



Full wwPDB EM Validation Report ⓘ

Jul 12, 2023 – 04:56 PM JST

PDB ID : 8I9Z
EMDB ID : EMD-35289
Title : Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit
- State Spb4
Authors : Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2023-02-07
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

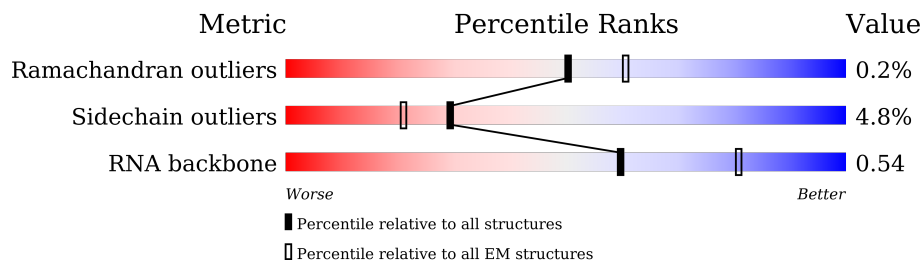
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C1	3341	
2	C2	319	
3	CA	316	
4	CB	391	
5	CC	801	
6	CD	495	
7	CE	598	
8	CF	270	

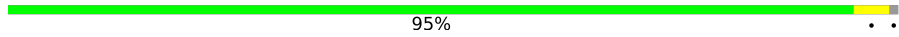


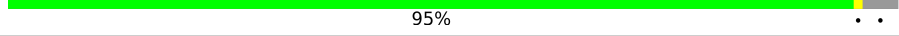

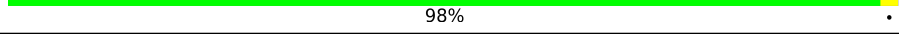


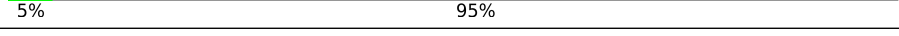
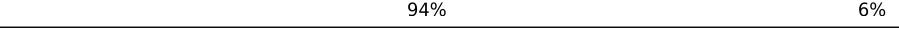
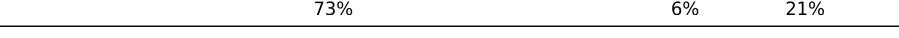
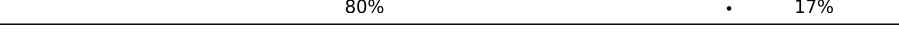
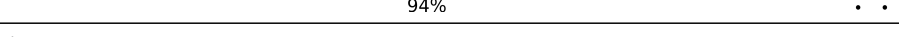
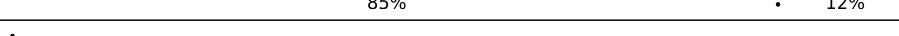
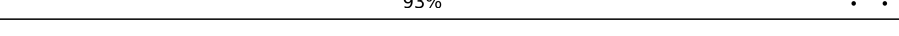
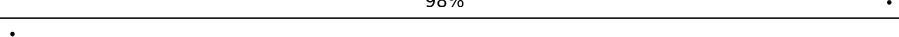
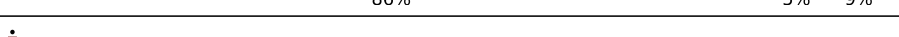

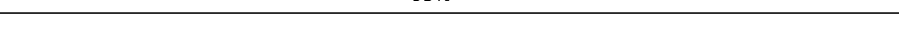






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Mol	Chain	Length	Quality of chain
9	CG	184	93%
10	CH	661	79% 18%
11	CI	414	34% 65%
12	CJ	679	69% 27%
13	CK	261	85% 12%
14	CL	558	50% 68% 30%
15	CM	249	84% 6% 10%
15	LF	249	96%
16	CN	246	98%
17	CO	120	50% 48%
18	CP	751	41% 57%
19	CQ	225	72% 8% 20%
20	CR	237	67% 30%
21	CS	834	72% 25%
22	CT	688	67% 29%
23	CU	451	38% 61%
24	CV	147	93% 5%
25	CW	679	70% 9% 21%
26	CX	203	41% 57%
27	CY	788	43% 5% 52%
28	Cz	123	55% 43%
29	LB	392	88% 9%
30	LC	365	96%
31	LE	200	90% 5% 6%
32	LG	262	74% 22%



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Mol	Chain	Length	Quality of chain
33	LH	192	 95%
34	LK	165	 82% 7% 12%
35	LL	213	 54% 45%
36	LM	142	 95%
37	LN	203	 87% 10%
38	LO	204	 98%
39	LP	187	 86% 10%
40	LQ	213	 60% 39%
41	LR	2898	 5% 95%
42	LS	174	 94% 6%
43	LT	160	 73% 6% 21%
44	LU	127	 80% 17%
45	LV	139	 94%
46	LX	156	 85% 12%
47	LY	138	 93%
48	LZ	135	 98%
49	Lc	108	 86% 5% 9%
50	Ld	120	 89% 9%
51	Le	131	 95%
52	Lf	109	 94% 5%
53	Lg	119	 97%
54	Lh	935	 13% 87%
55	Li	110	 78% 20%
56	Lj	95	 74% 22%
57	Lk	81	 89% 7%

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Mol	Chain	Length	Quality of chain
58	Ll	51	 71% 25%
59	Lq	217	 91% 5%

2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 167255 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 RNA (3341-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C1	2787	59633	26611	10807	19428	2787	0	0

- Molecule 2 is a RNA chain called RNA (319-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	256	5456	2435	974	1791	256	0	0

- Molecule 3 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CA	251	2069	1324	381	357	7	0	0

- Molecule 4 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CB	260	2063	1322	367	371	3	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CC	658	5289	3368	931	977	13	0	0

- Molecule 6 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CD	460	3468	2173	610	679	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CD	88	ASP	GLU	conflict	UNP G0SFB5

- Molecule 7 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	CE	465	3689	2362	646	670	11	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	543	LYS	-	insertion	UNP G0RYU9
CE	544	SER	-	insertion	UNP G0RYU9
CE	545	PHE	-	insertion	UNP G0RYU9
CE	546	GLY	-	insertion	UNP G0RYU9
CE	547	PHE	-	insertion	UNP G0RYU9
CE	548	SER	-	insertion	UNP G0RYU9
CE	549	THR	-	insertion	UNP G0RYU9
CE	550	PRO	-	insertion	UNP G0RYU9
CE	551	PRO	-	insertion	UNP G0RYU9
CE	552	ARG	-	insertion	UNP G0RYU9
CE	553	VAL	-	insertion	UNP G0RYU9
CE	554	ASP	-	insertion	UNP G0RYU9
CE	555	ILE	-	insertion	UNP G0RYU9
CE	556	THR	-	insertion	UNP G0RYU9
CE	557	LEU	-	insertion	UNP G0RYU9
CE	558	SER	-	insertion	UNP G0RYU9
CE	559	ALA	-	insertion	UNP G0RYU9
CE	560	SER	-	insertion	UNP G0RYU9
CE	561	LEU	-	insertion	UNP G0RYU9
CE	562	SER	-	insertion	UNP G0RYU9
CE	563	ARG	-	insertion	UNP G0RYU9
CE	564	ASP	-	insertion	UNP G0RYU9
CE	565	LYS	-	insertion	UNP G0RYU9
CE	566	LYS	-	insertion	UNP G0RYU9
CE	567	PRO	-	insertion	UNP G0RYU9
CE	568	GLN	-	insertion	UNP G0RYU9
CE	569	GLY	-	insertion	UNP G0RYU9
CE	570	ARG	-	insertion	UNP G0RYU9
CE	571	ARG	-	insertion	UNP G0RYU9
CE	572	ALA	-	insertion	UNP G0RYU9

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Chain	Residue	Modelled	Actual	Comment	Reference
CE	573	TYR	-	insertion	UNP G0RYU9
CE	574	GLY	-	insertion	UNP G0RYU9
CE	575	SER	-	insertion	UNP G0RYU9
CE	576	GLN	-	insertion	UNP G0RYU9
CE	577	PRO	-	insertion	UNP G0RYU9
CE	578	ARG	-	insertion	UNP G0RYU9
CE	579	GLN	-	insertion	UNP G0RYU9
CE	580	GLY	-	insertion	UNP G0RYU9
CE	581	GLY	-	insertion	UNP G0RYU9
CE	582	ARG	-	insertion	UNP G0RYU9
CE	583	TYR	-	insertion	UNP G0RYU9
CE	584	LYS	-	insertion	UNP G0RYU9

- Molecule 8 is a protein called Ribosome assembly factor mrt4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	CF	245	1945	1222	352	362	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CF	13	ILE	THR	conflict	UNP G0S616
CF	139	THR	PRO	conflict	UNP G0S616
CF	228	ASN	SER	conflict	UNP G0S616
CF	259	ILE	MET	conflict	UNP G0S616

- Molecule 9 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	CG	177	1396	884	247	253	12	0	0

- Molecule 10 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	CH	542	4388	2784	770	818	16	0	0

- Molecule 11 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CI	146	Total	C	N	O	S	0	0
			1196	763	224	204	5		

- Molecule 12 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CJ	494	Total	C	N	O	S	0	0
			4040	2575	719	734	12		

- Molecule 13 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CK	229	Total	C	N	O	S	0	0
			1835	1149	362	320	4		

- Molecule 14 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	CL	390	Total	C	N	O	0	0
			2173	1307	446	420		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CL	69	ARG	ILE	conflict	UNP G0SEW3

- Molecule 15 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CM	223	Total	C	N	O	S	0	0
			1820	1169	340	308	3		
15	LF	247	Total	C	N	O	S	0	0
			2017	1294	376	344	3		

- Molecule 16 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CN	246	Total	C	N	O	S	0	0
			1856	1158	322	369	7		

- Molecule 17 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CO	62	Total	C	N	O	S	0	0
			468	290	94	82	2		

- Molecule 18 is a protein called RNA methyltransferase nop2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CP	324	Total	C	N	O	S	0	0
			2535	1618	445	457	15		

- Molecule 19 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CQ	179	Total	C	N	O	S	0	0
			1485	926	304	245	10		

- Molecule 20 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CR	167	Total	C	N	O	S	0	0
			1354	827	278	247	2		

- Molecule 21 is a protein called AdoMet-dependent rRNA methyltransferase SPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CS	625	Total	C	N	O	S	0	0
			5036	3190	917	910	19		

- Molecule 22 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CT	488	Total	C	N	O	S	0	0
			3911	2486	690	719	16		

- Molecule 23 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CU	178	Total	C	N	O	S	0	0
			1415	876	265	271	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	CV	139	1073	672	213	188	0	0

- Molecule 25 is a protein called ATP-dependent RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	CW	537	4284	2733	760	777	14	0	0

- Molecule 26 is a protein called 60S ribosomal subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	CX	88	701	435	128	135	3	0	0

- Molecule 27 is a protein called Putative NOC2 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	CY	382	3035	1943	558	523	11	0	0

- Molecule 28 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Cz	70	592	368	120	101	3	0	0

- Molecule 29 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LB	356	2829	1798	518	501	12	0	0

- Molecule 30 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	LC	362	2752	1738	526	479	9	0	0

- Molecule 31 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LE	189	Total	C	N	O	S	0	0
			1475	944	267	261	3		

- Molecule 32 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LG	204	Total	C	N	O	S	0	0
			1644	1060	297	282	5		

- Molecule 33 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LH	190	Total	C	N	O	S	0	0
			1496	950	268	272	6		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	TYR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5

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Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LEU	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5

- Molecule 34 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LK	146	1112	701	203	206	2	0	0

- Molecule 35 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	LL	117	964	608	206	148	2	0	0

- Molecule 36 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	LM	137	1101	699	211	190	1	0	0

- Molecule 37 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	LN	183	1563	974	332	253	4	0	0

- Molecule 38 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	LO	204	1618	1039	306	267	6	0	0

- Molecule 39 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LP	169	1345	835	273	234	3	0	0

