



wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 02:56 pm BST

PDB ID : 7O7Y
EMDB ID : EMD-12756
Title : Rabbit 80S ribosome stalled close to the mutated SARS-CoV-2 slippery site by a pseudoknot (high resolution)
Authors : Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.
Deposited on : 2021-04-14
Resolution : 2.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

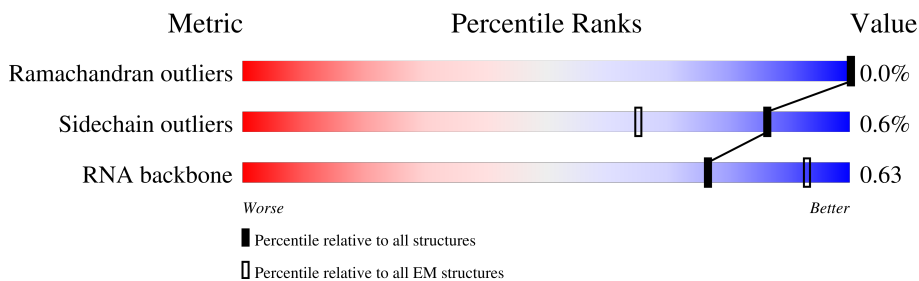
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 Å.

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



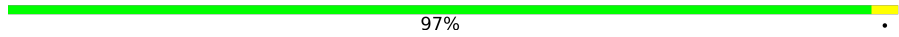





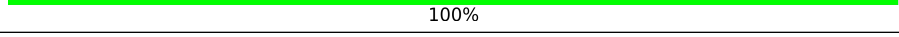
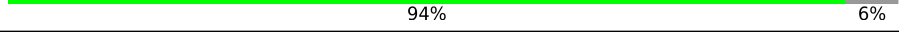
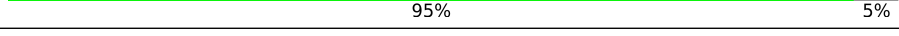

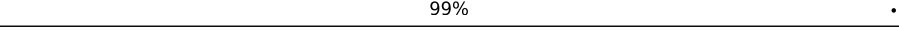
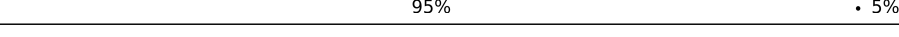

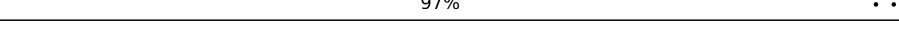
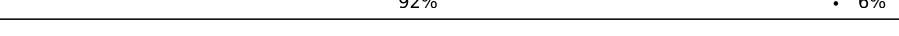
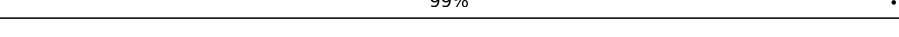
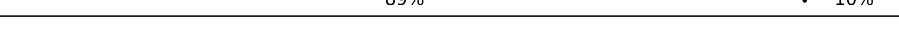

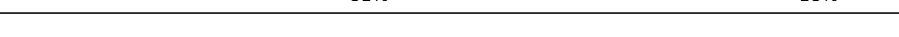






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A2	1870	
2	AA	84	
3	AB	69	
4	AC	156	
5	AD	133	
6	AE	115	
7	AF	317	
8	AG	56	
9	AH	217	

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Mol	Chain	Length	Quality of chain
10	AI	76	 97%
11	AT	76	 68% 29%
12	AZ	295	 74% 25%
13	Aa	264	 84% 15%
14	Ab	293	 74% 25%
15	Ac	281	 79% 20%
16	Ad	263	 100%
17	Ae	204	 94% 6%
18	Af	249	 95% 5%
19	Ag	432	 44% 56%
20	Ah	208	 99%
21	Ai	194	 95% 5%
22	Aj	165	 58% 42%
23	Ak	158	 97%
24	Al	132	 92% 6%
25	Am	151	 99%
26	An	151	 89% 10%
27	Ao	145	 88% 12%
28	Ap	172	 81% 18%
29	Aq	135	 99%
30	Ar	152	 95%
31	As	145	 99%
32	At	119	 87% 13%
33	Au	83	 98%
34	Av	130	 99%

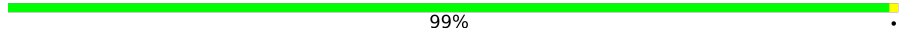
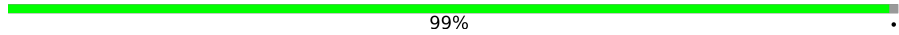

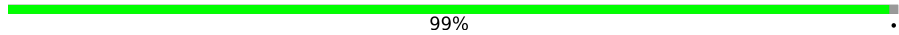


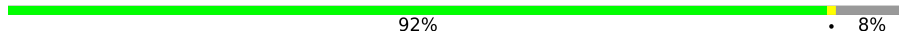
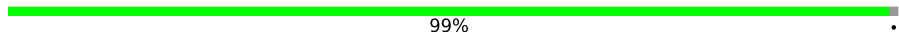
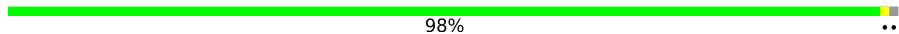

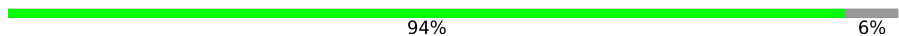

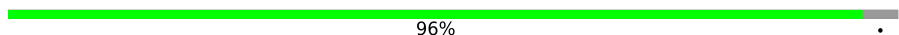
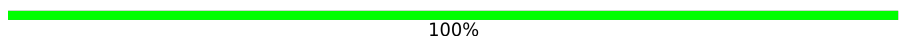
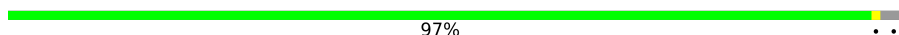
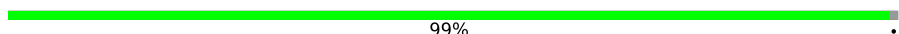
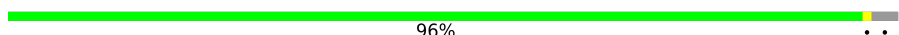

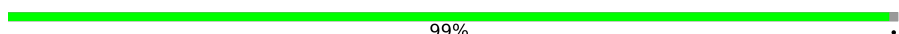
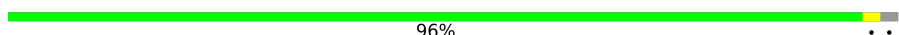

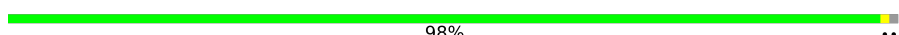
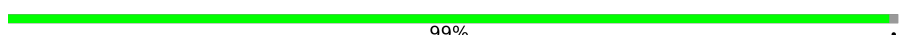


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Mol	Chain	Length	Quality of chain
35	Aw	143	97%
36	Ax	130	95%
37	Ay	124	69% 31%
38	Az	25	100%
39	B5	4808	66% 12% 22%
40	B7	120	92% 8%
41	B8	158	87% 12%
42	BA	257	98%
43	BB	403	99%
44	BC	413	87% 12%
45	BD	297	99%
46	BE	291	84% 16%
47	BF	247	91% 9%
48	BG	266	87% 12%
49	BH	192	99%
50	BI	214	99%
51	BJ	178	96%
52	BK	1071	97%
53	BL	211	98%
54	BM	218	63% 37%
55	BN	204	99%
56	BO	203	97%
57	BP	184	86% 14%
58	BQ	188	99%
59	BR	196	91% 8%

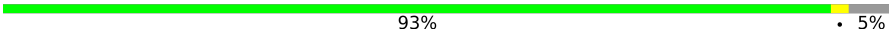
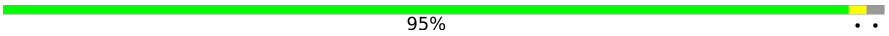
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Mol	Chain	Length	Quality of chain
60	BS	176	 99%
61	BT	160	 99%
62	BU	128	 77% 23%
63	BV	140	 99%
64	BW	157	 76% 23%
65	BX	156	 76% 24%
66	BY	145	 92% 8%
67	BZ	136	 99%
68	Ba	148	 98%
69	Bb	245	 44% 56%
70	Bc	115	 94% 6%
71	Bd	125	 85% 14%
72	Be	135	 96%
73	Bf	110	 100%
74	Bg	117	 97%
75	Bh	123	 99%
76	Bi	105	 96%
77	Bj	97	 89% 11%
78	Bk	70	 99%
79	Bl	51	 96%
80	Bm	128	 41% 59%
81	Bo	106	 98%
82	Bp	92	 99%
83	Br	137	 91% 8%
84	Bs	318	 62% 38%

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Mol	Chain	Length	Quality of chain
85	Bt	165	 93% . 5%
86	Bv	217	 95% ..

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 237077 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	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 2 is a protein called 40S ribosomal protein S27.

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

- Molecule 3 is a protein called Ribosomal protein S28.

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

- Molecule 4 is a protein called Ribosomal protein S27a.

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

- Molecule 5 is a protein called 40S ribosomal protein S30.

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

- Molecule 6 is a protein called Ribosomal protein eS26.

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

- Molecule 7 is a protein called RACK1.

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

- Molecule 8 is a protein called uS14.

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

- Molecule 9 is a RNA chain called mRNA containing SARS-CoV-2 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	AH	8	128	55	16	50	7	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AH	3466	U	A	conflict	GB NC_045512.2
AH	3468	A	C	conflict	GB NC_045512.2

- Molecule 10 is a RNA chain called E-site tRNA.

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

- Molecule 11 is a RNA chain called P-site Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	AT	76	1652	746	294	536	76	0	0

- Molecule 12 is a protein called 40S ribosomal protein SA.

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

- Molecule 13 is a protein called 40S ribosomal protein S3a.

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

- Molecule 14 is a protein called Ribosomal protein uS5.

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

- Molecule 15 is a protein called 40S ribosomal protein S3.

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

- Molecule 16 is a protein called Ribosomal protein eS4.

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

- Molecule 17 is a protein called Ribosomal protein S5.

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

- Molecule 18 is a protein called 40S ribosomal protein S6.

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

- Molecule 19 is a protein called 40S ribosomal protein S7.

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

- Molecule 20 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 21 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 22 is a protein called eS10.

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

- Molecule 23 is a protein called 40S ribosomal protein S11.

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

- Molecule 24 is a protein called 40S ribosomal protein S12.

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

- Molecule 25 is a protein called uS15.

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

- Molecule 26 is a protein called 40S ribosomal protein uS11.

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

- Molecule 27 is a protein called 40S ribosomal protein uS19.

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

- Molecule 28 is a protein called uS9.

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

- Molecule 29 is a protein called 40S ribosomal protein eS17.

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

- Molecule 30 is a protein called 40S ribosomal protein S18.

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

- Molecule 31 is a protein called Ribosomal protein eS19.

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

- Molecule 32 is a protein called 40S ribosomal protein uS10.

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

- Molecule 33 is a protein called Ribosomal protein eS21.

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

- Molecule 34 is a protein called Ribosomal protein S15a.

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

- Molecule 35 is a protein called 40S ribosomal protein S23.

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

- Molecule 36 is a protein called 40S ribosomal protein S24.

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

- Molecule 37 is a protein called 40S ribosomal protein S25.

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

- Molecule 38 is a protein called 60s ribosomal protein l41.

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

- Molecule 39 is a RNA chain called 28S rRNA.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 40 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
40	B7	120	2570	1141	456	851	122	0	0

- Molecule 41 is a RNA chain called 5.8S rRNA.

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

- Molecule 42 is a protein called Ribosomal protein uL2.

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

- Molecule 43 is a protein called Ribosomal protein L3.

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

- Molecule 44 is a protein called 60S ribosomal protein L4.

