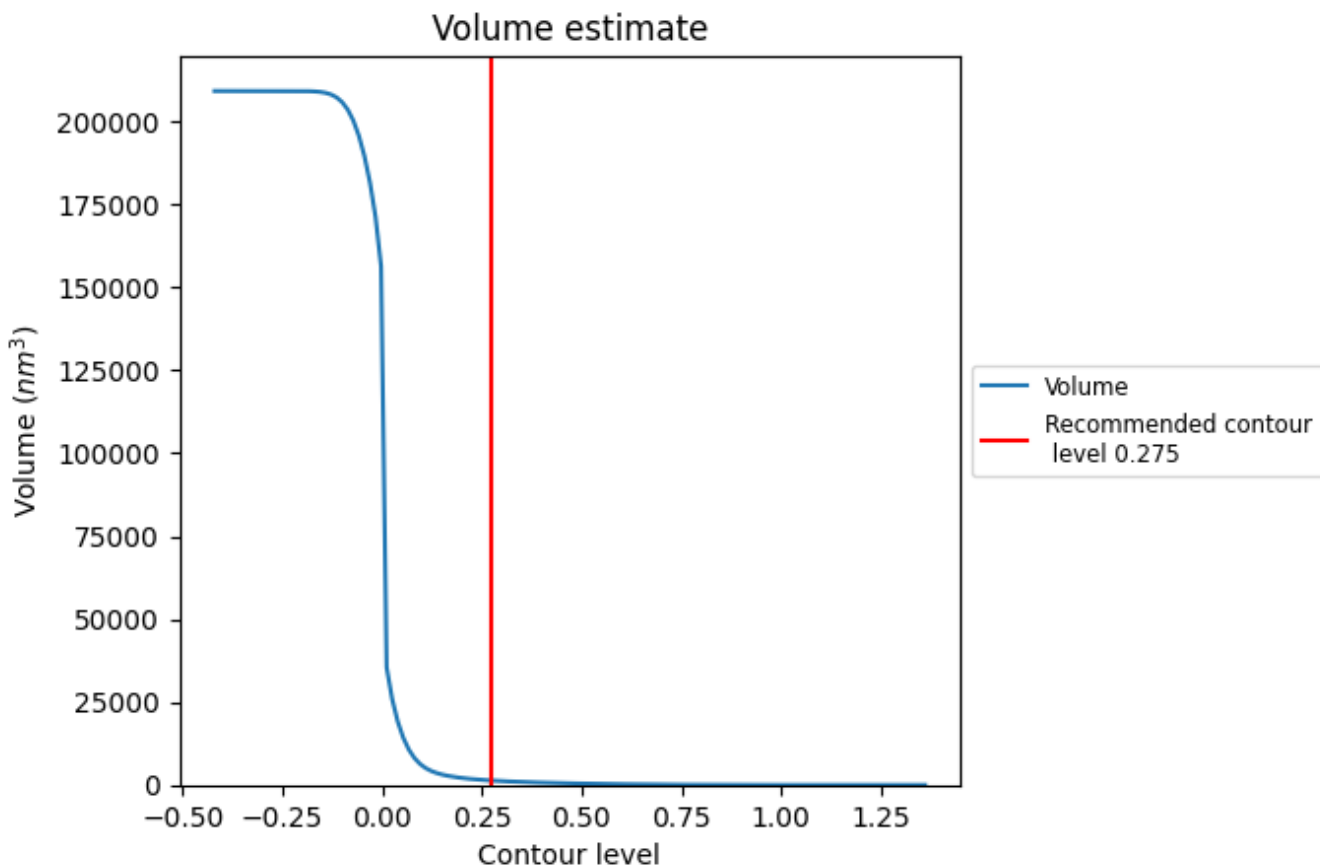
This section contains the results of statistical analysis of the map.

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.