- Molecule 40 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	LQ	129	1021	646	200	173	2	0	0

- Molecule 41 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	LR	148	1219	756	253	205	5	0	0

- Molecule 42 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	LS	174	1433	922	267	239	5	0	0

- Molecule 43 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	LT	126	1014	643	196	173	2	0	0

- Molecule 44 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	LU	105	850	551	147	151	1	0	0

- Molecule 45 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	LV	135	995	633	185	170	7	0	0

- Molecule 46 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	LX	137	1062	678	194	190		0	0

- Molecule 47 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	LY	134	1065	664	215	184	2	0	0

- Molecule 48 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	LZ	135	1112	713	207	188	4	0	0

- Molecule 49 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Lc	98	731	463	126	137	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Ld	109	890	563	171	155	1	0	0

- Molecule 51 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Le	127	1025	645	209	164	7	0	0

- Molecule 52 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Lf	108	862	546	171	144	1	0	0

- Molecule 53 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Lg	117	930	578	189	159	4	0	0

- Molecule 54 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	Lh	121	995	633	196	166	0	0

- Molecule 55 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Li	88	731	449	162	119	1	0	0

- Molecule 56 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	Lj	74	595	365	132	93	5	0	0

- Molecule 57 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	Lk	75	620	394	117	107	2	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lk	?	-	SER	deletion	UNP G0SG89
Lk	?	-	LYS	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89

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Chain	Residue	Modelled	Actual	Comment	Reference
Lk	?	-	ALA	deletion	UNP G0SG89
Lk	?	-	PHE	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89

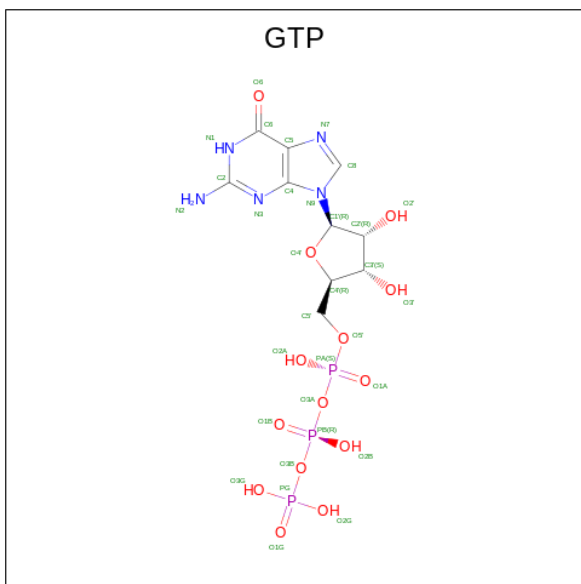
- Molecule 58 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	Ll	38	322	204	68	50	0	0

- Molecule 59 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	Lq	207	1600	1016	285	291	8	0	0

- Molecule 60 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

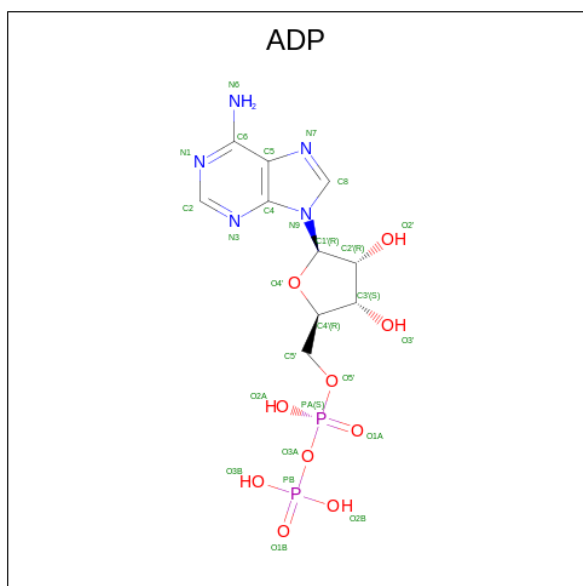


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	CH	1	32	10	5	14	3	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	CQ	1	Total	Zn	0
			1	1	
61	Lj	1	Total	Zn	0
			1	1	

- Molecule 62 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
62	CW	1	Total	C	N	O	P	0
			27	10	5	10	2	

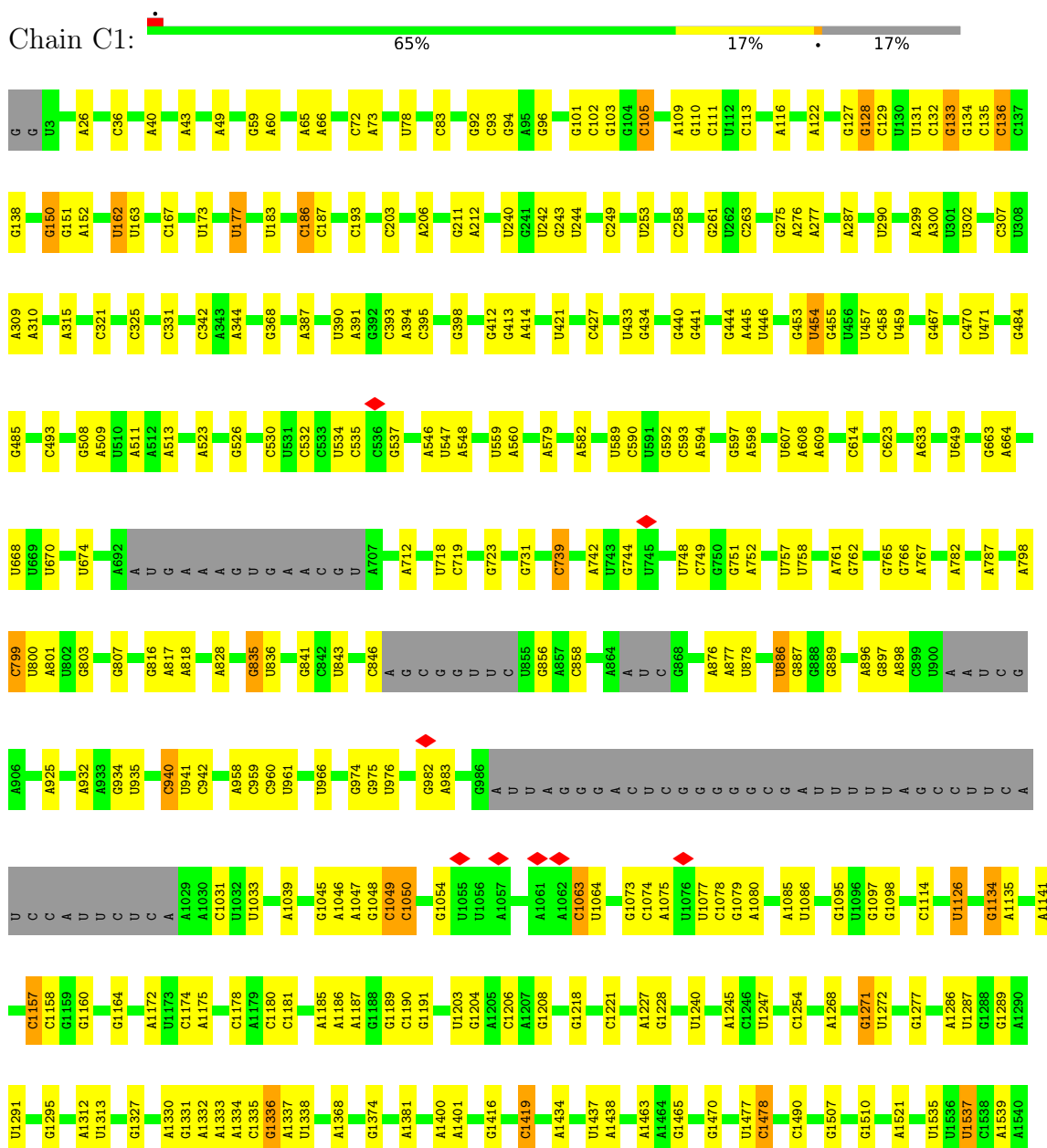
- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
63	CW	1	Total	Mg	0
			1	1	

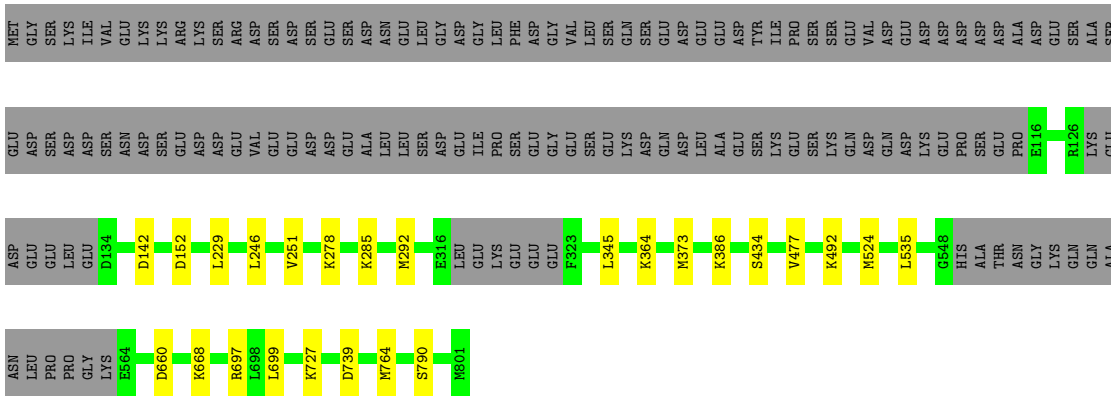
3 Residue-property plots

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

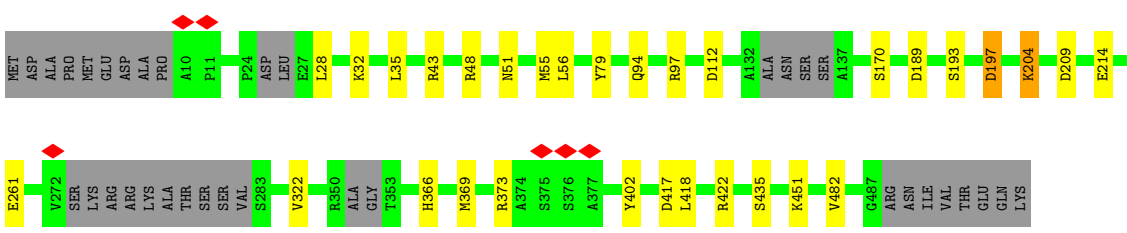
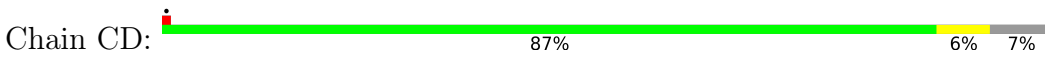
- Molecule 1: RNA (3341-MER)