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

- Molecule 45 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BD	294	2398	1516	439	429	14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BD	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 46 is a protein called 60S ribosomal protein L6.

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

- Molecule 47 is a protein called Ribosomal Protein uL30.

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

- Molecule 48 is a protein called Ribosomal protein eL8.

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

- Molecule 49 is a protein called 60S ribosomal protein L9.

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

- Molecule 50 is a protein called 60S ribosomal protein L10.

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

- Molecule 51 is a protein called Ribosomal protein L11.

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

- Molecule 52 is a protein called Replicase polyprotein 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BK	35	Total	C	N	O	S	0	0
			265	163	45	51	6		

- Molecule 53 is a protein called Ribosomal protein eL13.

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

- Molecule 54 is a protein called Ribosomal protein L14.

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

- Molecule 55 is a protein called Ribosomal protein L15.

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

- Molecule 56 is a protein called Ribosomal protein uL13.

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

- Molecule 57 is a protein called uL22.

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

- Molecule 58 is a protein called Ribosomal Protein eL18.

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

- Molecule 59 is a protein called 60S ribosomal protein L19.

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

- Molecule 60 is a protein called Ribosomal protein eL20.

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

- Molecule 61 is a protein called eL21.

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

- Molecule 62 is a protein called Ribosomal protein eL22.

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

- Molecule 63 is a protein called Ribosomal protein L23.

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

- Molecule 64 is a protein called eL24.

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

- Molecule 65 is a protein called uL23.

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

- Molecule 66 is a protein called Ribosomal protein L26.

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

- Molecule 67 is a protein called 60S ribosomal protein L27.

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

- Molecule 68 is a protein called 60S ribosomal protein L27a.

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

- Molecule 69 is a protein called 60S ribosomal protein L29.

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

- Molecule 70 is a protein called eL30.

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

- Molecule 71 is a protein called eL31.

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

- Molecule 72 is a protein called eL32.

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

- Molecule 73 is a protein called eL33.

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

- Molecule 74 is a protein called 60S ribosomal protein L34.

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

- Molecule 75 is a protein called uL29.

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

- Molecule 76 is a protein called 60S ribosomal protein L36.

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

- Molecule 77 is a protein called Ribosomal protein L37.

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

- Molecule 78 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	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	conflict	UNP G1U001

- Molecule 79 is a protein called eL39.

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

- Molecule 80 is a protein called 60S ribosomal protein L40.

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

- Molecule 81 is a protein called eL42.

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

- Molecule 82 is a protein called eL43.

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

- Molecule 83 is a protein called Ribosomal protein eL28.

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

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

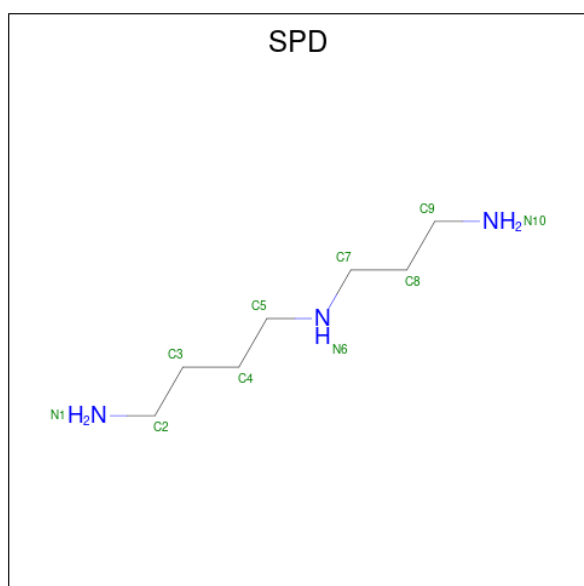
- Molecule 85 is a protein called Ribosomal protein L12.

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

- Molecule 86 is a protein called Ribosomal protein uL1.

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

- Molecule 87 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



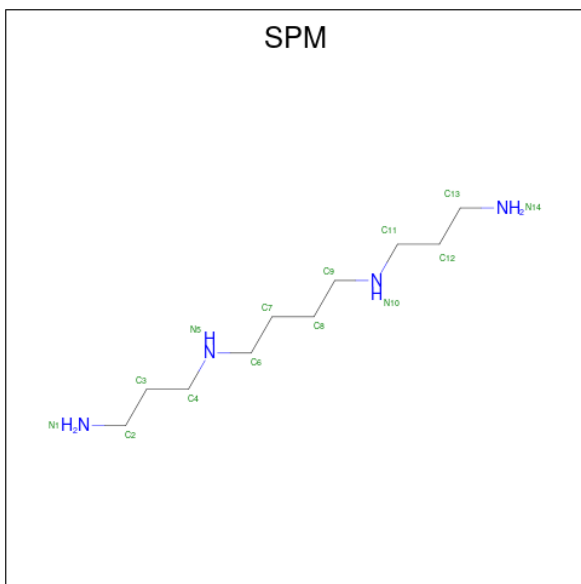
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
87	A2	1	10	7	3	0
87	A2	1	10	7	3	0
87	A2	1	10	7	3	0
87	A2	1	10	7	3	0
87	A2	1	10	7	3	0
87	A2	1	10	7	3	0
87	A2	1	10	7	3	0
87	A2	1	10	7	3	0

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

- Molecule 88 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



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

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
89	A2	110	110	110	0
89	AT	3	3	3	0
89	Af	1	1	1	0
89	B5	284	284	284	0
89	B7	9	9	9	0

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Mol	Chain	Residues	Atoms		AltConf
89	B8	9	Total 9	Mg 9	0
89	BP	1	Total 1	Mg 1	0
89	BR	1	Total 1	Mg 1	0
89	BV	1	Total 1	Mg 1	0
89	Ba	1	Total 1	Mg 1	0

- Molecule 90 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
90	A2	61	Total 61	X 61	0
90	AT	4	Total 4	X 4	0
90	Ad	1	Total 1	X 1	0
90	An	1	Total 1	X 1	0
90	Ar	1	Total 1	X 1	0
90	B5	225	Total 225	X 225	0
90	B7	6	Total 6	X 6	0
90	B8	7	Total 7	X 7	0
90	BA	4	Total 4	X 4	0
90	BB	3	Total 3	X 3	0
90	BC	1	Total 1	X 1	0
90	BH	1	Total 1	X 1	0
90	BI	1	Total 1	X 1	0
90	BL	1	Total 1	X 1	0

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Mol	Chain	Residues	Atoms	AltConf
90	BN	1	Total X 1 1	0
90	BQ	2	Total X 2 2	0
90	BT	2	Total X 2 2	0
90	Bb	1	Total X 1 1	0
90	Be	2	Total X 2 2	0
90	Bf	1	Total X 1 1	0
90	Bg	1	Total X 1 1	0
90	Bj	1	Total X 1 1	0
90	Bl	1	Total X 1 1	0
90	Bo	1	Total X 1 1	0

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

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

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	A2	1579	Total 1579	O 1579	0
92	AA	6	Total 6	O 6	0
92	AD	2	Total 2	O 2	0
92	AE	19	Total 19	O 19	0
92	AG	1	Total 1	O 1	0
92	AH	14	Total 14	O 14	0
92	AI	12	Total 12	O 12	0
92	AT	35	Total 35	O 35	0
92	AZ	1	Total 1	O 1	0
92	Aa	16	Total 16	O 16	0
92	Ab	10	Total 10	O 10	0
92	Ad	9	Total 9	O 9	0
92	Ae	4	Total 4	O 4	0
92	Af	6	Total 6	O 6	0
92	Ag	4	Total 4	O 4	0
92	Ah	22	Total 22	O 22	0
92	Ai	4	Total 4	O 4	0
92	Ak	31	Total 31	O 31	0
92	Am	22	Total 22	O 22	0
92	An	20	Total 20	O 20	0
92	Ap	10	Total 10	O 10	0
92	Ar	2	Total 2	O 2	0

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Mol	Chain	Residues	Atoms		AltConf
92	As	4	Total 4	O 4	0
92	At	4	Total 4	O 4	0
92	Au	1	Total 1	O 1	0
92	Av	16	Total 16	O 16	0
92	Aw	23	Total 23	O 23	0
92	Ax	1	Total 1	O 1	0
92	Ay	1	Total 1	O 1	0
92	Az	9	Total 9	O 9	0
92	B5	7033	Total 7033	O 7033	0
92	B7	199	Total 199	O 199	0
92	B8	250	Total 250	O 250	0
92	BA	114	Total 114	O 114	0
92	BB	131	Total 131	O 131	0
92	BC	148	Total 148	O 148	0
92	BD	45	Total 45	O 45	0
92	BE	34	Total 34	O 34	0
92	BF	88	Total 88	O 88	0
92	BG	34	Total 34	O 34	0
92	BH	34	Total 34	O 34	0
92	BI	64	Total 64	O 64	0
92	BJ	13	Total 13	O 13	0

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Mol	Chain	Residues	Atoms		AltConf
92	BK	5	Total 5	O 5	0
92	BL	79	Total 79	O 79	0
92	BM	20	Total 20	O 20	0
92	BN	139	Total 139	O 139	0
92	BO	69	Total 69	O 69	0
92	BP	51	Total 51	O 51	0
92	BQ	84	Total 84	O 84	0
92	BR	44	Total 44	O 44	0
92	BS	58	Total 58	O 58	0
92	BT	55	Total 55	O 55	0
92	BU	5	Total 5	O 5	0
92	BV	36	Total 36	O 36	0
92	BW	15	Total 15	O 15	0
92	BX	22	Total 22	O 22	0
92	BY	21	Total 21	O 21	0
92	BZ	12	Total 12	O 12	0
92	Ba	87	Total 87	O 87	0
92	Bb	24	Total 24	O 24	0
92	Bc	13	Total 13	O 13	0
92	Bd	31	Total 31	O 31	0
92	Be	77	Total 77	O 77	0