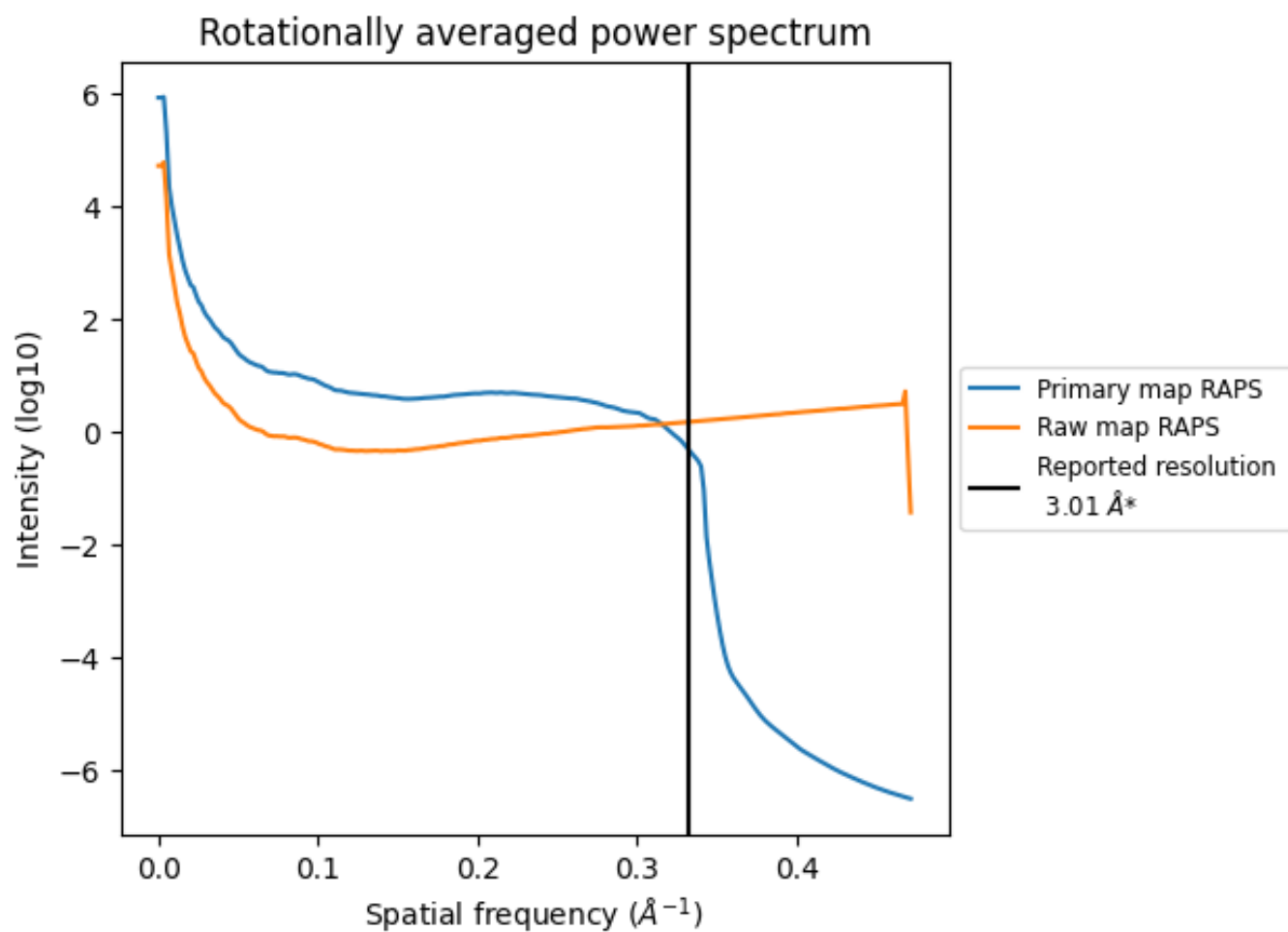
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 1330 nm^3 ; this corresponds to an approximate mass of 1201 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