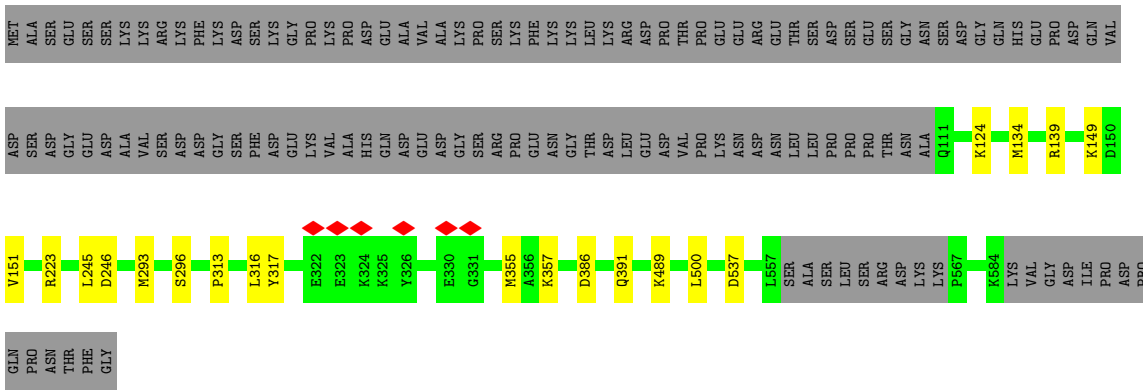
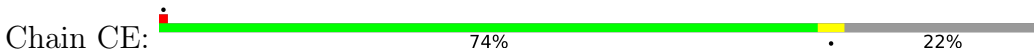
A1541	A1745	U1903	G1982	U2064	G2366	G2560	A2778	U2902
G1542	U1746	U1904	G1983	U2065	U	U	G	G2903
G1543	U1746	G1911	C1984	A2066	A	G	G2782	C2906
C1548	G1750	A1912	A1985	A2075	G	G	U2800	U2907
U1549	G1759	G1913	A1986	G2081	A	A	C2801	G2908
C1550	G1759	G	C1987	G	U	U	A2802	G
G1553	U1774	A	C1988	G	G	G	U2804	U
C1554	G1775	U	G1989	G	U	C	C2815	U
C1555	A1776	U	G1990	G	G	G	U2816	U
U1559	U1794	G1918	G1991	C	A	A	U	A
G1560	A1795	G1919	C1992	A	C	C	U	G2915
A1796	U1796	A1924	G1993	U	G	A	U	A2916
U1797	U1798	A1925	G1994	U	G	C	U	C2917
G1562	C1799	G1926	G1995	U	U	C	G	U2923
U1561	U1800	G1927	C1996	U	G	C	A	A2929
A1566	U1800	G1928	G1997	A	G	U	U	U2936
A1567	U1819	G1932	C1998	C	A	U	C	U
A1568	A1820	G1940	C1999	U	U	U	U	U
A1572	A1821	G1942	C2000	G	G	G	U	U
U1583	C1825	G1942	U2001	A	C	A	C	A
A1584	C1828	G1943	C2002	U	U	U	G	G2829
U1598	A1829	U1944	A2003	A	A	A	U	A2830
U1599	G1842	G1948	G2004	U	G	A	C	U2831
U1607	A1843	G1949	C2005	U	C	A	G	U2832
U1608	U1844	C1950	A2006	A	G	A	U	U2833
G1609	C1845	G1951	C2007	U	U	C	U	U2845
C1610	A1846	A1952	C2008	A	G	C	U	A2846
U1618	C1851	C1954	C2009	U	U	U	U	U2847
A1621	G1857	C1958	G2010	C	C	C	U	G2722
A1622	A1858	U1959	C2020	G	G	C	C	C2723
C1623	U1859	G1960	C2021	U	A	G	U	C2730
U1624	G1881	G1961	C2022	A	U	G	G	C2731
G1637	G1881	G1962	U2023	U	U	C	G	U2740
C1662	G1884	A1963	U2024	C	C	U	G	C2745
A1693	C1886	G1964	C2027	G	G	U	C	U2749
A1694	A	C1965	A	A	C	A	A	G2752
A1695	A	A1966	G	U	A	C	C	U
C1696	A	G1967	C	G	A	C	C	U
G1722	U	A1968	U	A	U	C	G	U
A1729	A	G1969	C	A	A	G	G	C
G1730	A	G1970	G	U	C	U	U	C
A1739	U1895	G1971	C	U	U	U	G	A2757
G1740	C1896	C1972	C	A	C	C	G	G2758
U1741	C1897	C1973	C	A	A	U	C	A2759
U1744	A1900	U1974	G	U	U	U	U	A2760
	A1901	C1975	C	C	C	U	U	A2761
	C1902	U1976	U	G	G	C	C	A2777
		A1977	C2041	G	G	U	U	
		G1978	C2042	A	U	U	U	
		C1979	G2043	U	U	U	U	
		C1980	G2044	C	C	U	U	
		G1981	G2048	U	U	U	U	
			C2049	G	G	C	C	
			A2054	U	U	U	U	



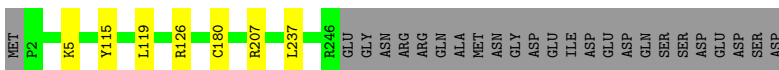
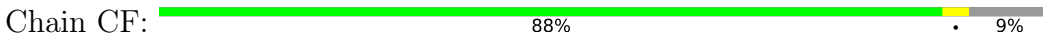
• Molecule 6: Ribosome biogenesis protein YTM1



• Molecule 7: RNA helicase



• Molecule 8: Ribosome assembly factor mrt4

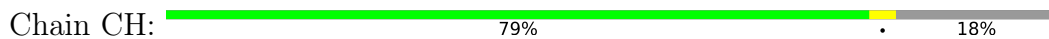


• Molecule 9: 60S ribosome subunit biogenesis protein NIP7

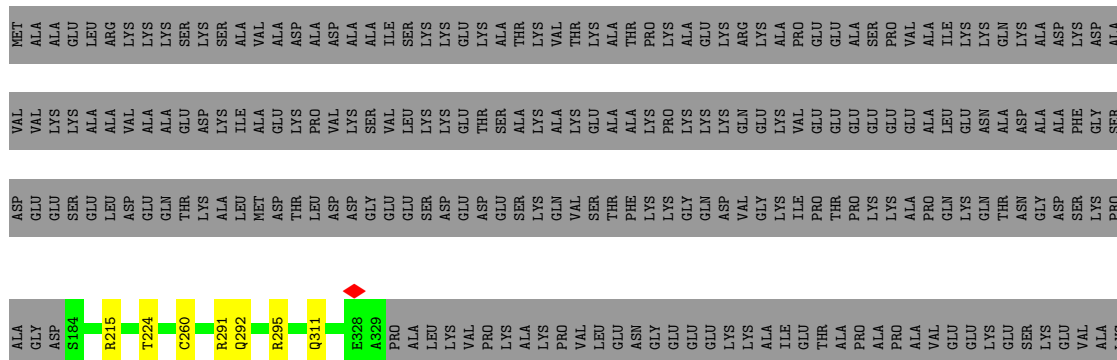




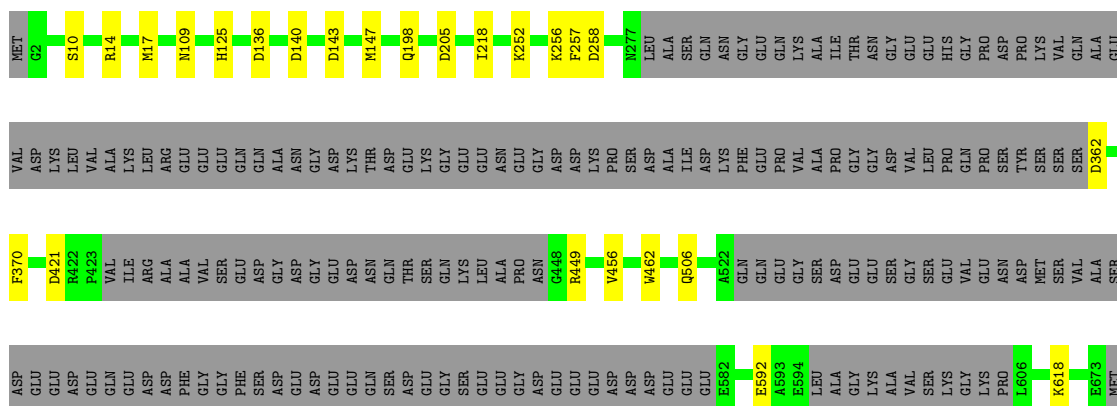
• Molecule 10: Nucleolar GTP-binding protein 1



• Molecule 11: Putative RNA-binding protein

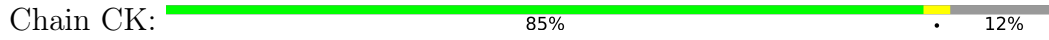


• Molecule 12: Pescadillo homolog

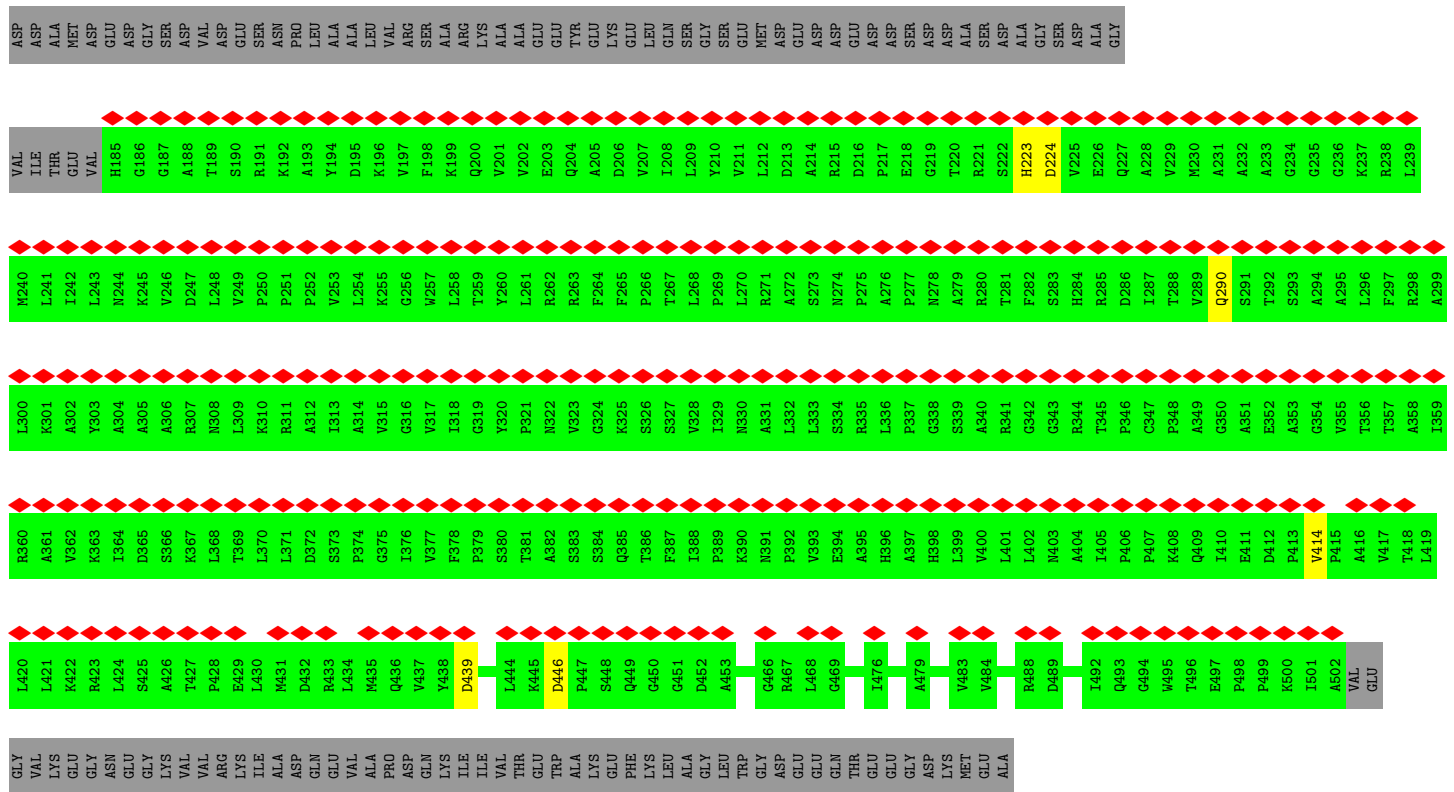
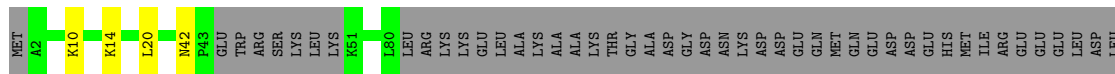