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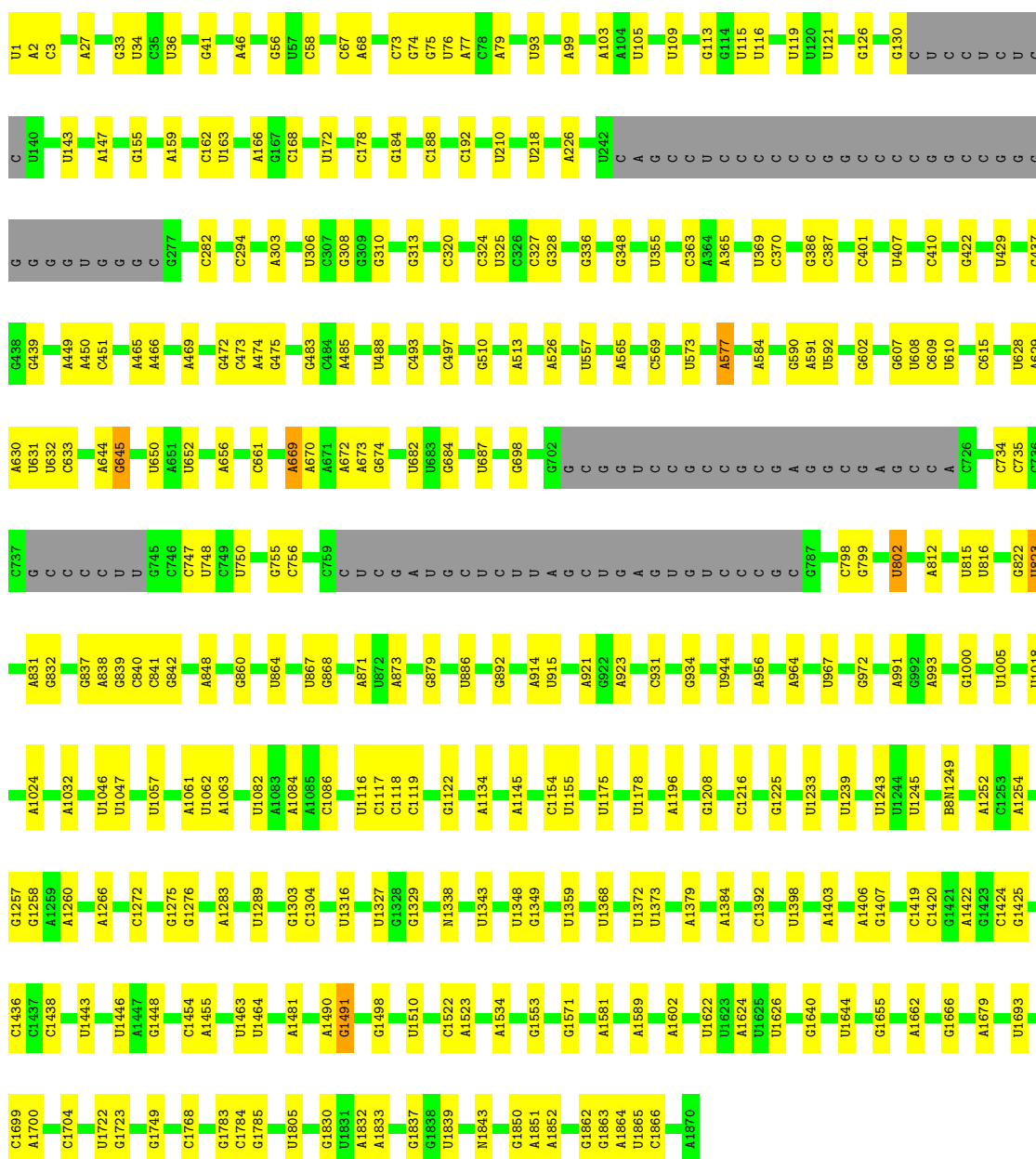
Mol	Chain	Residues	Atoms		AltConf
92	Bf	36	Total 36	O 36	0
92	Bg	45	Total 45	O 45	0
92	Bh	17	Total 17	O 17	0
92	Bi	19	Total 19	O 19	0
92	Bj	52	Total 52	O 52	0
92	Bk	1	Total 1	O 1	0
92	Bl	16	Total 16	O 16	0
92	Bm	14	Total 14	O 14	0
92	Bo	46	Total 46	O 46	0
92	Bp	32	Total 32	O 32	0
92	Br	41	Total 41	O 41	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

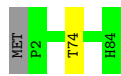
- Molecule 1: 18S rRNA

Chain A2:  79% 16% 5%



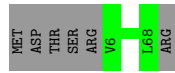
• Molecule 2: 40S ribosomal protein S27

Chain AA:  98%



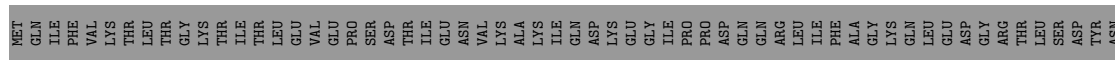
• Molecule 3: Ribosomal protein S28

Chain AB:  91%



• Molecule 4: Ribosomal protein S27a

Chain AC:  47%




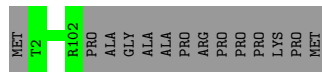
• Molecule 5: 40S ribosomal protein S30

Chain AD:  42%



• Molecule 6: Ribosomal protein eS26

Chain AE:  88%



• Molecule 7: RACK1

Chain AF:  98%



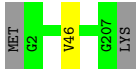
• Molecule 8: uS14

Chain AG:  98%



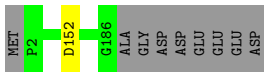
- Molecule 20: 40S ribosomal protein S8

Chain Ah: 99%



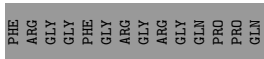
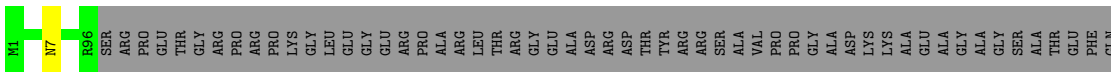
- Molecule 21: Ribosomal protein S9 (Predicted)

Chain Ai: 95% 5%



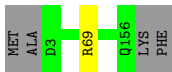
- Molecule 22: eS10

Chain Aj: 58% 42%



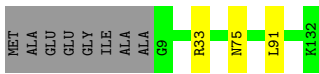
- Molecule 23: 40S ribosomal protein S11

Chain Ak: 97%



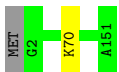
- Molecule 24: 40S ribosomal protein S12

Chain Al: 92% 6%



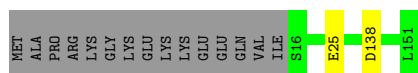
- Molecule 25: uS15

Chain Am: 99%




- Molecule 26: 40S ribosomal protein uS11

Chain An:  89% . 10%




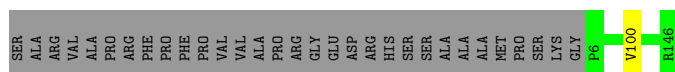
- Molecule 27: 40S ribosomal protein uS19

Chain Ao:  88% . 12%



- Molecule 28: uS9

Chain Ap:  81% . 18%



- Molecule 29: 40S ribosomal protein eS17

Chain Aq:  99% .



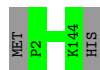
- Molecule 30: 40S ribosomal protein S18

Chain Ar:  95% . .




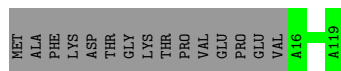
- Molecule 31: Ribosomal protein eS19

Chain As:  99% .



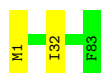
- Molecule 32: 40S ribosomal protein uS10

Chain At:  87% 13%



- Molecule 33: Ribosomal protein eS21

Chain Au:  98%



- Molecule 34: Ribosomal protein S15a

Chain Av:  99%



- Molecule 35: 40S ribosomal protein S23

Chain Aw:  97%



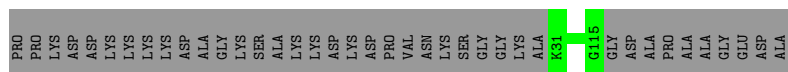
- Molecule 36: 40S ribosomal protein S24

Chain Ax:  95%



- Molecule 37: 40S ribosomal protein S25

Chain Ay:  69%  31%



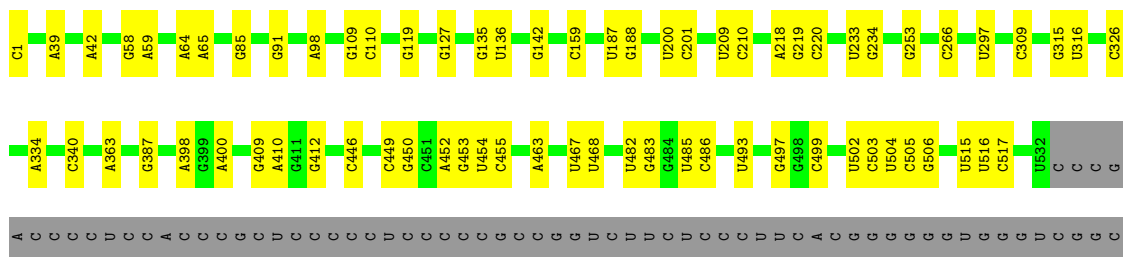
- Molecule 38: 60s ribosomal protein l41

Chain Az:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: 28S rRNA

Chain B5:  66%  12%  22%




G4756	G4761	C4762	C4763	C4764	U4765	C4766	G4780	C4789	C4793	A4797	C4801	U4805	U4808	G4637	G4638	G4639	G4640	C4641	G4642	G4643	G4644	G4645	G4646	G4647	G4648	G4649	A4650	G4651	G4655	G4658	A4705	U4711	U4715	U4728	C4729	U4740	A4746	U4749	A4753					
C	G	C	G	C	C	C	G	C	G	C	C	C	C	C	G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C			
G	C	C	C	C	U	C	G	C	C	C	C	C	C	C	C	G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C		
U	G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C		
C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C		
G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C		
C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C		
C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	
C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C

● Molecule 40: 5S rRNA



G1	G7	U33	A42	A50	U53	A54	G64	G110	U120
----	----	-----	-----	-----	-----	-----	-----	------	------

- Molecule 41: 5.8S rRNA

Chain B8:  87% 12%



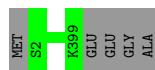
- Molecule 42: Ribosomal protein uL2

Chain BA:  98%




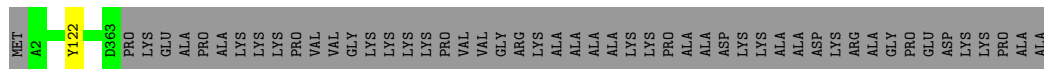
- Molecule 43: Ribosomal protein L3

Chain BB:  99%



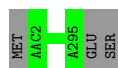
- Molecule 44: 60S ribosomal protein L4

Chain BC:  87% 12%




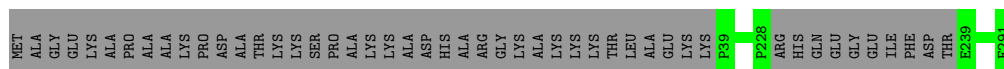
- Molecule 45: Ribosomal_L18_c domain-containing protein