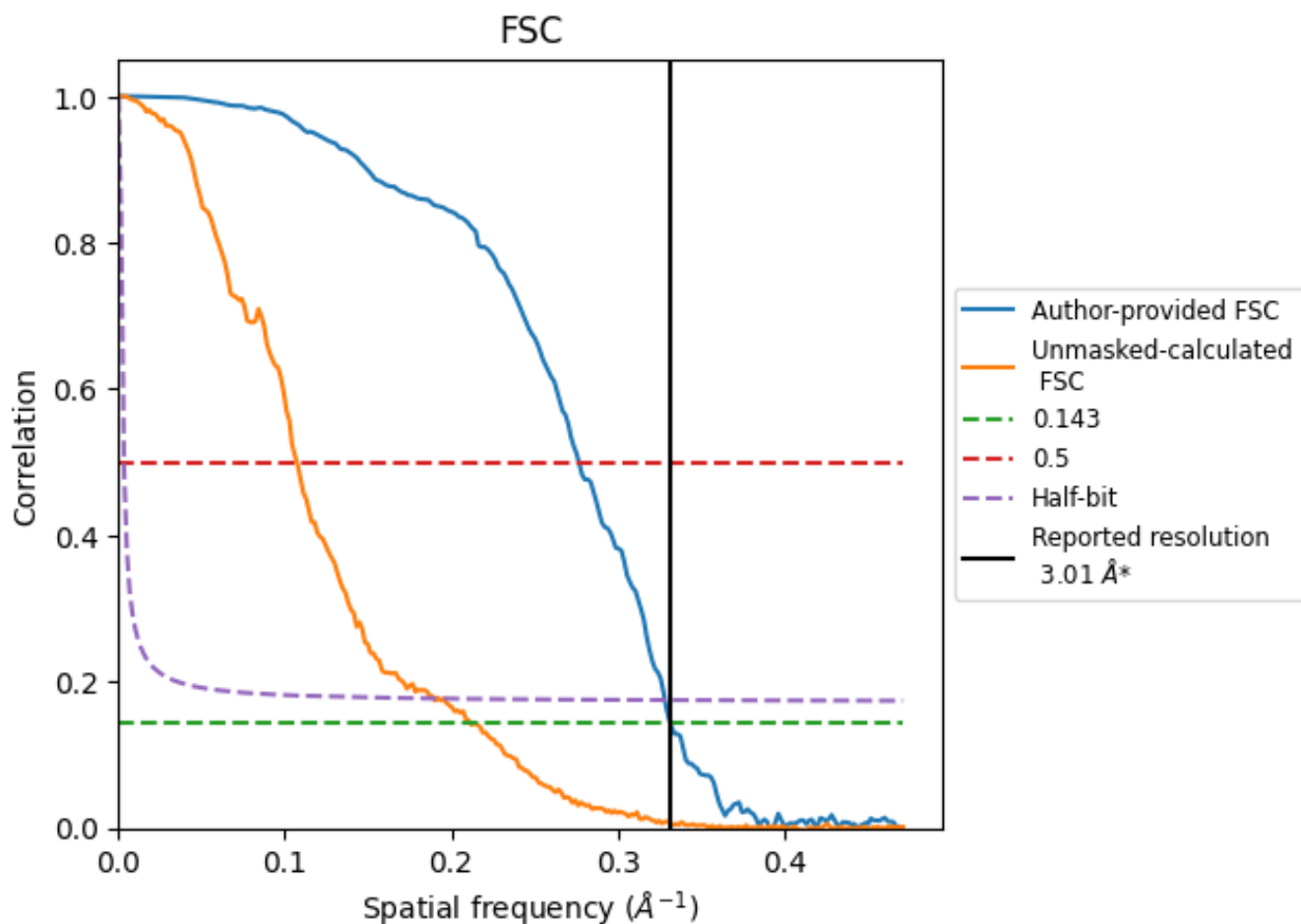


*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

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 0.332 Å⁻¹

7.2 Resolution estimates [i](#)

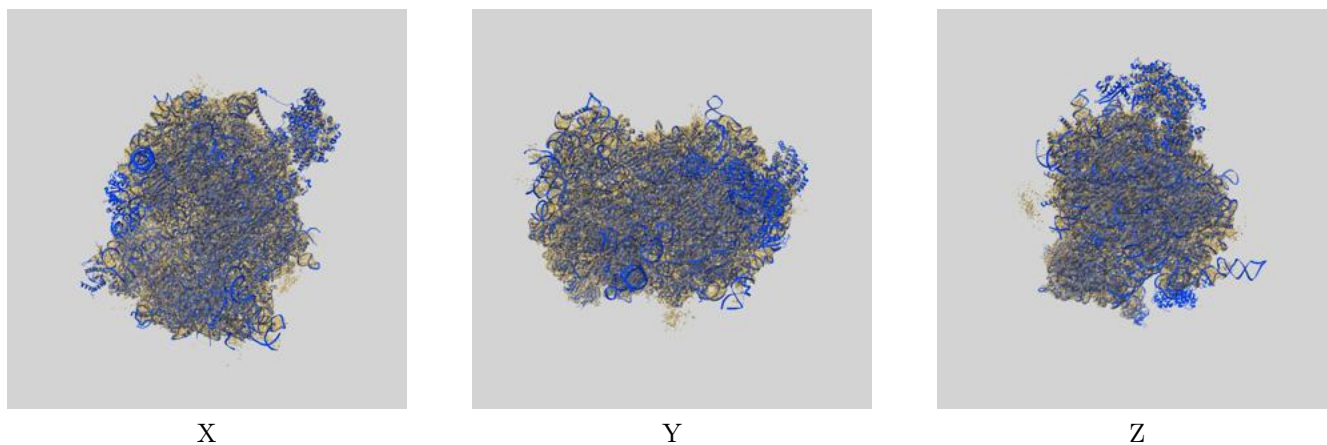
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.61	3.04
Unmasked-calculated*	4.73	9.33	5.27