ALA
ALA
LYS
LYS
ALA

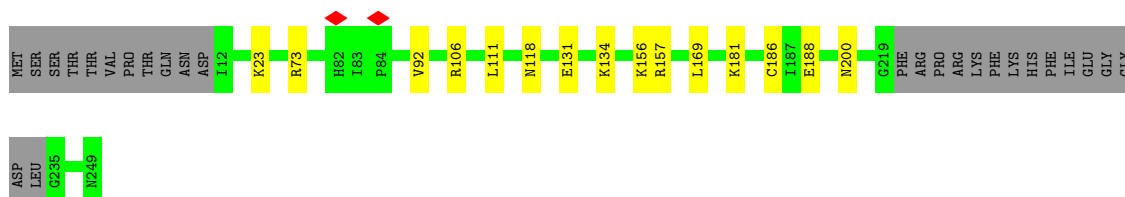
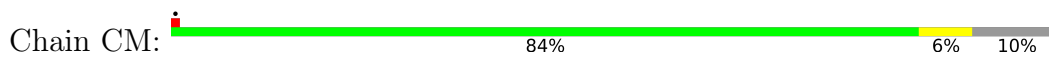
• Molecule 13: Ribosome biogenesis protein NSA2 homolog



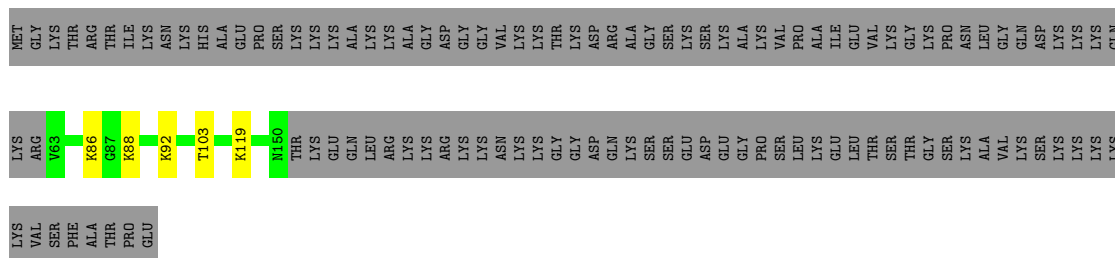
• Molecule 14: Putative GTP binding protein



• Molecule 15: 60S ribosomal protein l7-like protein

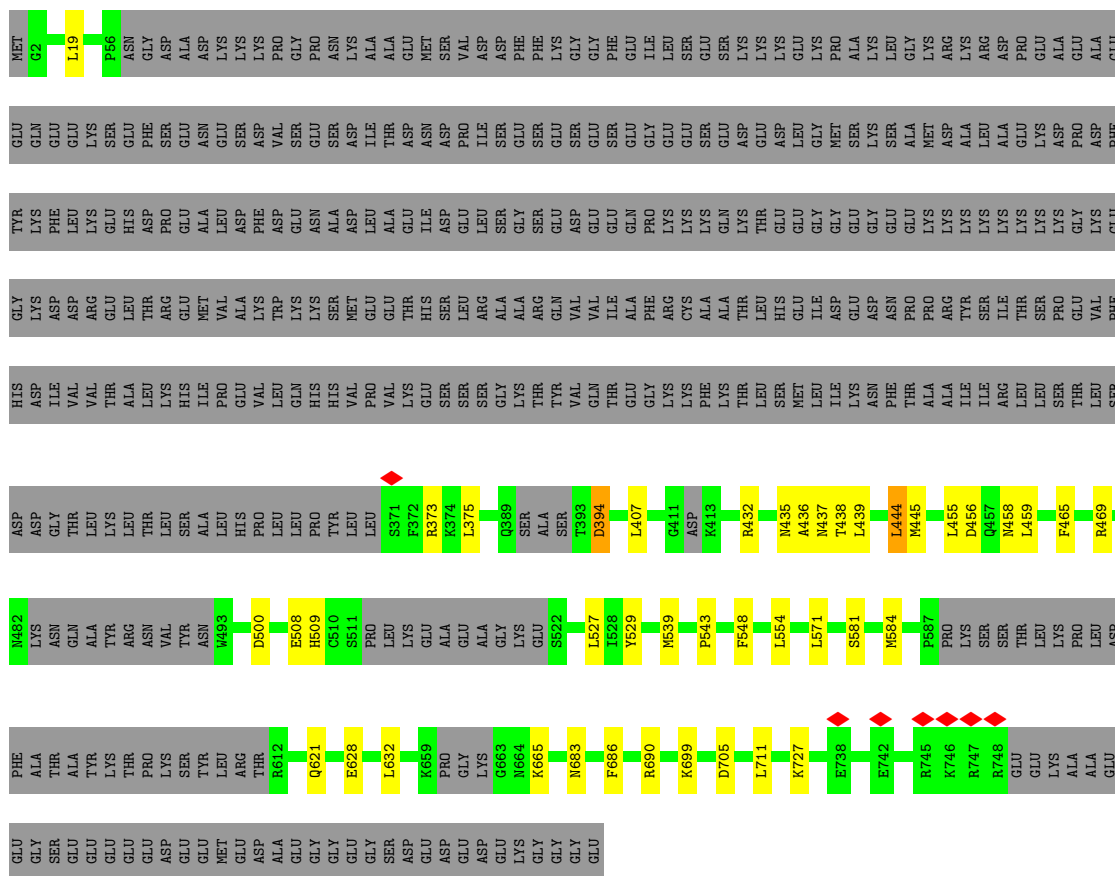


Chain CX: 41% 57%



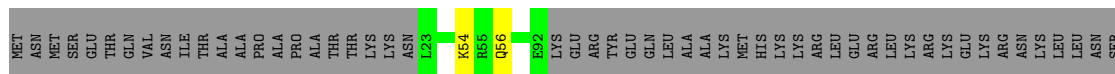
• Molecule 27: Putative NOC2 family protein

Chain CY: 43% 5% 52%



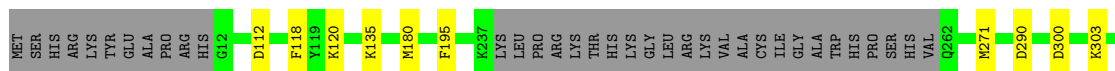
• Molecule 28: rRNA-processing protein

Chain Cz: 55% 43%

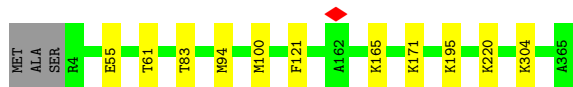


• Molecule 29: 60S ribosomal protein L3-like protein

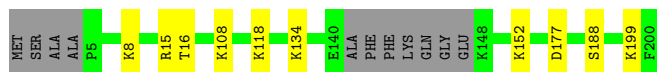
Chain LB: 88% 9%



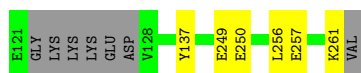
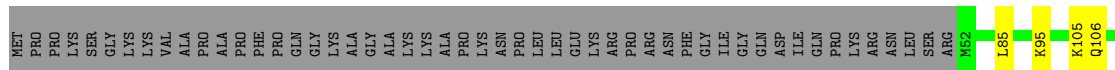
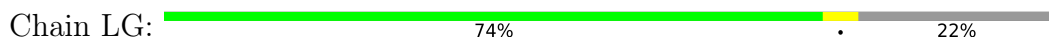
• Molecule 30: 60S ribosomal protein L4-like protein



• Molecule 31: 60S ribosomal protein L6



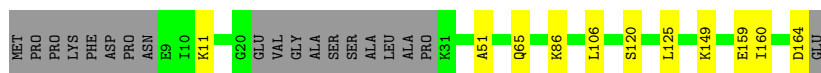
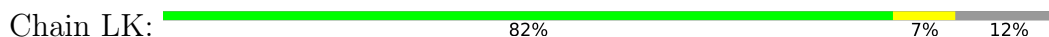
• Molecule 32: 60S ribosomal protein L8



• Molecule 33: 60S ribosomal protein l9-like protein

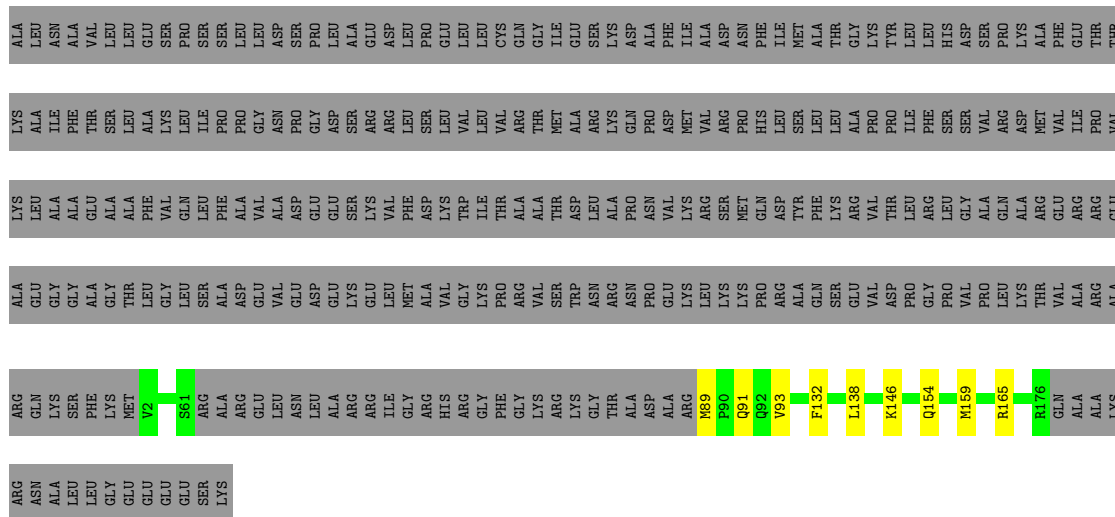


• Molecule 34: 60S ribosomal protein L12-like protein



• Molecule 35: 60S ribosomal protein L13

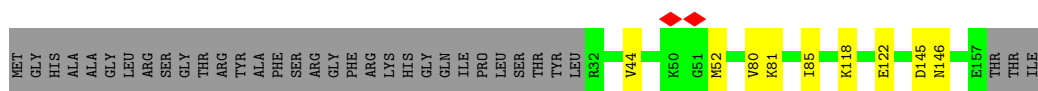
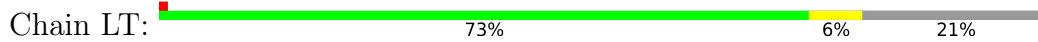




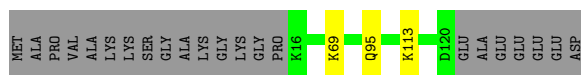
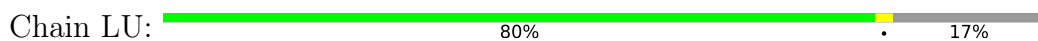
• Molecule 42: 60S ribosomal protein L20



• Molecule 43: 60S ribosomal protein l21-like protein



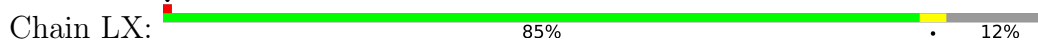
• Molecule 44: 60S ribosomal protein L22-like protein

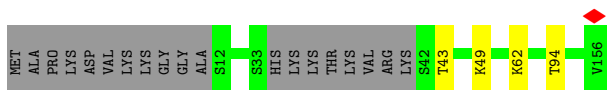


• Molecule 45: 60S ribosomal protein l23-like protein

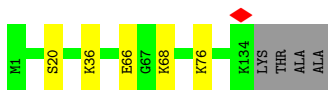


• Molecule 46: 60S ribosomal protein L25-like protein





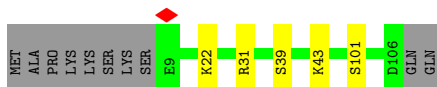
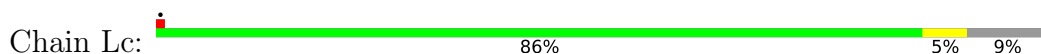
- Molecule 47: 60S ribosomal protein L26-like protein



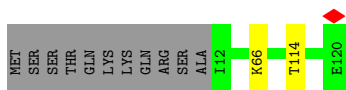
- Molecule 48: 60S ribosomal protein L27