Chain BD:  99%



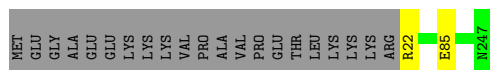
- Molecule 46: 60S ribosomal protein L6

Chain BE:  84% 16%



- Molecule 47: Ribosomal Protein uL30

Chain BF:  91% 9%



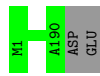
- Molecule 48: Ribosomal protein eL8

Chain BG: 87% 12%



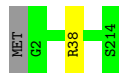
- Molecule 49: 60S ribosomal protein L9

Chain BH: 99%



- Molecule 50: 60S ribosomal protein L10

Chain BI: 99%



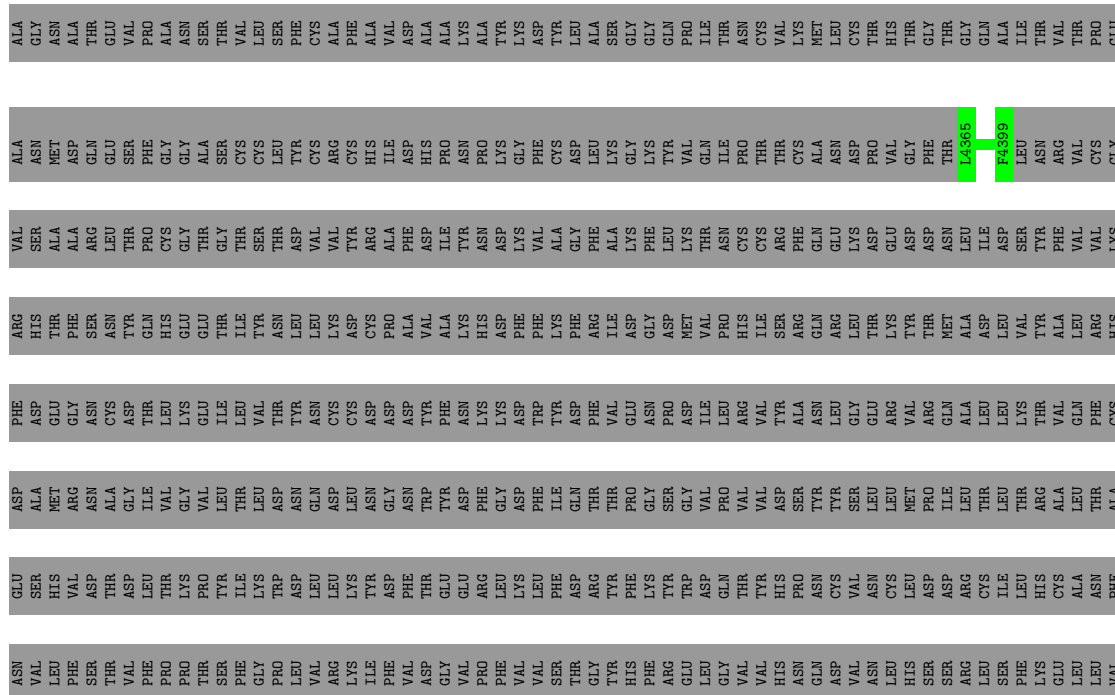
- Molecule 51: Ribosomal protein L11

Chain BJ: 96%

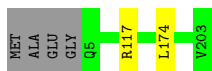


- Molecule 52: Replicase polyprotein 1ab


Chain BK: 97%

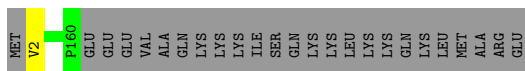


Chain BO:  97%



- Molecule 57: uL22

Chain BP:  86% 14%



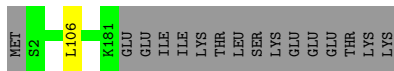
- Molecule 58: Ribosomal Protein eL18

Chain BQ:  99%



- Molecule 59: 60S ribosomal protein L19

Chain BR:  91% 8%



- Molecule 60: Ribosomal protein eL20

Chain BS:  99%




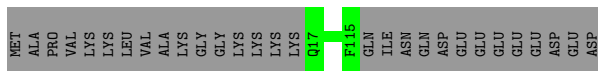
- Molecule 61: eL21

Chain BT:  99%



- Molecule 62: Ribosomal protein eL22

Chain BU:  77% 23%

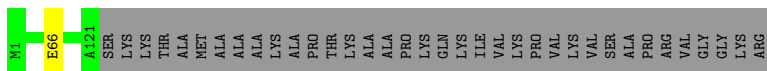
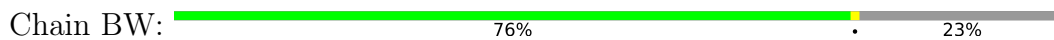


- Molecule 63: Ribosomal protein L23

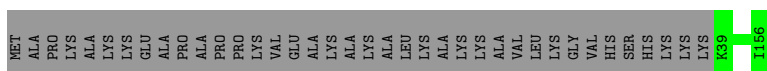
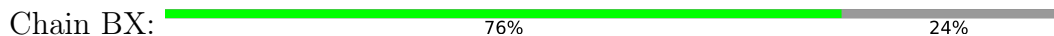
Chain BV:  99%



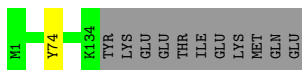
- Molecule 64: eL24



- Molecule 65: uL23



- Molecule 66: Ribosomal protein L26



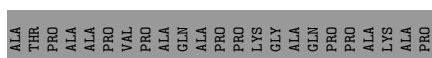
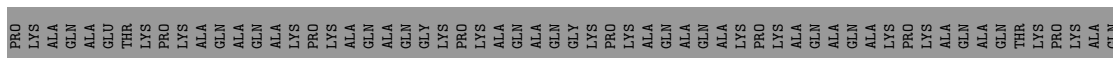
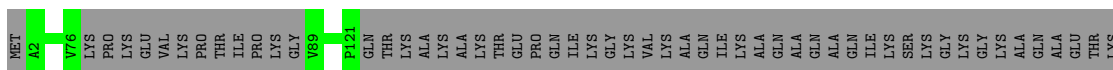
- Molecule 67: 60S ribosomal protein L27



- Molecule 68: 60S ribosomal protein L27a

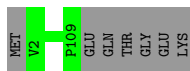


- Molecule 69: 60S ribosomal protein L29




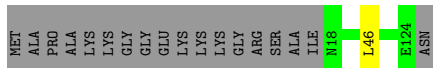
- Molecule 70: eL30

Chain Bc:  94% 6%



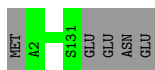
- Molecule 71: eL31

Chain Bd:  85% 14%



- Molecule 72: eL32

Chain Be:  96% .



- Molecule 73: eL33

Chain Bf:  100%

There are no outlier residues recorded for this chain.

- Molecule 74: 60S ribosomal protein L34

Chain Bg:  97% ..



- Molecule 75: uL29

Chain Bh:  99% .




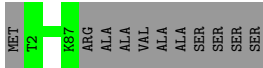
- Molecule 76: 60S ribosomal protein L36

Chain Bi:  96% ..



- Molecule 77: Ribosomal protein L37

Chain Bj:  89% 11%



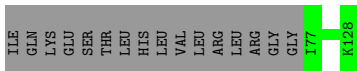
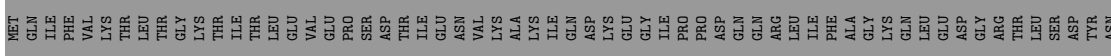
- Molecule 78: eL38



- Molecule 79: eL39



- Molecule 80: 60S ribosomal protein L40



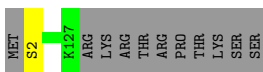
- Molecule 81: eL42



- Molecule 82: eL43



- Molecule 83: Ribosomal protein eL28



- Molecule 84: 60S acidic ribosomal protein P0

Chain Bs:  62% 38%

MET	GLU	PRO	ARG	GLU	D5	H206	PRO	GLU	VAL	LEU	ASP	ILE	THR	GLU	ASP	THR	LEU	HIS	SER	ARG	PHE	LEU	GLY	VAL	ARG	ASN	VAL	ALA	ALA	SER	VAL	CYS	LEU	GLN	ILE	GLY	TYR	PRO	THR	VAL	ALA	ALA	VAL	PRO	VAL	HIS	SER	ILE	ASN	GLY	TYR	LYS	ARG	VAL	LEU	ALA	LEU	SER	VAL	GLY
-----	-----	-----	-----	-----	----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLU	THR	LEU	TYR	THR	PHE	PRO	LEU	ALA	GLU	LYS	VAL	LYS	ALA	PHE	LEU	ALA	ASP	PRO	SER	ALA	VAL	VAL	ALA	ALA	PRO	VAL	ALA	ALA	SER	THR	ALA	PRO	ALA	ALA	ALA	PRO	LYS	VAL	GLU	LYS	ALA	GLU	GLY	GLU	SER	GLU	GLU	SER	GLU	ASP	GLU	ASP	MET	SER	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PHE	GLY	LEU	PHE	ASP
-----	-----	-----	-----	-----

- Molecule 85: Ribosomal protein L12

Chain Bt:  93% 5%

MET	PRO	LYS	PHE	ASP	PRO	ASN	E9	V73	V74	R92	A164	SER
-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	------	-----

- Molecule 86: Ribosomal protein uL1

Chain Bv:  95%

MET	GLY	ASP	ILE	LEU	S6	T88	F89	R60	H73	N96	V167	Y217
-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	695501	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	56604	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 1MA, MG, MA6, 5MC, HY3, 4AC, YYG, HIC, SAC, SPM, UR3, UY1, MLZ, 6MZ, PSU, V5N, OMU, H2U, SPD, B8N, M3L, UNX, 2MG, GTP, ZN, 7MG, AYA, OMG, A2M, NMM, AME, M2G, OMC, AAC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A2	0.18	1/40342 (0.0%)	0.70	9/62877 (0.0%)
2	AA	0.24	0/665	0.46	0/891
3	AB	0.24	0/497	0.58	0/666
4	AC	0.24	0/622	0.48	0/822
5	AD	0.25	0/462	0.54	0/607
6	AE	0.23	0/828	0.54	0/1109
7	AF	0.23	0/2493	0.47	0/3394
8	AG	0.23	0/470	0.52	0/623
9	AH	0.15	0/140	0.67	0/217
10	AI	0.33	0/68	0.79	0/103
11	AT	0.34	1/1440 (0.1%)	0.69	0/2242
12	AZ	0.23	0/1771	0.46	0/2406
13	Aa	0.23	0/1841	0.46	0/2459
14	Ab	0.24	0/1742	0.46	0/2354
15	Ac	0.24	0/1779	0.49	0/2395
16	Ad	0.24	0/2118	0.51	0/2849
17	Ae	0.23	0/1531	0.48	0/2059
18	Af	0.24	0/1946	0.53	0/2590
19	Ag	0.24	0/1552	0.47	0/2079
20	Ah	0.24	0/1715	0.52	0/2287
21	Ai	0.23	0/1550	0.52	0/2069
22	Aj	0.24	0/834	0.44	0/1125
23	Ak	0.25	0/1284	0.52	0/1717
24	Al	0.22	0/968	0.42	0/1296
25	Am	0.23	0/1232	0.48	0/1656
26	An	0.25	0/1029	0.55	0/1380
27	Ao	0.25	0/1069	0.49	0/1429
28	Ap	0.24	0/1142	0.51	0/1528
29	Aq	0.23	0/1094	0.49	0/1469
30	Ar	0.23	0/1226	0.54	0/1643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	As	0.23	0/1119	0.46	0/1498
32	At	0.23	0/831	0.52	0/1115
33	Au	0.24	0/636	0.49	0/852
34	Av	0.24	0/1051	0.49	0/1406
35	Aw	0.24	0/1107	0.51	0/1475
36	Ax	0.24	0/1032	0.51	0/1371
37	Ay	0.23	0/691	0.47	0/922
38	Az	0.22	0/240	0.68	0/305
39	B5	0.21	3/87403 (0.0%)	0.71	9/136359 (0.0%)
40	B7	0.19	0/2835	0.70	0/4418
41	B8	0.26	1/3635 (0.0%)	0.70	0/5661
42	BA	0.25	0/1965	0.55	0/2633
43	BB	0.24	0/3261	0.51	0/4364
44	BC	0.24	0/2932	0.51	0/3939
45	BD	0.24	0/2437	0.48	0/3264
46	BE	0.24	0/1998	0.50	0/2673
47	BF	0.24	0/1922	0.50	0/2563
48	BG	0.23	0/1908	0.48	0/2566
49	BH	0.24	0/1535	0.50	0/2063
50	BI	0.24	0/1756	0.51	0/2346
51	BJ	0.24	0/1385	0.51	0/1852
52	BK	0.25	0/269	0.46	0/361
53	BL	0.24	0/1733	0.54	0/2316
54	BM	0.24	0/1158	0.50	0/1547
55	BN	0.24	0/1746	0.56	0/2338
56	BO	0.24	0/1662	0.50	0/2222
57	BP	0.23	0/1317	0.50	0/1768
58	BQ	0.24	0/1539	0.57	0/2054
59	BR	0.22	0/1524	0.54	0/2013
60	BS	0.25	0/1497	0.54	0/2008
61	BT	0.24	0/1326	0.50	0/1770
62	BU	0.25	0/820	0.48	0/1100
63	BV	0.26	0/1048	0.53	0/1402
64	BW	0.24	0/1006	0.50	0/1334
65	BX	0.24	0/984	0.49	0/1323
66	BY	0.24	0/1132	0.52	0/1504
67	BZ	0.25	0/1130	0.49	0/1507
68	Ba	0.24	0/1179	0.51	0/1572
69	Bb	0.23	0/884	0.52	0/1169
70	Bc	0.24	0/847	0.44	0/1134
71	Bd	0.24	0/903	0.53	0/1216
72	Be	0.23	0/1088	0.53	0/1451
73	Bf	0.26	0/903	0.55	0/1208

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Bg	0.23	0/916	0.55	0/1220
75	Bh	0.23	0/1021	0.49	0/1348
76	Bi	0.23	0/841	0.53	0/1112
77	Bj	0.24	0/720	0.57	0/952
78	Bk	0.24	0/575	0.45	0/761
79	Bl	0.23	0/459	0.52	0/608
80	Bm	0.23	0/426	0.52	0/564
81	Bo	0.25	0/866	0.52	0/1141
82	Bp	0.23	0/718	0.50	0/953
83	Br	0.23	0/1020	0.54	0/1366
84	Bs	0.24	0/1530	0.46	0/2064
85	Bt	0.23	0/1193	0.48	0/1609
86	Bv	0.23	0/1735	0.45	0/2328
All	All	0.22	6/234844 (0.0%)	0.64	18/344329 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
81	Bo	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4761	U	C4-O4	12.87	1.33	1.23
41	B8	1	C	OP3-P	-10.64	1.48	1.61
1	A2	1	U	OP3-P	-10.58	1.48	1.61
39	B5	1	C	OP3-P	-10.58	1.48	1.61
11	AT	1	G	OP3-P	-10.57	1.48	1.61