*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 4.73 differs from the reported value 3.01 by more than 10 %

8 Map-model fit [i](#)

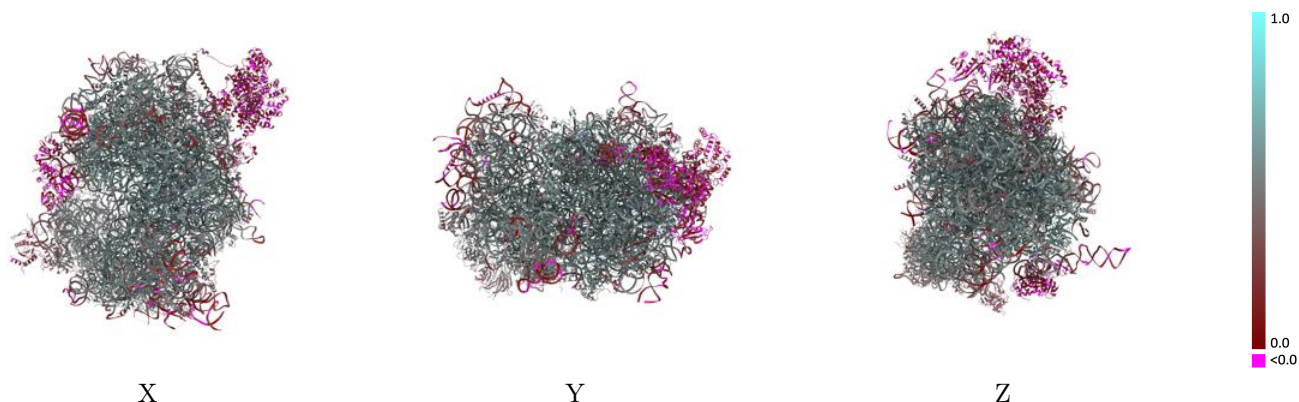
This section contains information regarding the fit between EMDB map EMD-50124 and PDB model 9F1B. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