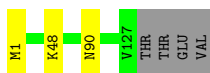
- Molecule 49: 60S ribosomal protein l30-like protein



- Molecule 50: Putative 60S ribosomal protein



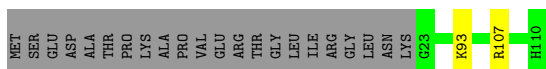
- Molecule 51: 60S ribosomal protein L32-like protein



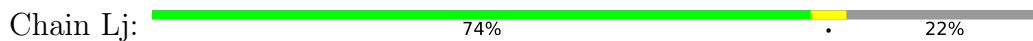
- Molecule 52: 60S ribosomal protein l33-like protein



- Molecule 53: Ribosomal protein l34-like protein



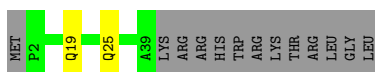
• Molecule 56: Ribosomal protein L37



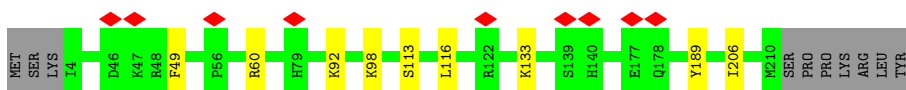
• Molecule 57: 60S ribosomal protein L38-like protein



• Molecule 58: 60S ribosomal protein L39



• Molecule 59: Ribosomal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173028	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 ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.758	Depositor
Minimum map value	-0.259	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	444.78, 444.78, 444.78	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.059, 1.059, 1.059	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: ADP, GTP, MG, ZN

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	C1	0.46	0/66718	0.97	166/104004 (0.2%)
2	C2	0.42	0/6097	0.91	3/9499 (0.0%)
3	CA	0.32	0/2115	0.56	1/2840 (0.0%)
4	CB	0.32	0/2109	0.66	3/2866 (0.1%)
5	CC	0.32	0/5438	0.62	6/7404 (0.1%)
6	CD	0.31	0/3543	0.73	7/4824 (0.1%)
7	CE	0.30	0/3760	0.61	1/5068 (0.0%)
8	CF	0.33	0/1982	0.63	1/2671 (0.0%)
9	CG	0.33	0/1422	0.60	1/1920 (0.1%)
10	CH	0.34	0/4468	0.64	5/6029 (0.1%)
11	CI	0.30	0/1225	0.58	0/1645
12	CJ	0.33	0/4125	0.64	5/5548 (0.1%)
13	CK	0.31	0/1863	0.56	0/2494
14	CL	0.28	0/2178	0.54	0/2983
15	CM	0.30	0/1851	0.60	1/2481 (0.0%)
15	LF	0.32	0/2055	0.57	2/2758 (0.1%)
16	CN	0.33	0/1881	0.65	2/2560 (0.1%)
17	CO	0.28	0/470	0.61	1/619 (0.2%)
18	CP	0.32	0/2594	0.58	0/3514
19	CQ	0.40	0/1507	0.68	0/1996
20	CR	0.28	0/1369	0.59	1/1828 (0.1%)
21	CS	0.29	0/5115	0.59	3/6841 (0.0%)
22	CT	0.33	0/3974	0.61	4/5357 (0.1%)
23	CU	0.28	0/1428	0.57	0/1910
24	CV	0.30	0/1091	0.59	0/1468
25	CW	0.37	0/4371	0.80	12/5917 (0.2%)
26	CX	0.28	0/705	0.60	0/938
27	CY	0.33	0/3079	0.77	11/4136 (0.3%)
28	Cz	0.27	0/598	0.51	0/785
29	LB	0.33	0/2885	0.60	1/3872 (0.0%)
30	LC	0.32	0/2809	0.56	0/3787
31	LE	0.30	0/1502	0.56	0/2020

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LG	0.36	0/1667	0.58	0/2230
33	LH	0.32	0/1516	0.55	0/2038
34	LK	0.28	0/1124	0.64	2/1507 (0.1%)
35	LL	0.30	0/983	0.64	0/1318
36	LM	0.30	0/1120	0.58	1/1507 (0.1%)
37	LN	0.33	0/1595	0.61	0/2132
38	LO	0.33	0/1652	0.57	0/2215
39	LP	0.27	0/1367	0.56	1/1838 (0.1%)
40	LQ	0.30	0/1033	0.61	0/1391
41	LR	0.29	0/1235	0.62	1/1644 (0.1%)
42	LS	0.32	0/1468	0.59	0/1975
43	LT	0.27	0/1033	0.59	0/1389
44	LU	0.29	0/863	0.48	0/1155
45	LV	0.30	0/1013	0.53	0/1361
46	LX	0.26	0/1078	0.48	0/1451
47	LY	0.28	0/1079	0.60	0/1443
48	LZ	0.32	0/1135	0.55	0/1519
49	Lc	0.31	0/740	0.59	0/995
50	Ld	0.29	0/904	0.57	0/1209
51	Le	0.29	0/1043	0.56	0/1389
52	Lf	0.35	0/883	0.61	0/1187
53	Lg	0.31	0/943	0.62	0/1258
54	Lh	0.27	0/1006	0.54	1/1338 (0.1%)
55	Li	0.32	0/738	0.64	0/971
56	Lj	0.33	0/606	0.65	0/803
57	Lk	0.33	0/628	0.59	0/835
58	Ll	0.28	0/329	0.62	0/440
59	Lq	0.27	0/1621	0.64	1/2180 (0.0%)
All	All	0.38	0/176729	0.79	244/253300 (0.1%)

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
14	CL	0	1
22	CT	0	1
59	Lq	0	1
All	All	0	3

There are no bond length outliers.