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	4761	U	N3-C4-C5	12.14	121.88	114.60
39	B5	4761	U	C2-N3-C4	-11.53	120.08	127.00
39	B5	4761	U	C5-C4-O4	-9.45	120.23	125.90
1	A2	1454	C	C2-N1-C1'	7.31	126.84	118.80
39	B5	4761	U	N1-C2-N3	7.14	119.19	114.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
81	Bo	53	MLZ	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	72/156 (46%)	69 (96%)	3 (4%)	0	100	100
5	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
6	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
7	AF	311/317 (98%)	303 (97%)	8 (3%)	0	100	100
8	AG	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
12	AZ	219/295 (74%)	213 (97%)	6 (3%)	0	100	100
13	Aa	220/264 (83%)	217 (99%)	3 (1%)	0	100	100
14	Ab	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
15	Ac	223/281 (79%)	221 (99%)	2 (1%)	0	100	100
16	Ad	260/263 (99%)	258 (99%)	2 (1%)	0	100	100
17	Ae	189/204 (93%)	186 (98%)	3 (2%)	0	100	100
18	Af	235/249 (94%)	235 (100%)	0	0	100	100
19	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
20	Ah	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
21	Ai	183/194 (94%)	180 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	Aj	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
23	Ak	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
24	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
25	Am	148/151 (98%)	148 (100%)	0	0	100	100
26	An	134/151 (89%)	130 (97%)	4 (3%)	0	100	100
27	Ao	126/145 (87%)	123 (98%)	2 (2%)	1 (1%)	19	19
28	Ap	139/172 (81%)	135 (97%)	3 (2%)	1 (1%)	22	22
29	Aq	132/135 (98%)	132 (100%)	0	0	100	100
30	Ar	146/152 (96%)	142 (97%)	4 (3%)	0	100	100
31	As	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
32	At	102/119 (86%)	101 (99%)	1 (1%)	0	100	100
33	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
34	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
35	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
36	Ax	123/130 (95%)	123 (100%)	0	0	100	100
37	Ay	83/124 (67%)	82 (99%)	1 (1%)	0	100	100
38	Az	23/25 (92%)	23 (100%)	0	0	100	100
42	BA	250/257 (97%)	243 (97%)	7 (3%)	0	100	100
43	BB	395/403 (98%)	389 (98%)	6 (2%)	0	100	100
44	BC	360/413 (87%)	358 (99%)	2 (1%)	0	100	100
45	BD	291/297 (98%)	289 (99%)	2 (1%)	0	100	100
46	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
47	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
48	BG	229/266 (86%)	229 (100%)	0	0	100	100
49	BH	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
50	BI	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
51	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
52	BK	33/1071 (3%)	33 (100%)	0	0	100	100
53	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
54	BM	136/218 (62%)	135 (99%)	1 (1%)	0	100	100
55	BN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	BO	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
57	BP	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
58	BQ	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
59	BR	178/196 (91%)	178 (100%)	0	0	100	100
60	BS	174/176 (99%)	174 (100%)	0	0	100	100
61	BT	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
62	BU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
63	BV	137/140 (98%)	137 (100%)	0	0	100	100
64	BW	119/157 (76%)	118 (99%)	1 (1%)	0	100	100
65	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
66	BY	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
67	BZ	133/136 (98%)	133 (100%)	0	0	100	100
68	Ba	144/148 (97%)	139 (96%)	4 (3%)	1 (1%)	22	22
69	Bb	103/245 (42%)	97 (94%)	6 (6%)	0	100	100
70	Bc	106/115 (92%)	106 (100%)	0	0	100	100
71	Bd	105/125 (84%)	105 (100%)	0	0	100	100
72	Be	128/135 (95%)	128 (100%)	0	0	100	100
73	Bf	108/110 (98%)	108 (100%)	0	0	100	100
74	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
75	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
76	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
77	Bj	84/97 (87%)	84 (100%)	0	0	100	100
78	Bk	67/70 (96%)	67 (100%)	0	0	100	100
79	Bl	48/51 (94%)	48 (100%)	0	0	100	100
80	Bm	49/128 (38%)	49 (100%)	0	0	100	100
81	Bo	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
82	Bp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
83	Br	124/137 (90%)	121 (98%)	3 (2%)	0	100	100
84	Bs	194/318 (61%)	188 (97%)	6 (3%)	0	100	100
85	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
86	Bv	210/217 (97%)	201 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11943/14908 (80%)	11781 (99%)	159 (1%)	3 (0%)	100 100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	Ao	137	HIS
28	Ap	100	VAL
68	Ba	15	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AA	75/76 (99%)	74 (99%)	1 (1%)	69 81
3	AB	56/62 (90%)	56 (100%)	0	100 100
4	AC	67/140 (48%)	67 (100%)	0	100 100
5	AD	47/106 (44%)	46 (98%)	1 (2%)	53 67
6	AE	88/98 (90%)	88 (100%)	0	100 100
7	AF	272/275 (99%)	270 (99%)	2 (1%)	84 91
8	AG	48/49 (98%)	48 (100%)	0	100 100
12	AZ	182/243 (75%)	179 (98%)	3 (2%)	62 76
13	Aa	203/231 (88%)	202 (100%)	1 (0%)	88 94
14	Ab	185/223 (83%)	182 (98%)	3 (2%)	62 76
15	Ac	189/232 (82%)	185 (98%)	4 (2%)	53 67
16	Ad	224/225 (100%)	224 (100%)	0	100 100
17	Ae	161/170 (95%)	161 (100%)	0	100 100
18	Af	207/218 (95%)	206 (100%)	1 (0%)	88 94
19	Ag	170/360 (47%)	169 (99%)	1 (1%)	86 93
20	Ah	178/180 (99%)	177 (99%)	1 (1%)	86 93
21	Ai	161/168 (96%)	160 (99%)	1 (1%)	86 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	Aj	87/136 (64%)	86 (99%)	1 (1%)	73	85
23	Ak	139/142 (98%)	138 (99%)	1 (1%)	84	91
24	Al	104/108 (96%)	101 (97%)	3 (3%)	42	54
25	Am	130/131 (99%)	129 (99%)	1 (1%)	81	90
26	An	106/119 (89%)	104 (98%)	2 (2%)	57	71
27	Ao	114/130 (88%)	114 (100%)	0	100	100
28	Ap	117/140 (84%)	117 (100%)	0	100	100
29	Aq	120/121 (99%)	120 (100%)	0	100	100
30	Ar	127/131 (97%)	124 (98%)	3 (2%)	49	62
31	As	112/114 (98%)	112 (100%)	0	100	100
32	At	94/107 (88%)	94 (100%)	0	100	100
33	Au	67/67 (100%)	66 (98%)	1 (2%)	65	78
34	Av	112/113 (99%)	112 (100%)	0	100	100
35	Aw	112/114 (98%)	111 (99%)	1 (1%)	78	88
36	Ax	107/112 (96%)	106 (99%)	1 (1%)	78	88
37	Ay	75/102 (74%)	75 (100%)	0	100	100
38	Az	24/24 (100%)	24 (100%)	0	100	100
42	BA	194/198 (98%)	193 (100%)	1 (0%)	88	94
43	BB	344/347 (99%)	344 (100%)	0	100	100
44	BC	302/337 (90%)	301 (100%)	1 (0%)	92	97
45	BD	247/250 (99%)	247 (100%)	0	100	100
46	BE	216/251 (86%)	216 (100%)	0	100	100
47	BF	197/215 (92%)	195 (99%)	2 (1%)	76	86
48	BG	199/223 (89%)	197 (99%)	2 (1%)	76	86
49	BH	169/171 (99%)	169 (100%)	0	100	100
50	BI	180/181 (99%)	179 (99%)	1 (1%)	86	93
51	BJ	143/149 (96%)	143 (100%)	0	100	100
52	BK	30/936 (3%)	30 (100%)	0	100	100
53	BL	175/176 (99%)	172 (98%)	3 (2%)	60	74
54	BM	117/161 (73%)	117 (100%)	0	100	100
55	BN	171/172 (99%)	169 (99%)	2 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	BO	171/173 (99%)	169 (99%)	2 (1%)	71	83
57	BP	140/163 (86%)	139 (99%)	1 (1%)	84	91
58	BQ	164/165 (99%)	163 (99%)	1 (1%)	86	93
59	BR	159/175 (91%)	158 (99%)	1 (1%)	86	93
60	BS	154/154 (100%)	153 (99%)	1 (1%)	86	93
61	BT	139/140 (99%)	139 (100%)	0	100	100
62	BU	88/113 (78%)	88 (100%)	0	100	100
63	BV	106/107 (99%)	106 (100%)	0	100	100
64	BW	100/126 (79%)	99 (99%)	1 (1%)	76	86
65	BX	106/134 (79%)	106 (100%)	0	100	100
66	BY	124/135 (92%)	123 (99%)	1 (1%)	81	90
67	BZ	117/118 (99%)	117 (100%)	0	100	100
68	Ba	118/119 (99%)	118 (100%)	0	100	100
69	Bb	87/183 (48%)	87 (100%)	0	100	100
70	Bc	92/98 (94%)	92 (100%)	0	100	100
71	Bd	98/110 (89%)	97 (99%)	1 (1%)	76	86
72	Be	116/121 (96%)	116 (100%)	0	100	100
73	Bf	89/89 (100%)	89 (100%)	0	100	100
74	Bg	98/100 (98%)	97 (99%)	1 (1%)	76	86
75	Bh	109/110 (99%)	109 (100%)	0	100	100
76	Bi	86/89 (97%)	85 (99%)	1 (1%)	71	83
77	Bj	73/80 (91%)	73 (100%)	0	100	100
78	Bk	64/65 (98%)	64 (100%)	0	100	100
79	Bl	47/48 (98%)	46 (98%)	1 (2%)	53	67
80	Bm	47/115 (41%)	47 (100%)	0	100	100
81	Bo	92/93 (99%)	92 (100%)	0	100	100
82	Bp	74/75 (99%)	74 (100%)	0	100	100
83	Br	109/120 (91%)	109 (100%)	0	100	100
84	Bs	164/258 (64%)	164 (100%)	0	100	100
85	Bt	128/137 (93%)	125 (98%)	3 (2%)	50	63
86	Bv	191/195 (98%)	186 (97%)	5 (3%)	46	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10394/12642 (82%)	10329 (99%)	65 (1%)	86 93

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
85	Bt	73	VAL
85	Bt	92	ARG
25	Am	70	LYS
24	Al	91	LEU
86	Bv	58	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
78	Bk	58	GLN
83	Br	4	HIS
27	Ao	104	GLN
24	Al	72	HIS
83	Br	6	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1758/1870 (94%)	225 (12%)	0
10	AI	3/76 (3%)	2 (66%)	0
11	AT	75/76 (98%)	10 (13%)	0
39	B5	3750/4808 (77%)	472 (12%)	3 (0%)
40	B7	118/120 (98%)	9 (7%)	0
41	B8	155/158 (98%)	15 (9%)	0
9	AH	5/217 (2%)	0	0
All	All	5864/7325 (80%)	733 (12%)	3 (0%)