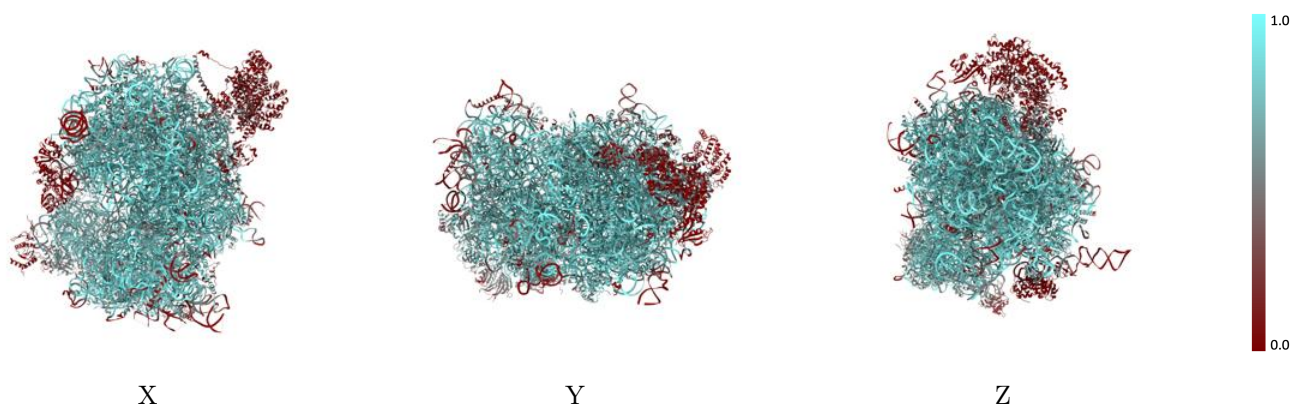
The images above show the 3D surface view of the map at the recommended contour level 0.275 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



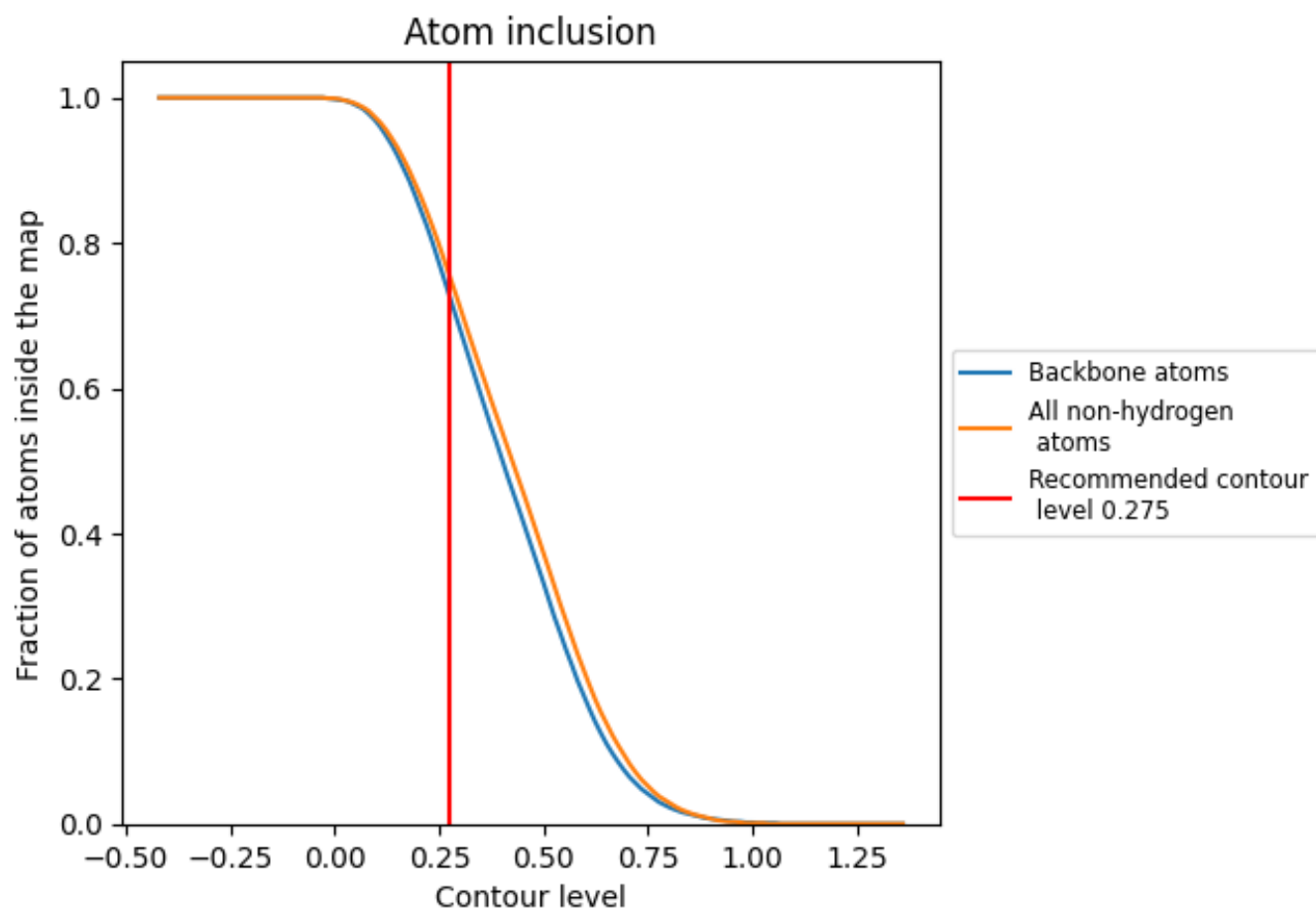
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.275).







































