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2021	C	N3-C2-O2	-11.80	113.64	121.90
1	C1	1583	U	C2-N1-C1'	10.78	130.64	117.70
25	CW	277	PRO	CA-N-CD	-10.77	96.43	111.50
10	CH	72	ASP	CB-CG-OD1	10.72	127.95	118.30
1	C1	2022	C	N3-C2-O2	-10.09	114.84	121.90
5	CC	739	ASP	CB-CG-OD1	9.73	127.06	118.30
22	CT	146	PRO	CA-N-CD	-9.73	97.88	111.50
27	CY	632	LEU	CA-CB-CG	9.71	137.63	115.30
1	C1	136	C	N3-C2-O2	-9.59	115.19	121.90
1	C1	1583	U	N1-C2-O2	9.40	129.38	122.80
1	C1	2041	C	N3-C2-O2	-9.34	115.36	121.90
1	C1	1925	A	O5'-P-OP1	-9.06	97.55	105.70
27	CY	394	ASP	CB-CG-OD1	8.77	126.19	118.30
1	C1	1583	U	N3-C2-O2	-8.74	116.08	122.20
1	C1	1477	U	C2-N1-C1'	8.68	128.12	117.70
5	CC	660	ASP	CB-CG-OD1	8.52	125.97	118.30
1	C1	2021	C	N1-C2-O2	8.40	123.94	118.90
29	LB	290	ASP	CB-CG-OD1	8.23	125.71	118.30
12	CJ	258	ASP	CB-CG-OD1	8.12	125.61	118.30
9	CG	34	ASP	CB-CG-OD1	8.10	125.59	118.30
1	C1	835	G	P-O3'-C3'	7.92	129.21	119.70
1	C1	1049	C	N1-C2-O2	7.91	123.65	118.90
5	CC	142	ASP	CB-CG-OD1	7.84	125.35	118.30
1	C1	2723	C	N3-C2-O2	-7.83	116.42	121.90
6	CD	209	ASP	CB-CG-OD2	7.79	125.32	118.30
1	C1	2000	C	N3-C2-O2	-7.76	116.47	121.90
6	CD	197	ASP	CB-CG-OD1	7.76	125.28	118.30
15	CM	169	LEU	CA-CB-CG	7.65	132.90	115.30
1	C1	1477	U	N1-C2-O2	7.64	128.15	122.80
6	CD	417	ASP	CB-CG-OD1	7.57	125.11	118.30
1	C1	187	C	N3-C2-O2	-7.53	116.63	121.90
1	C1	1050	C	N3-C2-O2	-7.38	116.74	121.90
36	LM	42	ASP	CB-CG-OD1	7.37	124.93	118.30
1	C1	739	C	C2-N1-C1'	7.36	126.89	118.80
1	C1	2041	C	N1-C2-O2	7.32	123.29	118.90
1	C1	3110	C	N1-C2-O2	7.25	123.25	118.90
1	C1	1583	U	C6-N1-C1'	-7.24	111.06	121.20
1	C1	187	C	C6-N1-C2	-7.16	117.44	120.30
25	CW	483	ASP	CB-CG-OD1	7.11	124.70	118.30
1	C1	2745	G	N1-C6-O6	-7.11	115.63	119.90
1	C1	2000	C	C6-N1-C2	-7.07	117.47	120.30
16	CN	176	LEU	CA-CB-CG	7.07	131.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1336	G	C4-N9-C1'	7.05	135.67	126.50
10	CH	453	ASP	CB-CG-OD1	7.04	124.63	118.30
1	C1	1902	C	N3-C2-O2	-7.04	116.97	121.90
1	C1	136	C	N1-C2-O2	6.95	123.07	118.90
1	C1	1924	A	OP1-P-O3'	6.94	120.47	105.20
27	CY	375	LEU	CA-CB-CG	6.83	131.02	115.30
1	C1	1477	U	N3-C2-O2	-6.81	117.43	122.20
10	CH	442	ASP	CB-CG-OD1	6.77	124.40	118.30
4	CB	103	ASP	CB-CA-C	6.77	123.93	110.40
1	C1	799	C	N3-C2-O2	-6.73	117.19	121.90
34	LK	125	LEU	CA-CB-CG	6.65	130.60	115.30
1	C1	263	C	N1-C2-O2	6.65	122.89	118.90
1	C1	2417	U	C2-N1-C1'	6.60	125.62	117.70
1	C1	2923	U	C2-N1-C1'	6.58	125.60	117.70
27	CY	444	LEU	CA-CB-CG	6.54	130.35	115.30
1	C1	1537	U	N3-C2-O2	-6.54	117.62	122.20
1	C1	2731	C	N3-C2-O2	-6.53	117.33	121.90
15	LF	233	ASP	CB-CG-OD1	6.52	124.17	118.30
27	CY	571	LEU	CA-CB-CG	6.48	130.21	115.30
1	C1	532	C	N1-C2-O2	6.44	122.76	118.90
1	C1	398	G	O4'-C1'-N9	6.43	113.35	108.20
1	C1	102	C	N1-C2-O2	6.43	122.76	118.90
1	C1	127	G	N3-C4-N9	6.36	129.81	126.00
1	C1	3227	C	C2-N1-C1'	6.35	125.78	118.80
1	C1	2558	C	C2-N1-C1'	6.34	125.78	118.80
1	C1	1624	U	C2-N1-C1'	6.30	125.26	117.70
1	C1	1336	G	N3-C4-N9	6.30	129.78	126.00
1	C1	36	C	N1-C2-O2	6.25	122.65	118.90
25	CW	380	ASP	CB-CG-OD1	6.23	123.91	118.30
27	CY	19	LEU	CA-CB-CG	6.23	129.62	115.30
12	CJ	205	ASP	CB-CG-OD1	6.22	123.90	118.30
1	C1	1063	C	P-O3'-C3'	6.20	127.14	119.70
12	CJ	362	ASP	CB-CG-OD2	6.20	123.88	118.30
1	C1	150	G	OP2-P-O3'	6.20	118.83	105.20
1	C1	2406	C	C2-N1-C1'	6.18	125.59	118.80
1	C1	2731	C	N1-C2-O2	6.17	122.60	118.90
1	C1	150	G	P-O3'-C3'	6.17	127.10	119.70
1	C1	1924	A	P-O3'-C3'	6.15	127.08	119.70
1	C1	2406	C	N1-C2-O2	6.13	122.58	118.90
5	CC	535	LEU	CA-CB-CG	6.13	129.40	115.30
1	C1	3088	U	C2-N1-C1'	6.12	125.05	117.70
1	C1	1336	G	C8-N9-C1'	-6.12	119.05	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	133	G	N3-C4-C5	-6.11	125.54	128.60
1	C1	1336	G	N3-C4-C5	-6.11	125.55	128.60
1	C1	1999	C	N1-C2-O2	6.10	122.56	118.90
1	C1	1948	G	N1-C2-N2	-6.07	110.74	116.20
1	C1	78	U	N3-C2-O2	-6.07	117.95	122.20
1	C1	249	C	N3-C2-O2	-6.07	117.65	121.90
12	CJ	421	ASP	CB-CG-OD2	6.01	123.71	118.30
21	CS	364	LEU	CA-CB-CG	6.00	129.10	115.30
1	C1	2417	U	N1-C2-O2	6.00	127.00	122.80
1	C1	1206	C	N1-C2-O2	5.98	122.49	118.90
1	C1	3110	C	N3-C2-O2	-5.96	117.73	121.90
4	CB	104	PRO	CA-N-CD	-5.95	103.17	111.50
25	CW	601	MET	CA-CB-CG	5.94	123.40	113.30
1	C1	1624	U	N3-C2-O2	-5.93	118.05	122.20
1	C1	1950	C	C2-N1-C1'	5.92	125.32	118.80
1	C1	136	C	C6-N1-C2	-5.92	117.93	120.30
34	LK	164	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C1	1477	U	C6-N1-C1'	-5.91	112.93	121.20
25	CW	267	MET	CG-SD-CE	5.90	109.64	100.20
7	CE	355	MET	CB-CG-SD	5.89	130.06	112.40
1	C1	1478	C	C2-N1-C1'	5.88	125.27	118.80
1	C1	177	U	C2-N1-C1'	5.87	124.75	117.70
1	C1	1271	G	O4'-C1'-N9	5.87	112.90	108.20
1	C1	2885	C	N1-C2-O2	5.87	122.42	118.90
1	C1	2342	U	O4'-C1'-N1	5.86	112.89	108.20
1	C1	2745	G	C5-C6-O6	5.86	132.12	128.60
1	C1	1049	C	N3-C2-O2	-5.86	117.80	121.90
59	Lq	116	LEU	CA-CB-CG	5.85	128.76	115.30
1	C1	3281	U	O4'-C1'-N1	-5.83	103.54	108.20
1	C1	173	U	C2-N1-C1'	5.81	124.67	117.70
1	C1	966	U	N3-C2-O2	-5.80	118.14	122.20
1	C1	243	G	C4-N9-C1'	5.80	134.04	126.50
2	C2	102	U	P-O3'-C3'	5.80	126.66	119.70
1	C1	2022	C	N1-C2-O2	5.79	122.38	118.90
1	C1	133	G	N3-C4-N9	5.78	129.47	126.00
1	C1	1049	C	C2-N1-C1'	5.78	125.16	118.80
1	C1	614	C	C2-N1-C1'	5.78	125.16	118.80
6	CD	369	MET	CB-CG-SD	5.78	129.74	112.40
22	CT	146	PRO	N-CD-CG	-5.77	94.54	103.20
6	CD	35	LEU	CA-CB-CG	5.77	128.57	115.30
1	C1	2022	C	C6-N1-C2	-5.77	117.99	120.30
1	C1	2417	U	N3-C2-O2	-5.76	118.17	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	186	C	N1-C2-O2	5.75	122.35	118.90
25	CW	271	MET	CA-CB-CG	5.75	123.07	113.30
20	CR	234	LEU	CA-CB-CG	5.74	128.49	115.30
25	CW	132	PRO	CA-N-CD	-5.72	103.50	111.50
1	C1	2355	G	P-O3'-C3'	5.72	126.56	119.70
21	CS	319	LEU	CA-CB-CG	5.70	128.40	115.30
1	C1	2467	U	C2-N1-C1'	5.69	124.53	117.70
25	CW	485	ASP	CB-CG-OD1	5.69	123.42	118.30
15	LF	13	LEU	CA-CB-CG	5.68	128.36	115.30
27	CY	539	MET	CB-CG-SD	5.67	129.43	112.40
27	CY	711	LEU	CA-CB-CG	5.67	128.35	115.30
1	C1	1157	C	O4'-C1'-N1	5.67	112.73	108.20
1	C1	2467	U	N1-C2-O2	5.66	126.76	122.80
1	C1	263	C	N3-C2-O2	-5.64	117.95	121.90
1	C1	1940	G	N1-C6-O6	-5.64	116.52	119.90
17	CO	38	MET	CB-CG-SD	5.63	129.30	112.40
1	C1	3227	C	N1-C2-O2	5.63	122.28	118.90
25	CW	316	LEU	CA-CB-CG	5.61	128.20	115.30
1	C1	940	C	P-O3'-C3'	5.60	126.42	119.70
1	C1	1948	G	N1-C6-O6	-5.59	116.54	119.90
12	CJ	218	ILE	CG1-CB-CG2	-5.59	99.09	111.40
1	C1	1134	G	P-O3'-C3'	5.59	126.41	119.70
1	C1	127	G	C8-N9-C1'	-5.58	119.75	127.00
1	C1	1419	C	C2-N1-C1'	5.57	124.93	118.80
1	C1	102	C	N3-C2-O2	-5.57	118.00	121.90
1	C1	3177	C	C2-N1-C1'	5.56	124.92	118.80
1	C1	249	C	N1-C2-O2	5.56	122.24	118.90
1	C1	799	C	N1-C2-O2	5.52	122.21	118.90
1	C1	1948	G	C5-C6-O6	5.51	131.91	128.60
1	C1	127	G	C4-N9-C1'	5.50	133.66	126.50
22	CT	166	LEU	CA-CB-CG	5.50	127.94	115.30
27	CY	407	LEU	CA-CB-CG	5.50	127.94	115.30
25	CW	596	LEU	CA-CB-CG	5.49	127.93	115.30
1	C1	133	G	C2-N3-C4	5.49	114.64	111.90
1	C1	1221	C	C2-N1-C1'	5.49	124.83	118.80
1	C1	36	C	N3-C2-O2	-5.46	118.08	121.90
2	C2	156	U	C2-N1-C1'	5.46	124.25	117.70
1	C1	3162	A	P-O3'-C3'	5.45	126.24	119.70
16	CN	203	LEU	CA-CB-CG	5.45	127.82	115.30
1	C1	3297	U	P-O3'-C3'	5.43	126.22	119.70
27	CY	554	LEU	CA-CB-CG	5.43	127.79	115.30
1	C1	2467	U	N3-C2-O2	-5.42	118.40	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	CH	297	LEU	CA-CB-CG	5.42	127.77	115.30
1	C1	263	C	C6-N1-C2	-5.41	118.14	120.30
54	Lh	34	LEU	CA-CB-CG	5.41	127.75	115.30
1	C1	72	C	C2-N3-C4	-5.40	117.20	119.90
1	C1	2731	C	C6-N1-C2	-5.38	118.15	120.30
41	LR	138	LEU	CA-CB-CG	5.38	127.66	115.30
2	C2	64	U	N3-C2-O2	-5.37	118.44	122.20
25	CW	333	LEU	CA-CB-CG	5.36	127.63	115.30
1	C1	128	G	C5-C6-O6	5.35	131.81	128.60
8	CF	119	LEU	CA-CB-CG	5.35	127.60	115.30
1	C1	83	C	C6-N1-C1'	5.35	127.22	120.80
1	C1	1583	U	C5-C6-N1	5.35	125.37	122.70
1	C1	2991	C	N1-C2-O2	5.34	122.11	118.90
1	C1	1950	C	N1-C2-O2	5.34	122.11	118.90
1	C1	113	C	C2-N1-C1'	5.34	124.67	118.80
1	C1	177	U	N1-C2-O2	5.33	126.53	122.80
1	C1	263	C	C2-N1-C1'	5.32	124.65	118.80
5	CC	246	LEU	CA-CB-CG	5.31	127.52	115.30
22	CT	161	LEU	CA-CB-CG	5.31	127.52	115.30
1	C1	2021	C	C6-N1-C2	-5.30	118.18	120.30
1	C1	1624	U	N1-C2-O2	5.30	126.51	122.80
1	C1	1126	U	N1-C2-O2	5.29	126.50	122.80
1	C1	3289	C	N1-C2-O2	5.29	122.07	118.90
1	C1	3209	U	P-O3'-C3'	5.28	126.04	119.70
1	C1	1902	C	N1-C2-O2	5.28	122.07	118.90
1	C1	162	U	N3-C2-O2	-5.28	118.51	122.20
1	C1	83	C	N3-C2-O2	-5.26	118.22	121.90
1	C1	1954	C	C5-C6-N1	5.24	123.62	121.00
1	C1	243	G	N3-C4-C5	-5.23	125.98	128.60
1	C1	1940	G	C5-C6-O6	5.23	131.74	128.60
1	C1	105	C	C6-N1-C2	-5.23	118.21	120.30
21	CS	201	PHE	CB-CG-CD1	5.22	124.46	120.80
1	C1	3131	A	P-O3'-C3'	5.22	125.96	119.70
1	C1	2723	C	C6-N1-C2	-5.22	118.21	120.30
6	CD	204	LYS	CA-CB-CG	5.22	124.88	113.40
1	C1	167	C	C2-N1-C1'	5.21	124.53	118.80
3	CA	39	LEU	CA-CB-CG	5.21	127.28	115.30
1	C1	3289	C	N3-C2-O2	-5.20	118.26	121.90
1	C1	3015	U	C2-N1-C1'	5.19	123.93	117.70
39	LP	107	LEU	CA-CB-CG	5.17	127.20	115.30
1	C1	3110	C	C2-N1-C1'	5.17	124.48	118.80
1	C1	1050	C	C6-N1-C2	-5.17	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2328	C	C2-N1-C1'	5.16	124.48	118.80
1	C1	1537	U	N1-C2-O2	5.16	126.41	122.80
1	C1	101	G	C4-N9-C1'	5.15	133.20	126.50
1	C1	187	C	N1-C2-N3	5.15	122.80	119.20
1	C1	739	C	C6-N1-C1'	-5.15	114.62	120.80
1	C1	1073	G	C5-C6-O6	5.15	131.69	128.60
10	CH	527	LEU	CA-CB-CG	5.14	127.13	115.30
1	C1	105	C	C2-N1-C1'	5.14	124.45	118.80
1	C1	103	G	C5-C6-O6	5.13	131.68	128.60
1	C1	1507	G	C4-N9-C1'	5.13	133.17	126.50
1	C1	1662	C	N1-C2-O2	5.12	121.97	118.90
1	C1	427	C	C2-N1-C1'	5.11	124.42	118.80
1	C1	133	G	C4-N9-C1'	5.11	133.14	126.50
1	C1	1851	C	N1-C2-O2	5.11	121.96	118.90
25	CW	267	MET	CB-CG-SD	5.10	127.71	112.40
1	C1	886	U	P-O3'-C3'	5.10	125.82	119.70
4	CB	64	LEU	CA-CB-CG	5.09	127.02	115.30
1	C1	307	C	C2-N1-C1'	5.09	124.40	118.80
1	C1	2991	C	N3-C2-O2	-5.08	118.34	121.90
1	C1	3297	U	N3-C2-O2	-5.08	118.64	122.20
1	C1	3297	U	N1-C2-O2	5.07	126.35	122.80
1	C1	1172	A	C4-N9-C1'	5.07	135.42	126.30
1	C1	1857	G	C4-N9-C1'	5.07	133.09	126.50
6	CD	56	LEU	CA-CB-CG	5.06	126.94	115.30
27	CY	543	PRO	CA-N-CD	-5.06	104.42	111.50
1	C1	3113	C	C2-N1-C1'	5.05	124.36	118.80
1	C1	2466	U	C2-N1-C1'	5.05	123.76	117.70
1	C1	1073	G	N1-C6-O6	-5.05	116.87	119.90
1	C1	3110	C	O4'-C1'-N1	5.04	112.23	108.20
1	C1	2923	U	N1-C2-O2	5.03	126.32	122.80
1	C1	1542	G	O4'-C1'-N9	5.03	112.22	108.20
1	C1	454	U	C2-N1-C1'	5.02	123.72	117.70
5	CC	345	LEU	CA-CB-CG	5.02	126.84	115.30
1	C1	935	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	CL	223	HIS	Peptide
22	CT	253	VAL	Peptide
59	Lq	60	ARG	Peptide