5 of 733 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	3	C
1	A2	33	G
1	A2	41	G
1	A2	46	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
39	B5	1545	C
39	B5	1588	G
39	B5	4445	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	A2	684	1	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
39	A2M	B5	3450	39	18,25,26	1.01	1 (5%)	18,36,39	1.19	2 (11%)
39	PSU	B5	3496	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
1	A2M	A2	159	1	18,25,26	1.01	1 (5%)	18,36,39	1.28	2 (11%)
39	PSU	B5	1638	39	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
39	PSU	B5	1718	39	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1047	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
1	PSU	A2	1348	1	18,21,22	1.32	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	119	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
39	5MC	B5	4193	39	18,22,23	0.99	2 (11%)	26,32,35	1.20	2 (7%)
11	H2U	AT	16	11	18,21,22	1.00	2 (11%)	21,30,33	1.51	2 (9%)
39	PSU	B5	2475	39	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	A2	93	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	A2	967	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	4116	39	18,26,27	0.89	1 (5%)	19,38,41	1.11	2 (10%)
1	PSU	A2	218	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
39	A2M	B5	1810	39,89	18,25,26	1.02	1 (5%)	18,36,39	1.29	2 (11%)
1	OMU	A2	121	1	19,22,23	1.22	3 (15%)	26,31,34	1.68	4 (15%)
39	OMG	B5	3942	39,11	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
1	6MZ	A2	1833	89,1	18,25,26	0.89	1 (5%)	16,36,39	2.11	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	PSU	B5	3490	39	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
39	PSU	B5	4045	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
39	PSU	B5	4419	39	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	A2	1626	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	1683	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
39	OMU	B5	3973	39	19,22,23	1.24	3 (15%)	26,31,34	1.71	4 (15%)
39	OMG	B5	1477	39	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	A2	1446	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	3576	39	18,21,22	1.39	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	A2	1368	1	18,21,22	1.34	2 (11%)	22,30,33	1.93	4 (18%)
1	OMU	A2	1443	89,1	19,22,23	1.22	3 (15%)	26,31,34	1.70	4 (15%)
39	OMC	B5	4282	39,89	19,22,23	0.81	0	26,31,34	0.80	0
11	PSU	AT	55	11	18,21,22	1.32	2 (11%)	22,30,33	1.91	4 (18%)
39	PSU	B5	3494	39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
39	PSU	B5	4382	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	4 (18%)
39	PSU	B5	3502	39	18,21,22	1.33	2 (11%)	22,30,33	1.92	4 (18%)
39	OMC	B5	3573	39	19,22,23	0.79	0	26,31,34	0.83	0
39	A2M	B5	3599	39	18,25,26	0.99	1 (5%)	18,36,39	1.21	2 (11%)
11	PSU	AT	27	11	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
11	1MA	AT	14	11	16,25,26	1.56	2 (12%)	18,37,40	1.02	3 (16%)
1	OMC	A2	1704	1	19,22,23	0.80	0	26,31,34	0.83	1 (3%)
1	PSU	A2	823	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
1	OMU	A2	116	1	19,22,23	1.19	3 (15%)	26,31,34	1.69	5 (19%)
1	PSU	A2	1057	1	18,21,22	1.36	2 (11%)	22,30,33	1.95	3 (13%)
1	A2M	A2	1384	1	18,25,26	1.04	1 (5%)	18,36,39	1.21	2 (11%)
39	A2M	B5	3492	39,1	18,25,26	1.02	1 (5%)	18,36,39	1.27	2 (11%)
39	PSU	B5	3616	39	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
41	PSU	B8	55	41	18,21,22	1.33	2 (11%)	22,30,33	1.89	4 (18%)
39	PSU	B5	4099	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
39	OMG	B5	3476	39	18,26,27	0.93	1 (5%)	19,38,41	1.05	2 (10%)
39	A2M	B5	1270	39	18,25,26	0.99	1 (5%)	18,36,39	1.22	2 (11%)
42	V5N	BA	216	42	4,11,12	0.78	0	5,14,16	1.61	1 (20%)
39	A2M	B5	3562	39	18,25,26	1.01	1 (5%)	18,36,39	1.25	2 (11%)
1	A2M	A2	485	1	18,25,26	1.00	1 (5%)	18,36,39	1.21	2 (11%)
39	PSU	B5	1491	39	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	PSU	B5	3652	39,89	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
39	PSU	B5	4058	39	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
11	7MG	AT	46	11	22,26,27	1.30	3 (13%)	29,39,42	2.53	7 (24%)
39	A2M	B5	2658	39,89	18,25,26	1.02	1 (5%)	18,36,39	1.24	2 (11%)
39	PSU	B5	3585	39,89	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
11	1MA	AT	58	11	16,25,26	1.61	2 (12%)	18,37,40	1.04	2 (11%)
39	OMG	B5	1260	39	18,26,27	0.95	1 (5%)	19,38,41	1.16	2 (10%)
1	PSU	A2	682	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	3500	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4107	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	A2M	B5	3517	39	18,25,26	0.91	1 (5%)	18,36,39	1.38	2 (11%)
1	PSU	A2	1233	1	18,21,22	1.35	2 (11%)	22,30,33	1.94	4 (18%)
41	OMG	B8	75	41	18,26,27	0.91	1 (5%)	19,38,41	1.07	2 (10%)
1	OMC	A2	518	1	19,22,23	0.80	0	26,31,34	0.80	0
1	MA6	A2	1851	1	18,26,27	0.92	1 (5%)	19,38,41	1.38	3 (15%)
39	PSU	B5	3447	39	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
39	OMC	B5	1284	39	19,22,23	0.80	0	26,31,34	0.74	0
33	AME	Au	1	33	9,10,11	0.47	0	9,11,13	0.87	1 (11%)
39	1MA	B5	1266	39,89	16,25,26	1.49	2 (12%)	18,37,40	1.06	3 (16%)
1	OMG	A2	868	1	18,26,27	0.93	1 (5%)	19,38,41	1.11	2 (10%)
1	PSU	A2	105	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4740	39	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	OMG	B5	3524	39	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
12	SAC	AZ	2	12	7,8,9	0.53	0	8,9,11	0.87	1 (12%)
1	A2M	A2	99	89,1	18,25,26	1.04	1 (5%)	18,36,39	1.23	2 (11%)
39	OMG	B5	1580	39	18,26,27	0.95	1 (5%)	19,38,41	1.04	2 (10%)
39	OMU	B5	4052	39	19,22,23	1.23	3 (15%)	26,31,34	1.68	4 (15%)
1	A2M	A2	166	1	18,25,26	1.06	2 (11%)	18,36,39	1.26	2 (11%)
39	OMG	B5	3631	39	18,26,27	0.90	1 (5%)	19,38,41	1.17	2 (10%)
11	5MU	AT	54	11	19,22,23	1.38	5 (26%)	28,32,35	2.04	7 (25%)
1	MA6	A2	1852	1	18,26,27	0.95	1 (5%)	19,38,41	1.26	2 (10%)
39	PSU	B5	4042	39	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
39	A2M	B5	4317	39	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
39	PSU	B5	2351	39	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	OMU	A2	355	1	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	PSU	B5	4267	39,89	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
1	OMC	A2	174	89,1	19,22,23	0.81	0	26,31,34	0.80	0
39	A2M	B5	4269	39,89	18,25,26	1.02	1 (5%)	18,36,39	1.27	2 (11%)
1	7MG	A2	1640	11,1	22,26,27	1.33	3 (13%)	29,39,42	2.51	7 (24%)
41	PSU	B8	69	41	18,21,22	1.36	2 (11%)	22,30,33	1.92	5 (22%)
43	HIC	BB	245	43	8,11,12	0.87	0	6,14,16	0.81	0
39	PSU	B5	4203	39	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
39	PSU	B5	4298	39	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
39	5MC	B5	3514	39,89	18,22,23	0.94	2 (11%)	26,32,35	1.11	3 (11%)
1	A2M	A2	669	89,1	18,25,26	0.98	1 (5%)	18,36,39	1.40	2 (11%)
1	PSU	A2	1245	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	A2	1392	1	19,22,23	0.83	0	26,31,34	0.94	2 (7%)
39	PSU	B5	4322	39	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
39	OMG	B5	4369	39	18,26,27	0.92	1 (5%)	19,38,41	1.12	2 (10%)
35	HY3	Aw	62	35	6,8,9	1.94	1 (16%)	5,10,12	1.12	1 (20%)
1	A2M	A2	27	89,1	18,25,26	1.01	1 (5%)	18,36,39	1.21	2 (11%)
1	PSU	A2	1693	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
39	OMU	B5	2258	39	19,22,23	1.21	2 (10%)	26,31,34	1.68	4 (15%)
39	PSU	B5	3369	39	18,21,22	1.37	2 (11%)	22,30,33	1.92	4 (18%)
39	PSU	B5	3554	39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
39	A2M	B5	400	39	18,25,26	1.01	1 (5%)	18,36,39	1.22	2 (11%)
1	A2M	A2	1032	1	18,25,26	0.97	1 (5%)	18,36,39	1.29	3 (16%)
39	PSU	B5	1632	39	18,21,22	1.39	3 (16%)	22,30,33	1.92	4 (18%)
1	PSU	A2	802	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	1178	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	3466	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	OMU	B5	4366	39	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
1	OMG	A2	510	89,1	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
39	OMU	B5	3657	39	19,22,23	1.21	2 (10%)	26,31,34	1.74	5 (19%)
11	OMG	AT	34	11,9	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
39	PSU	B5	3462	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	407	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
40	GTP	B7	1	40	26,34,34	0.94	2 (7%)	32,54,54	0.82	0
1	OMU	A2	1289	1	19,22,23	1.23	3 (15%)	26,31,34	1.68	5 (19%)
1	OMG	A2	1329	1	18,26,27	0.95	1 (5%)	19,38,41	1.08	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A2	864	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	34	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
11	2MG	AT	10	11	18,26,27	0.87	1 (5%)	16,38,41	1.09	2 (12%)
39	PSU	B5	4169	39	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	36	1	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
39	A2M	B5	2244	39,89	18,25,26	1.01	1 (5%)	18,36,39	1.18	2 (11%)
1	PSU	A2	210	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
39	OMC	B5	3619	39	19,22,23	0.80	0	26,31,34	0.83	1 (3%)
39	A2M	B5	4336	39	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
39	PSU	B5	4435	39	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
44	AYA	BC	2	44	6,7,8	0.71	0	5,8,10	0.29	0
39	A2M	B5	398	39	18,25,26	1.04	1 (5%)	18,36,39	1.22	2 (11%)
11	M2G	AT	26	11	20,27,28	1.41	3 (15%)	22,40,43	0.98	2 (9%)
39	PSU	B5	4149	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
39	PSU	B5	4246	39	18,21,22	1.33	2 (11%)	22,30,33	1.92	3 (13%)
39	OMG	B5	4383	39	18,26,27	0.93	1 (5%)	19,38,41	1.12	2 (10%)
1	PSU	A2	1175	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4188	39	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	OMG	B5	3974	39	18,26,27	0.91	1 (5%)	19,38,41	1.13	2 (10%)
1	OMG	A2	645	1	18,26,27	0.92	1 (5%)	19,38,41	1.11	2 (10%)
11	PSU	AT	39	11	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
39	PSU	B5	3427	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	1239	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	A2	650	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4177	39	18,21,22	1.36	2 (11%)	22,30,33	1.89	4 (18%)
1	PSU	A2	1644	89,1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
39	OMC	B5	3601	39	19,22,23	0.78	0	26,31,34	0.77	0
39	PSU	B5	4039	39	18,21,22	1.36	2 (11%)	22,30,33	1.95	3 (13%)
39	PSU	B5	1799	39	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	OMC	B5	2704	39	19,22,23	0.81	0	26,31,34	0.80	0
39	OMG	B5	3359	39	18,26,27	0.93	1 (5%)	19,38,41	1.14	2 (10%)
1	4AC	A2	1338	1	21,24,25	1.09	2 (9%)	29,34,37	1.12	2 (6%)
39	OMC	B5	3433	39	19,22,23	0.77	0	26,31,34	0.79	0
1	B8N	A2	1249	1	24,29,30	1.27	3 (12%)	29,42,45	1.26	3 (10%)
39	OMG	B5	3676	39	18,26,27	0.95	1 (5%)	19,38,41	1.12	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	OMU	B5	4244	39	19,22,23	1.20	2 (10%)	26,31,34	1.66	5 (19%)
1	A2M	A2	1679	1	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
39	UY1	B5	3550	39	19,22,23	1.33	3 (15%)	22,31,34	2.04	5 (22%)
39	PSU	B5	4166	39	18,21,22	1.38	2 (11%)	22,30,33	1.84	4 (18%)
39	OMG	B5	2207	39	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
11	H2U	AT	17	11	18,21,22	1.00	2 (11%)	21,30,33	1.67	2 (9%)
1	PSU	A2	867	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	4217	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4325	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
11	OMC	AT	32	11	19,22,23	0.79	0	26,31,34	0.77	0
39	OMC	B5	2647	39	19,22,23	0.79	0	26,31,34	0.78	0
39	OMC	B5	4202	39	19,22,23	0.78	0	26,31,34	0.75	0
1	OMU	A2	172	1	19,22,23	1.20	2 (10%)	26,31,34	1.71	5 (19%)
83	SAC	Br	2	83	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
39	PSU	B5	1731	39	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
11	YYG	AT	37	11	31,42,43	1.69	4 (12%)	33,62,65	2.12	10 (30%)
1	OMU	A2	1805	1	19,22,23	1.21	3 (15%)	26,31,34	1.70	4 (15%)
1	PSU	A2	815	1	18,21,22	1.33	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	A2	1005	1	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	A2	513	1	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
39	PSU	B5	1720	39	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
39	A2M	B5	1489	39,89	18,25,26	1.01	1 (5%)	18,36,39	1.40	2 (11%)
1	PSU	A2	816	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	4 (18%)
39	OMC	B5	2194	39,89	19,22,23	0.81	0	26,31,34	0.96	1 (3%)
80	M3L	Bm	98	80	10,11,12	0.81	0	9,14,16	0.41	0
39	PSU	B5	1537	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	OMU	A2	429	1	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
39	PSU	B5	3583	39	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	OMC	B5	2265	39,89	19,22,23	0.81	0	26,31,34	0.82	0
81	MLZ	Bo	53	81	8,9,10	0.48	0	4,9,11	0.16	0
1	PSU	A2	610	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	OMU	B5	2680	39	19,22,23	1.23	2 (10%)	26,31,34	1.79	5 (19%)
1	PSU	A2	687	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	3371	39	18,21,22	1.37	2 (11%)	22,30,33	1.87	4 (18%)