8.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 76% 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 (0.275) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.4750
A2	 0.8340	 0.4770
AA	 0.6760	 0.4940
AB	 0.6040	 0.4780
AC	 0.1580	 0.2200
AD	 0.5770	 0.4370
AE	 0.7980	 0.5180
AF	 0.4480	 0.3760
AG	 0.8120	 0.4960
AH	 0.1110	 0.3930
AT	 0.5350	 0.4300
AZ	 0.7000	 0.5000
Aa	 0.6880	 0.5030
Ab	 0.7800	 0.5250
Ac	 0.6100	 0.4320
Ad	 0.7770	 0.5190
Ae	 0.6640	 0.4740
Af	 0.6150	 0.4160
Ag	 0.5810	 0.4320
Ah	 0.7380	 0.5060
Ai	 0.7500	 0.4960
Aj	 0.5520	 0.3920
Ak	 0.7490	 0.5000
Al	 0.0760	 0.1840
Am	 0.7700	 0.5270
An	 0.7710	 0.5310
Ao	 0.5590	 0.4140
Ap	 0.7010	 0.4760
Aq	 0.6430	 0.4560
Ar	 0.6120	 0.4400
As	 0.6700	 0.4420
At	 0.6020	 0.4150
Au	 0.7330	 0.5060
Av	 0.8070	 0.5460
Aw	 0.8050	 0.5450





























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Chain	Atom inclusion	Q-score
Ax	0.7070	0.4830
Ay	0.5010	0.3960
Az	0.7390	0.5400
B	0.7510	0.5210
B5	0.8560	0.5010
B7	0.9420	0.5520
B8	0.9030	0.5280
BA	0.8510	0.5690
BB	0.8300	0.5580
BC	0.8460	0.5570
BE	0.7190	0.4990
BF	0.8490	0.5600
BG	0.7080	0.4880
BH	0.7620	0.5330
BI	0.7880	0.5470
BJ	0.6930	0.5030
BK	0.3310	0.3920
BL	0.7930	0.5170
BM	0.7900	0.5200
BN	0.9040	0.5760
BO	0.8470	0.5610
BP	0.8530	0.5640
BQ	0.8600	0.5680
BR	0.7950	0.5200
BS	0.8660	0.5670
BT	0.7900	0.5340
BU	0.6780	0.4800
BV	0.7760	0.5450
BW	0.5410	0.3730
BX	0.8060	0.5380
BY	0.7740	0.5400
BZ	0.7880	0.5270
Ba	0.8760	0.5730
Bb	0.6860	0.4710
Bc	0.6760	0.4860
Bd	0.8030	0.5370
Be	0.8540	0.5620
Bf	0.8500	0.5750
Bg	0.7930	0.5360
Bh	0.7850	0.5290
Bi	0.7700	0.5150
Bj	0.9140	0.5780

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Chain	Atom inclusion	Q-score
Bk	 0.6550	 0.4820
Bl	 0.8760	 0.5530
Bm	 0.8190	 0.5500
Bo	 0.7960	 0.5480
Bp	 0.7920	 0.5460
Br	 0.8380	 0.5520
Bs	 0.0050	 0.0570
Bt	 0.0020	 0.0470
Ct	 0.1020	 0.1340
Cu	 0.2310	 0.2170
DA	 0.0050	 0.0410
DB	 0.1280	 0.1010
DC	 0.1200	 0.0860