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	
3	CA	247/316 (78%)	235 (95%)	12 (5%)	0	100	100
4	CB	256/391 (66%)	242 (94%)	12 (5%)	2 (1%)	19	43
5	CC	650/801 (81%)	625 (96%)	24 (4%)	1 (0%)	47	73
6	CD	450/495 (91%)	429 (95%)	21 (5%)	0	100	100
7	CE	461/598 (77%)	440 (95%)	20 (4%)	1 (0%)	47	73
8	CF	243/270 (90%)	232 (96%)	10 (4%)	1 (0%)	34	60
9	CG	175/184 (95%)	169 (97%)	6 (3%)	0	100	100
10	CH	538/661 (81%)	517 (96%)	21 (4%)	0	100	100
11	CI	144/414 (35%)	139 (96%)	5 (4%)	0	100	100
12	CJ	484/679 (71%)	468 (97%)	16 (3%)	0	100	100
13	CK	223/261 (85%)	216 (97%)	7 (3%)	0	100	100
14	CL	384/558 (69%)	353 (92%)	25 (6%)	6 (2%)	9	24
15	CM	219/249 (88%)	208 (95%)	11 (5%)	0	100	100
15	LF	245/249 (98%)	236 (96%)	9 (4%)	0	100	100
16	CN	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
17	CO	56/120 (47%)	55 (98%)	1 (2%)	0	100	100
18	CP	322/751 (43%)	309 (96%)	13 (4%)	0	100	100
19	CQ	173/225 (77%)	169 (98%)	4 (2%)	0	100	100
20	CR	159/237 (67%)	154 (97%)	5 (3%)	0	100	100
21	CS	607/834 (73%)	577 (95%)	29 (5%)	1 (0%)	47	73
22	CT	478/688 (70%)	454 (95%)	23 (5%)	1 (0%)	47	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	CU	174/451 (39%)	169 (97%)	4 (2%)	1 (1%)	25	50
24	CV	137/147 (93%)	131 (96%)	5 (4%)	1 (1%)	22	46
25	CW	531/679 (78%)	495 (93%)	34 (6%)	2 (0%)	34	60
26	CX	86/203 (42%)	85 (99%)	1 (1%)	0	100	100
27	CY	366/788 (46%)	346 (94%)	19 (5%)	1 (0%)	41	66
28	Cz	68/123 (55%)	65 (96%)	3 (4%)	0	100	100
29	LB	352/392 (90%)	338 (96%)	14 (4%)	0	100	100
30	LC	360/365 (99%)	345 (96%)	15 (4%)	0	100	100
31	LE	185/200 (92%)	172 (93%)	13 (7%)	0	100	100
32	LG	200/262 (76%)	189 (94%)	11 (6%)	0	100	100
33	LH	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
34	LK	142/165 (86%)	132 (93%)	8 (6%)	2 (1%)	11	28
35	LL	115/213 (54%)	109 (95%)	6 (5%)	0	100	100
36	LM	135/142 (95%)	129 (96%)	6 (4%)	0	100	100
37	LN	179/203 (88%)	173 (97%)	6 (3%)	0	100	100
38	LO	202/204 (99%)	200 (99%)	2 (1%)	0	100	100
39	LP	165/187 (88%)	162 (98%)	3 (2%)	0	100	100
40	LQ	127/213 (60%)	122 (96%)	5 (4%)	0	100	100
41	LR	144/2898 (5%)	143 (99%)	1 (1%)	0	100	100
42	LS	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
43	LT	124/160 (78%)	118 (95%)	5 (4%)	1 (1%)	19	43
44	LU	103/127 (81%)	101 (98%)	2 (2%)	0	100	100
45	LV	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
46	LX	133/156 (85%)	130 (98%)	3 (2%)	0	100	100
47	LY	132/138 (96%)	126 (96%)	6 (4%)	0	100	100
48	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
49	Lc	96/108 (89%)	95 (99%)	1 (1%)	0	100	100
50	Ld	107/120 (89%)	104 (97%)	3 (3%)	0	100	100
51	Le	125/131 (95%)	123 (98%)	2 (2%)	0	100	100
52	Lf	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
53	Lg	115/119 (97%)	112 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	Lh	119/935 (13%)	117 (98%)	2 (2%)	0	100	100
55	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100	100
56	Lj	72/95 (76%)	70 (97%)	2 (3%)	0	100	100
57	Lk	73/81 (90%)	70 (96%)	3 (4%)	0	100	100
58	Ll	36/51 (71%)	36 (100%)	0	0	100	100
59	Lq	205/217 (94%)	184 (90%)	21 (10%)	0	100	100
All	All	12684/20359 (62%)	12128 (96%)	535 (4%)	21 (0%)	50	73

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CB	103	ASP
4	CB	104	PRO
7	CE	313	PRO
14	CL	224	ASP
14	CL	414	VAL
27	CY	436	ALA
34	LK	51	ALA
14	CL	439	ASP
21	CS	14	ASP
22	CT	237	PRO
25	CW	36	GLU
14	CL	42	ASN
25	CW	63	SER
34	LK	160	ILE
8	CF	126	ARG
23	CU	226	THR
24	CV	24	ARG
14	CL	290	GLN
14	CL	446	ASP
43	LT	44	VAL
5	CC	251	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	
3	CA	223/276 (81%)	217 (97%)	6 (3%)	44	74
4	CB	222/329 (68%)	208 (94%)	14 (6%)	18	40
5	CC	580/710 (82%)	562 (97%)	18 (3%)	40	69
6	CD	381/410 (93%)	355 (93%)	26 (7%)	16	36
7	CE	400/517 (77%)	382 (96%)	18 (4%)	27	55
8	CF	214/236 (91%)	209 (98%)	5 (2%)	50	78
9	CG	150/155 (97%)	145 (97%)	5 (3%)	38	67
10	CH	481/575 (84%)	465 (97%)	16 (3%)	38	67
11	CI	121/336 (36%)	114 (94%)	7 (6%)	20	43
12	CJ	428/579 (74%)	408 (95%)	20 (5%)	26	54
13	CK	195/225 (87%)	187 (96%)	8 (4%)	30	59
14	CL	65/458 (14%)	62 (95%)	3 (5%)	27	54
15	CM	191/215 (89%)	177 (93%)	14 (7%)	14	33
15	LF	213/215 (99%)	206 (97%)	7 (3%)	38	67
16	CN	206/206 (100%)	202 (98%)	4 (2%)	57	82
17	CO	48/99 (48%)	47 (98%)	1 (2%)	53	80
18	CP	273/632 (43%)	255 (93%)	18 (7%)	16	38
19	CQ	150/192 (78%)	133 (89%)	17 (11%)	6	13
20	CR	144/206 (70%)	137 (95%)	7 (5%)	25	52
21	CS	527/716 (74%)	504 (96%)	23 (4%)	28	56
22	CT	427/600 (71%)	405 (95%)	22 (5%)	23	49
23	CU	149/376 (40%)	144 (97%)	5 (3%)	37	66
24	CV	109/112 (97%)	107 (98%)	2 (2%)	59	83
25	CW	473/577 (82%)	422 (89%)	51 (11%)	6	15
26	CX	76/172 (44%)	71 (93%)	5 (7%)	16	38
27	CY	315/686 (46%)	283 (90%)	32 (10%)	7	17
28	Cz	60/107 (56%)	58 (97%)	2 (3%)	38	67
29	LB	301/331 (91%)	290 (96%)	11 (4%)	34	63
30	LC	283/285 (99%)	272 (96%)	11 (4%)	32	61
31	LE	159/166 (96%)	149 (94%)	10 (6%)	18	40
32	LG	175/222 (79%)	165 (94%)	10 (6%)	20	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	LH	167/169 (99%)	159 (95%)	8 (5%)	25	53
34	LK	121/136 (89%)	114 (94%)	7 (6%)	20	43
35	LL	99/176 (56%)	97 (98%)	2 (2%)	55	81
36	LM	115/117 (98%)	114 (99%)	1 (1%)	78	92
37	LN	164/180 (91%)	157 (96%)	7 (4%)	29	57
38	LO	163/163 (100%)	159 (98%)	4 (2%)	47	76
39	LP	137/152 (90%)	130 (95%)	7 (5%)	24	50
40	LQ	110/178 (62%)	109 (99%)	1 (1%)	78	92
41	LR	128/2396 (5%)	120 (94%)	8 (6%)	18	40
42	LS	154/154 (100%)	144 (94%)	10 (6%)	17	38
43	LT	109/135 (81%)	101 (93%)	8 (7%)	14	33
44	LU	93/108 (86%)	90 (97%)	3 (3%)	39	68
45	LV	99/102 (97%)	95 (96%)	4 (4%)	31	60
46	LX	114/129 (88%)	110 (96%)	4 (4%)	36	65
47	LY	117/119 (98%)	112 (96%)	5 (4%)	29	57
48	LZ	121/121 (100%)	118 (98%)	3 (2%)	47	76
49	Lc	79/88 (90%)	74 (94%)	5 (6%)	18	40
50	Ld	95/105 (90%)	93 (98%)	2 (2%)	53	80
51	Le	110/114 (96%)	107 (97%)	3 (3%)	44	74
52	Lf	89/90 (99%)	84 (94%)	5 (6%)	21	45
53	Lg	101/102 (99%)	99 (98%)	2 (2%)	55	81
54	Lh	108/781 (14%)	106 (98%)	2 (2%)	57	82
55	Li	75/93 (81%)	73 (97%)	2 (3%)	44	74
56	Lj	61/78 (78%)	57 (93%)	4 (7%)	16	38
57	Lk	71/76 (93%)	68 (96%)	3 (4%)	30	58
58	Ll	34/46 (74%)	32 (94%)	2 (6%)	19	43
59	Lq	179/189 (95%)	172 (96%)	7 (4%)	32	61
All	All	10752/17218 (62%)	10235 (95%)	517 (5%)	29	53

All (517) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CA	23	ARG

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Mol	Chain	Res	Type
3	CA	72	SER
3	CA	179	VAL
3	CA	275	LYS
3	CA	278	ARG
3	CA	287	ARG
4	CB	60	THR
4	CB	71	HIS
4	CB	91	THR
4	CB	98	CYS
4	CB	104	PRO
4	CB	129	ASP
4	CB	136	LYS
4	CB	173	LYS
4	CB	206	ARG
4	CB	209	LEU
4	CB	226	LYS
4	CB	264	ARG
4	CB	269	ARG
4	CB	275	TRP
5	CC	152	ASP
5	CC	229	LEU
5	CC	278	LYS
5	CC	285	LYS
5	CC	292	MET
5	CC	364	LYS
5	CC	373	MET
5	CC	386	LYS
5	CC	434	SER
5	CC	477	VAL
5	CC	492	LYS
5	CC	524	MET
5	CC	668	LYS
5	CC	697	ARG
5	CC	699	LEU
5	CC	727	LYS
5	CC	764	MET
5	CC	790	SER
6	CD	28	LEU
6	CD	32	LYS
6	CD	43	ARG
6	CD	48	ARG
6	CD	51	ASN