39	A2M	B5	1479	39	18,25,26	1.00	1 (5%)	18,36,39	1.24	2 (11%)
1	OMG	A2	1448	1	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	A2M	B5	2206	39,89	18,25,26	1.04	1 (5%)	18,36,39	1.19	2 (11%)
1	A2M	A2	469	1	18,25,26	1.04	1 (5%)	18,36,39	1.27	2 (11%)
31	NMM	As	67	31	9,11,12	0.59	0	6,12,14	0.46	0
1	OMU	A2	1327	89,1	19,22,23	1.21	2 (10%)	26,31,34	1.70	5 (19%)
69	MLZ	Bb	5	69	8,9,10	0.48	0	4,9,11	0.16	0
1	A2M	A2	577	1	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
1	OMG	A2	602	1	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
39	OMG	B5	4240	39	18,26,27	0.91	1 (5%)	19,38,41	1.08	2 (10%)
39	PSU	B5	4749	39	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
39	6MZ	B5	3966	39	18,25,26	0.88	1 (5%)	16,36,39	2.07	4 (25%)
1	PSU	A2	1046	1	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	A2	591	1	18,25,26	1.04	1 (5%)	18,36,39	1.19	2 (11%)
39	OMG	B5	4364	39	18,26,27	0.92	1 (5%)	19,38,41	1.11	2 (10%)
11	PSU	AT	28	11	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	1721	39	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
39	PSU	B5	1801	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
39	OMG	B5	2267	39	18,26,27	0.95	1 (5%)	19,38,41	1.03	2 (10%)
39	A2M	B5	3456	39	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
39	OMG	B5	4138	39	18,26,27	0.90	1 (5%)	19,38,41	1.05	2 (10%)
1	OMG	A2	1491	89,1	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
39	PSU	B5	4374	39	18,21,22	1.36	2 (11%)	22,30,33	1.97	3 (13%)
39	OMC	B5	3540	39	19,22,23	0.80	0	26,31,34	0.79	0
39	PSU	B5	4711	39	18,21,22	1.36	2 (11%)	22,30,33	1.89	4 (18%)
39	A2M	B5	2630	39,89	18,25,26	1.00	1 (5%)	18,36,39	1.25	2 (11%)
1	PSU	A2	652	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	OMC	B5	2667	39	19,22,23	0.81	0	26,31,34	0.81	0
1	4AC	A2	1843	1	21,24,25	0.99	1 (4%)	29,34,37	1.08	3 (10%)
1	OMC	A2	463	1	19,22,23	0.81	0	26,31,34	0.80	0
1	PSU	A2	1082	1	18,21,22	1.38	2 (11%)	22,30,33	1.90	4 (18%)
39	OMG	B5	2719	39	18,26,27	0.95	1 (5%)	19,38,41	1.02	2 (10%)
68	V5N	Ba	39	68	4,11,12	0.76	0	5,14,16	1.69	1 (20%)
11	5MC	AT	49	11	18,22,23	0.95	2 (11%)	26,32,35	1.15	3 (11%)
1	OMG	A2	437	1	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	A2	573	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
39	OMC	B5	1820	39,89	19,22,23	0.78	0	26,31,34	0.86	0
39	OMG	B5	4245	39	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	UR3	B5	4276	39	19,22,23	1.00	1 (5%)	26,32,35	1.45	1 (3%)
39	PSU	B5	4278	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	OMC	B5	2208	39,89	19,22,23	0.79	0	26,31,34	0.78	0
39	A2M	B5	3557	39	18,25,26	0.99	1 (5%)	18,36,39	1.24	2 (11%)
1	OMU	A2	628	1	19,22,23	1.16	2 (10%)	26,31,34	1.71	5 (19%)
30	SAC	Ar	2	30	7,8,9	0.53	0	8,9,11	0.88	1 (12%)
1	PSU	A2	109	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	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
1	OMG	A2	684	1	-	0/5/27/28	0/3/3/3
39	A2M	B5	3450	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	3496	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	159	1	-	2/5/27/28	0/3/3/3
39	PSU	B5	1638	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1718	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
39	5MC	B5	4193	39	-	4/7/25/26	0/2/2/2
11	H2U	AT	16	11	-	1/7/38/39	0/2/2/2
39	PSU	B5	2475	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	4116	39	-	0/5/27/28	0/3/3/3
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	1810	39,89	-	0/5/27/28	0/3/3/3
1	OMU	A2	121	1	-	0/9/27/28	0/2/2/2
39	OMG	B5	3942	39,11	-	0/5/27/28	0/3/3/3
1	6MZ	A2	1833	89,1	-	2/5/27/28	0/3/3/3
39	PSU	B5	3490	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4045	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4419	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1683	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	3973	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	1477	39	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3576	39	-	1/7/25/26	0/2/2/2
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	1443	89,1	-	1/9/27/28	0/2/2/2
39	OMC	B5	4282	39,89	-	0/9/27/28	0/2/2/2
11	PSU	AT	55	11	-	0/7/25/26	0/2/2/2
39	PSU	B5	3494	39	-	2/7/25/26	0/2/2/2
39	PSU	B5	4382	39	-	3/7/25/26	0/2/2/2
39	PSU	B5	3502	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	3573	39	-	0/9/27/28	0/2/2/2
39	A2M	B5	3599	39	-	2/5/27/28	0/3/3/3
11	PSU	AT	27	11	-	0/7/25/26	0/2/2/2
11	1MA	AT	14	11	-	0/3/25/26	0/3/3/3
1	OMC	A2	1704	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	823	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	1384	1	-	0/5/27/28	0/3/3/3
39	A2M	B5	3492	39,1	-	0/5/27/28	0/3/3/3
39	PSU	B5	3616	39	-	0/7/25/26	0/2/2/2
41	PSU	B8	55	41	-	0/7/25/26	0/2/2/2
39	PSU	B5	4099	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3476	39	-	0/5/27/28	0/3/3/3
39	A2M	B5	1270	39	-	1/5/27/28	0/3/3/3
42	V5N	BA	216	42	-	1/5/10/12	0/1/1/1
39	A2M	B5	3562	39	-	0/5/27/28	0/3/3/3
1	A2M	A2	485	1	-	0/5/27/28	0/3/3/3
39	PSU	B5	1491	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3652	39,89	-	0/7/25/26	0/2/2/2
39	PSU	B5	4058	39	-	0/7/25/26	0/2/2/2
11	7MG	AT	46	11	-	1/7/37/38	0/3/3/3
39	A2M	B5	2658	39,89	-	1/5/27/28	0/3/3/3
39	PSU	B5	3585	39,89	-	0/7/25/26	0/2/2/2
11	1MA	AT	58	11	-	0/3/25/26	0/3/3/3
39	OMG	B5	1260	39	-	0/5/27/28	0/3/3/3
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3500	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4107	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3517	39	-	2/5/27/28	0/3/3/3
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
41	OMG	B8	75	41	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	A2	518	1	-	1/9/27/28	0/2/2/2
1	MA6	A2	1851	1	-	0/7/29/30	0/3/3/3
39	PSU	B5	3447	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	1284	39	-	0/9/27/28	0/2/2/2
33	AME	Au	1	33	-	2/9/10/12	-
39	1MA	B5	1266	39,89	-	0/3/25/26	0/3/3/3
1	OMG	A2	868	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4740	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3524	39	-	1/5/27/28	0/3/3/3
12	SAC	AZ	2	12	-	2/7/8/10	-
1	A2M	A2	99	89,1	-	2/5/27/28	0/3/3/3
39	OMG	B5	1580	39	-	0/5/27/28	0/3/3/3
39	OMU	B5	4052	39	-	0/9/27/28	0/2/2/2
1	A2M	A2	166	1	-	0/5/27/28	0/3/3/3
39	OMG	B5	3631	39	-	0/5/27/28	0/3/3/3
11	5MU	AT	54	11	-	0/7/25/26	0/2/2/2
1	MA6	A2	1852	1	-	1/7/29/30	0/3/3/3
39	PSU	B5	4042	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4317	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	2351	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	355	1	-	0/9/27/28	0/2/2/2
39	PSU	B5	4267	39,89	-	1/7/25/26	0/2/2/2
1	OMC	A2	174	89,1	-	0/9/27/28	0/2/2/2
39	A2M	B5	4269	39,89	-	0/5/27/28	0/3/3/3
1	7MG	A2	1640	11,1	-	0/7/37/38	0/3/3/3
41	PSU	B8	69	41	-	0/7/25/26	0/2/2/2
43	HIC	BB	245	43	-	1/5/6/8	0/1/1/1
39	PSU	B5	4203	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4298	39	-	0/7/25/26	0/2/2/2
39	5MC	B5	3514	39,89	-	0/7/25/26	0/2/2/2
1	A2M	A2	669	89,1	-	2/5/27/28	0/3/3/3
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
1	OMC	A2	1392	1	-	2/9/27/28	0/2/2/2
39	PSU	B5	4322	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	4369	39	-	0/5/27/28	0/3/3/3
35	HY3	Aw	62	35	-	1/1/12/14	0/1/1/1
1	A2M	A2	27	89,1	-	0/5/27/28	0/3/3/3
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	2258	39	-	1/9/27/28	0/2/2/2
39	PSU	B5	3369	39	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	B5	3554	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	400	39	-	0/5/27/28	0/3/3/3
1	A2M	A2	1032	1	-	0/5/27/28	0/3/3/3
39	PSU	B5	1632	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	802	1	-	2/7/25/26	0/2/2/2
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3466	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	4366	39	-	0/9/27/28	0/2/2/2
1	OMG	A2	510	89,1	-	0/5/27/28	0/3/3/3
39	OMU	B5	3657	39	-	0/9/27/28	0/2/2/2
11	OMG	AT	34	11,9	-	1/5/27/28	0/3/3/3
39	PSU	B5	3462	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
40	GTP	B7	1	40	-	0/18/38/38	0/3/3/3
1	OMU	A2	1289	1	-	1/9/27/28	0/2/2/2
1	OMG	A2	1329	1	-	1/5/27/28	0/3/3/3
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
11	2MG	AT	10	11	-	0/5/27/28	0/3/3/3
39	PSU	B5	4169	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	2244	39,89	-	0/5/27/28	0/3/3/3
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	3619	39	-	1/9/27/28	0/2/2/2
39	A2M	B5	4336	39	-	1/5/27/28	0/3/3/3
39	PSU	B5	4435	39	-	0/7/25/26	0/2/2/2
44	AYA	BC	2	44	-	2/4/6/8	-
39	A2M	B5	398	39	-	2/5/27/28	0/3/3/3
11	M2G	AT	26	11	-	0/7/29/30	0/3/3/3
39	PSU	B5	4149	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4246	39	-	1/7/25/26	0/2/2/2
39	OMG	B5	4383	39	-	0/5/27/28	0/3/3/3
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4188	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3974	39	-	0/5/27/28	0/3/3/3
1	OMG	A2	645	1	-	4/5/27/28	0/3/3/3
11	PSU	AT	39	11	-	0/7/25/26	0/2/2/2
39	PSU	B5	3427	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4177	39	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A2	1644	89,1	-	0/7/25/26	0/2/2/2
39	OMC	B5	3601	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	4039	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1799	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	2704	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	3359	39	-	0/5/27/28	0/3/3/3
1	4AC	A2	1338	1	-	4/11/29/30	0/2/2/2
39	OMC	B5	3433	39	-	4/9/27/28	0/2/2/2
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
39	OMG	B5	3676	39	-	0/5/27/28	0/3/3/3
39	OMU	B5	4244	39	-	0/9/27/28	0/2/2/2
1	A2M	A2	1679	1	-	0/5/27/28	0/3/3/3
39	UY1	B5	3550	39	-	3/9/27/28	0/2/2/2
39	PSU	B5	4166	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	2207	39	-	2/5/27/28	0/3/3/3
11	H2U	AT	17	11	-	6/7/38/39	0/2/2/2
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4217	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4325	39	-	0/7/25/26	0/2/2/2
11	OMC	AT	32	11	-	0/9/27/28	0/2/2/2
39	OMC	B5	2647	39	-	0/9/27/28	0/2/2/2
39	OMC	B5	4202	39	-	2/9/27/28	0/2/2/2
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
83	SAC	Br	2	83	-	0/7/8/10	-
39	PSU	B5	1731	39	-	0/7/25/26	0/2/2/2
11	YYG	AT	37	11	-	1/20/42/43	0/3/4/4
1	OMU	A2	1805	1	-	0/9/27/28	0/2/2/2
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	513	1	-	3/5/27/28	0/3/3/3
39	PSU	B5	1720	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	1489	39,89	-	1/5/27/28	0/3/3/3
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	2194	39,89	-	2/9/27/28	0/2/2/2
80	M3L	Bm	98	80	-	0/9/10/12	-
39	PSU	B5	1537	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	429	1	-	4/9/27/28	0/2/2/2
39	PSU	B5	3583	39	-	2/7/25/26	0/2/2/2
39	OMC	B5	2265	39,89	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	MLZ	B ₀	53	81	-	0/7/8/10	-
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	2680	39	-	2/9/27/28	0/2/2/2
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3371	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	1479	39	-	0/5/27/28	0/3/3/3
1	OMG	A2	1448	1	-	3/5/27/28	0/3/3/3
39	A2M	B5	2206	39,89	-	0/5/27/28	0/3/3/3
1	A2M	A2	469	1	-	1/5/27/28	0/3/3/3
31	NMM	A _s	67	31	-	0/9/11/13	-
1	OMU	A2	1327	89,1	-	0/9/27/28	0/2/2/2
69	MLZ	B _b	5	69	-	1/7/8/10	-
1	A2M	A2	577	1	-	2/5/27/28	0/3/3/3
1	OMG	A2	602	1	-	1/5/27/28	0/3/3/3
39	OMG	B5	4240	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4749	39	-	0/7/25/26	0/2/2/2
39	6MZ	B5	3966	39	-	0/5/27/28	0/3/3/3
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	591	1	-	0/5/27/28	0/3/3/3
39	OMG	B5	4364	39	-	0/5/27/28	0/3/3/3
11	PSU	A _T	28	11	-	0/7/25/26	0/2/2/2
39	PSU	B5	1721	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1801	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	2267	39	-	0/5/27/28	0/3/3/3
39	A2M	B5	3456	39	-	0/5/27/28	0/3/3/3
39	OMG	B5	4138	39	-	0/5/27/28	0/3/3/3
1	OMG	A2	1491	89,1	-	1/5/27/28	0/3/3/3
39	PSU	B5	4374	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	3540	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	4711	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	2630	39,89	-	0/5/27/28	0/3/3/3
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	2667	39	-	0/9/27/28	0/2/2/2
1	4AC	A2	1843	1	-	2/11/29/30	0/2/2/2
1	OMC	A2	463	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	1082	1	-	1/7/25/26	0/2/2/2
39	OMG	B5	2719	39	-	0/5/27/28	0/3/3/3
68	V5N	B _a	39	68	-	0/5/10/12	0/1/1/1
11	5MC	A _T	49	11	-	0/7/25/26	0/2/2/2
1	OMG	A2	437	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	OMC	B5	1820	39,89	-	0/9/27/28	0/2/2/2
39	OMG	B5	4245	39	-	1/5/27/28	0/3/3/3
39	UR3	B5	4276	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4278	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	2208	39,89	-	0/9/27/28	0/2/2/2
39	A2M	B5	3557	39	-	0/5/27/28	0/3/3/3
1	OMU	A2	628	1	-	4/9/27/28	0/2/2/2
30	SAC	Ar	2	30	-	0/7/8/10	-
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2

The worst 5 of 359 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AT	37	YYG	O23-C21	6.59	1.45	1.34
11	AT	37	YYG	O18-C16	5.20	1.45	1.33
11	AT	58	1MA	C2-N3	4.96	1.35	1.29
11	AT	14	1MA	C2-N3	4.82	1.34	1.29
39	B5	1266	1MA	C2-N3	4.51	1.34	1.29

The worst 5 of 630 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1640	7MG	N9-C4-N3	8.94	138.85	125.47
11	AT	46	7MG	N9-C4-N3	8.82	138.66	125.47
1	A2	1833	6MZ	C2-N1-C6	7.00	122.59	116.59
11	AT	17	H2U	C4-N3-C2	-6.83	120.13	125.79
39	B5	4374	PSU	N1-C2-N3	6.34	122.31	115.13

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	645	OMG	O4'-C4'-C5'-O5'
1	A2	645	OMG	C3'-C4'-C5'-O5'
1	A2	1833	6MZ	C5-C6-N6-C9
1	A2	1833	6MZ	N1-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 791 ligands modelled in this entry, 428 are monoatomic and 330 are unknown - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
87	SPD	B5	4906	-	9,9,9	0.15	0	8,8,8	0.25	0
87	SPD	A2	1906	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4914	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4904	-	9,9,9	0.16	0	8,8,8	0.20	0
87	SPD	B5	4921	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	A2	1902	-	9,9,9	0.15	0	8,8,8	0.16	0
87	SPD	B5	4918	-	9,9,9	0.16	0	8,8,8	0.17	0
88	SPM	A2	1909	-	13,13,13	0.14	0	12,12,12	0.19	0
87	SPD	B5	4916	-	9,9,9	0.15	0	8,8,8	0.20	0
87	SPD	A2	1903	-	9,9,9	0.16	0	8,8,8	0.16	0
87	SPD	B5	4902	-	9,9,9	0.15	0	8,8,8	0.15	0
87	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	B5	4903	-	9,9,9	0.15	0	8,8,8	0.28	0
87	SPD	B5	4907	-	9,9,9	0.15	0	8,8,8	0.23	0
87	SPD	B5	4913	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	A2	1904	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4923	-	9,9,9	0.15	0	8,8,8	0.21	0
87	SPD	B5	4905	-	9,9,9	0.14	0	8,8,8	0.17	0
87	SPD	B5	4922	-	9,9,9	0.16	0	8,8,8	0.19	0
87	SPD	A2	1908	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4911	-	9,9,9	0.15	0	8,8,8	0.16	0
87	SPD	B5	4920	-	9,9,9	0.15	0	8,8,8	0.28	0
88	SPM	B5	4915	-	13,13,13	0.16	0	12,12,12	0.29	0
87	SPD	B5	4910	-	9,9,9	0.15	0	8,8,8	0.16	0
87	SPD	A2	1905	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4917	-	9,9,9	0.15	0	8,8,8	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	SPD	B5	4909	-	9,9,9	0.17	0	8,8,8	0.19	0
87	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.19	0
87	SPD	BN	301	-	9,9,9	0.15	0	8,8,8	0.14	0
87	SPD	B5	4919	-	9,9,9	0.15	0	8,8,8	0.19	0
88	SPM	B5	4912	-	13,13,13	0.15	0	12,12,12	0.23	0
87	SPD	B5	4908	-	9,9,9	0.14	0	8,8,8	0.21	0
87	SPD	B5	4924	-	9,9,9	0.16	0	8,8,8	0.14	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
87	SPD	B5	4906	-	-	0/7/7/7	-
87	SPD	A2	1906	-	-	1/7/7/7	-
87	SPD	B5	4914	-	-	0/7/7/7	-
87	SPD	B5	4904	-	-	1/7/7/7	-
87	SPD	B5	4921	-	-	1/7/7/7	-
87	SPD	A2	1902	-	-	0/7/7/7	-
87	SPD	B5	4918	-	-	0/7/7/7	-
88	SPM	A2	1909	-	-	1/11/11/11	-
87	SPD	B5	4916	-	-	0/7/7/7	-
87	SPD	A2	1903	-	-	0/7/7/7	-
87	SPD	B5	4902	-	-	1/7/7/7	-
87	SPD	A2	1907	-	-	1/7/7/7	-
87	SPD	B5	4903	-	-	2/7/7/7	-
87	SPD	B5	4907	-	-	0/7/7/7	-
87	SPD	B5	4913	-	-	0/7/7/7	-
87	SPD	A2	1904	-	-	0/7/7/7	-
87	SPD	B5	4923	-	-	0/7/7/7	-
87	SPD	B5	4905	-	-	0/7/7/7	-
87	SPD	B5	4922	-	-	1/7/7/7	-
87	SPD	A2	1908	-	-	0/7/7/7	-
87	SPD	B5	4911	-	-	0/7/7/7	-
87	SPD	B5	4920	-	-	0/7/7/7	-
88	SPM	B5	4915	-	-	0/11/11/11	-
87	SPD	B5	4910	-	-	1/7/7/7	-
87	SPD	A2	1905	-	-	0/7/7/7	-
87	SPD	B5	4917	-	-	0/7/7/7	-
87	SPD	B5	4909	-	-	1/7/7/7	-
87	SPD	A2	1901	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	BN	301	-	-	1/7/7/7	-
87	SPD	B5	4919	-	-	0/7/7/7	-
88	SPM	B5	4912	-	-	0/11/11/11	-
87	SPD	B5	4908	-	-	0/7/7/7	-
87	SPD	B5	4924	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	A2	1909	SPM	C12-C11-N10-C9
87	B5	4903	SPD	C2-C3-C4-C5
87	B5	4903	SPD	C3-C4-C5-N6
87	B5	4902	SPD	C4-C5-N6-C7
87	B5	4924	SPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12756. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.