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Mol	Chain	Res	Type
6	CD	55	MET
6	CD	79	TYR
6	CD	94	GLN
6	CD	97	ARG
6	CD	112	ASP
6	CD	170	SER
6	CD	189	ASP
6	CD	193	SER
6	CD	197	ASP
6	CD	204	LYS
6	CD	214	GLU
6	CD	261	GLU
6	CD	322	VAL
6	CD	366	HIS
6	CD	373	ARG
6	CD	402	TYR
6	CD	418	LEU
6	CD	422	ARG
6	CD	435	SER
6	CD	451	LYS
6	CD	482	VAL
7	CE	124	LYS
7	CE	134	MET
7	CE	139	ARG
7	CE	149	LYS
7	CE	151	VAL
7	CE	223	ARG
7	CE	245	LEU
7	CE	246	ASP
7	CE	293	MET
7	CE	296	SER
7	CE	316	LEU
7	CE	317	TYR
7	CE	357	LYS
7	CE	386	ASP
7	CE	391	GLN
7	CE	489	LYS
7	CE	500	LEU
7	CE	537	ASP
8	CF	5	LYS
8	CF	115	TYR
8	CF	180	CYS

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Mol	Chain	Res	Type
8	CF	207	ARG
8	CF	237	LEU
9	CG	14	ASP
9	CG	25	SER
9	CG	79	LYS
9	CG	124	GLU
9	CG	164	CYS
10	CH	6	ASP
10	CH	10	VAL
10	CH	58	GLU
10	CH	65	SER
10	CH	69	VAL
10	CH	79	ASP
10	CH	128	LYS
10	CH	268	ASN
10	CH	281	MET
10	CH	293	LYS
10	CH	423	LYS
10	CH	469	GLU
10	CH	508	MET
10	CH	525	LYS
10	CH	540	ASP
10	CH	547	ARG
11	CI	215	ARG
11	CI	224	THR
11	CI	260	CYS
11	CI	291	ARG
11	CI	292	GLN
11	CI	295	ARG
11	CI	311	GLN
12	CJ	10	SER
12	CJ	14	ARG
12	CJ	17	MET
12	CJ	109	ASN
12	CJ	125	HIS
12	CJ	136	ASP
12	CJ	140	ASP
12	CJ	143	ASP
12	CJ	147	MET
12	CJ	198	GLN
12	CJ	252	LYS
12	CJ	256	LYS

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Mol	Chain	Res	Type
12	CJ	257	PHE
12	CJ	370	PHE
12	CJ	449	ARG
12	CJ	456	VAL
12	CJ	462	TRP
12	CJ	506	GLN
12	CJ	592	GLU
12	CJ	618	LYS
13	CK	6	TYR
13	CK	9	ARG
13	CK	46	ARG
13	CK	52	LYS
13	CK	128	SER
13	CK	145	LYS
13	CK	164	ARG
13	CK	169	GLU
14	CL	10	LYS
14	CL	14	LYS
14	CL	20	LEU
15	CM	23	LYS
15	CM	73	ARG
15	CM	92	VAL
15	CM	106	ARG
15	CM	111	LEU
15	CM	118	ASN
15	CM	131	GLU
15	CM	134	LYS
15	CM	156	LYS
15	CM	157	ARG
15	CM	181	LYS
15	CM	186	CYS
15	CM	188	GLU
15	CM	200	ASN
16	CN	28	LEU
16	CN	67	ARG
16	CN	191	ASN
16	CN	237	MET
17	CO	110	MET
18	CP	268	LYS
18	CP	318	ARG
18	CP	369	SER
18	CP	411	ASN

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Mol	Chain	Res	Type
18	CP	412	ASP
18	CP	417	ARG
18	CP	441	ARG
18	CP	443	PHE
18	CP	445	ARG
18	CP	470	SER
18	CP	472	LYS
18	CP	478	LYS
18	CP	502	SER
18	CP	530	ARG
18	CP	531	ARG
18	CP	571	TYR
18	CP	574	ASP
18	CP	576	PHE
19	CQ	1	MET
19	CQ	48	LYS
19	CQ	63	MET
19	CQ	74	ARG
19	CQ	86	TRP
19	CQ	88	LYS
19	CQ	136	ARG
19	CQ	144	ARG
19	CQ	148	LEU
19	CQ	151	GLU
19	CQ	152	ARG
19	CQ	156	VAL
19	CQ	158	GLU
19	CQ	164	LEU
19	CQ	166	LYS
19	CQ	167	LEU
19	CQ	181	ARG
20	CR	8	ARG
20	CR	12	SER
20	CR	131	VAL
20	CR	165	LYS
20	CR	192	ARG
20	CR	209	MET
20	CR	223	SER
21	CS	201	PHE
21	CS	210	ARG
21	CS	310	LYS
21	CS	322	LYS

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Mol	Chain	Res	Type
21	CS	370	LYS
21	CS	372	ARG
21	CS	379	ARG
21	CS	397	MET
21	CS	438	MET
21	CS	490	TYR
21	CS	505	GLU
21	CS	563	SER
21	CS	576	GLN
21	CS	577	LYS
21	CS	660	MET
21	CS	668	THR
21	CS	673	LYS
21	CS	675	ASP
21	CS	676	LEU
21	CS	688	GLN
21	CS	704	ASP
21	CS	743	ARG
21	CS	752	LYS
22	CT	125	ARG
22	CT	143	GLU
22	CT	152	LEU
22	CT	201	LYS
22	CT	219	LYS
22	CT	257	ASN
22	CT	273	ARG
22	CT	276	ASP
22	CT	318	ASP
22	CT	319	GLU
22	CT	413	LYS
22	CT	497	ASP
22	CT	524	SER
22	CT	526	ASN
22	CT	562	THR
22	CT	599	LEU
22	CT	602	GLN
22	CT	603	VAL
22	CT	647	THR
22	CT	652	ASN
22	CT	665	ARG
22	CT	666	LYS
23	CU	212	THR

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Mol	Chain	Res	Type
23	CU	217	HIS
23	CU	301	GLU
23	CU	310	LYS
23	CU	319	LYS
24	CV	14	ARG
24	CV	69	LYS
25	CW	22	LEU
25	CW	25	TRP
25	CW	33	MET
25	CW	35	TYR
25	CW	36	GLU
25	CW	37	GLN
25	CW	39	THR
25	CW	53	LYS
25	CW	56	VAL
25	CW	99	GLU
25	CW	100	LEU
25	CW	103	GLN
25	CW	108	LEU
25	CW	136	LYS
25	CW	150	LYS
25	CW	154	ASP
25	CW	162	SER
25	CW	220	ARG
25	CW	235	ARG
25	CW	236	LEU
25	CW	241	MET
25	CW	243	TYR
25	CW	246	LYS
25	CW	271	MET
25	CW	291	LYS
25	CW	307	PHE
25	CW	315	VAL
25	CW	330	HIS
25	CW	332	LYS
25	CW	340	LYS
25	CW	344	ARG
25	CW	345	PHE
25	CW	356	THR
25	CW	364	LEU
25	CW	376	ASP
25	CW	382	LYS

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Mol	Chain	Res	Type
25	CW	387	ARG
25	CW	393	ARG
25	CW	408	ARG
25	CW	414	GLN
25	CW	428	HIS
25	CW	439	ASP
25	CW	457	GLN
25	CW	471	MET
25	CW	473	HIS
25	CW	480	ARG
25	CW	501	MET
25	CW	505	ARG
25	CW	572	TRP
25	CW	597	LYS
25	CW	610	ARG
26	CX	86	LYS
26	CX	88	LYS
26	CX	92	LYS
26	CX	103	THR
26	CX	119	LYS
27	CY	373	ARG
27	CY	394	ASP
27	CY	432	ARG
27	CY	435	ASN
27	CY	437	ASN
27	CY	438	THR
27	CY	439	LEU
27	CY	444	LEU
27	CY	445	MET
27	CY	455	LEU
27	CY	456	ASP
27	CY	458	ASN
27	CY	459	LEU
27	CY	465	PHE
27	CY	469	ARG
27	CY	500	ASP
27	CY	508	GLU
27	CY	509	HIS
27	CY	527	LEU
27	CY	529	TYR
27	CY	548	PHE
27	CY	581	SER

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Mol	Chain	Res	Type
27	CY	584	MET
27	CY	621	GLN
27	CY	628	GLU
27	CY	665	LYS
27	CY	683	ASN
27	CY	686	PHE
27	CY	690	ARG
27	CY	699	LYS
27	CY	705	ASP
27	CY	727	LYS
28	Cz	54	LYS
28	Cz	56	GLN
29	LB	112	ASP
29	LB	118	PHE
29	LB	120	LYS
29	LB	135	LYS
29	LB	180	MET
29	LB	195	PHE
29	LB	271	MET
29	LB	300	ASP
29	LB	303	LYS
29	LB	359	TRP
29	LB	365	GLU
30	LC	55	GLU
30	LC	61	THR
30	LC	83	THR
30	LC	94	MET
30	LC	100	MET
30	LC	121	PHE
30	LC	165	LYS
30	LC	171	LYS
30	LC	195	LYS
30	LC	220	LYS
30	LC	304	LYS
31	LE	8	LYS
31	LE	15	ARG
31	LE	16	THR
31	LE	108	LYS
31	LE	118	LYS
31	LE	134	LYS
31	LE	152	LYS
31	LE	177	ASP

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Mol	Chain	Res	Type
31	LE	188	SER
31	LE	199	LYS
15	LF	16	GLU
15	LF	77	GLN
15	LF	99	ASN
15	LF	127	LYS
15	LF	134	LYS
15	LF	189	ASP
15	LF	226	LYS
32	LG	85	LEU
32	LG	95	LYS
32	LG	105	LYS
32	LG	106	GLN
32	LG	137	TYR
32	LG	249	GLU
32	LG	250	GLU
32	LG	256	LEU
32	LG	257	GLU
32	LG	261	LYS
33	LH	19	SER
33	LH	21	LYS
33	LH	23	ARG
33	LH	33	LYS
33	LH	36	LYS
33	LH	55	LEU
33	LH	109	THR
33	LH	172	LYS
34	LK	11	LYS
34	LK	65	GLN
34	LK	86	LYS
34	LK	106	LEU
34	LK	120	SER
34	LK	149	LYS
34	LK	159	GLU
35	LL	53	LYS
35	LL	67	ARG
36	LM	121	MET
37	LN	27	CYS
37	LN	43	SER
37	LN	66	VAL
37	LN	122	ASN
37	LN	125	SER

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Mol	Chain	Res	Type
37	LN	140	LYS
37	LN	144	ARG
38	LO	69	ARG
38	LO	80	ARG
38	LO	178	ARG
38	LO	194	LYS
39	LP	8	GLU
39	LP	16	ARG
39	LP	30	ARG
39	LP	43	ARG
39	LP	79	SER
39	LP	82	ARG
39	LP	182	ARG
40	LQ	44	ARG
41	LR	89	MET
41	LR	91	GLN
41	LR	93	VAL
41	LR	132	PHE
41	LR	146	LYS
41	LR	154	GLN
41	LR	159	MET
41	LR	165	ARG
42	LS	34	GLU
42	LS	39	SER
42	LS	45	LEU
42	LS	67	LYS
42	LS	106	MET
42	LS	119	ARG
42	LS	133	GLU
42	LS	141	LYS
42	LS	149	SER
42	LS	160	SER
43	LT	52	MET
43	LT	80	VAL
43	LT	81	LYS
43	LT	85	ILE
43	LT	118	LYS
43	LT	122	GLU
43	LT	145	ASP
43	LT	146	ASN
44	LU	69	LYS
44	LU	95	GLN

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Mol	Chain	Res	Type
44	LU	113	LYS
45	LV	15	MET
45	LV	27	CYS
45	LV	95	LEU
45	LV	139	MET
46	LX	43	THR
46	LX	49	LYS
46	LX	62	LYS
46	LX	94	THR
47	LY	20	SER
47	LY	36	LYS
47	LY	66	GLU
47	LY	68	LYS
47	LY	76	LYS
48	LZ	14	ARG
48	LZ	29	ASP
48	LZ	115	LYS
49	Lc	22	LYS
49	Lc	31	ARG
49	Lc	39	SER
49	Lc	43	LYS
49	Lc	101	SER
50	Ld	66	LYS
50	Ld	114	THR
51	Le	1	MET
51	Le	48	LYS
51	Le	90	ASN
52	Lf	56	ARG
52	Lf	59	LYS
52	Lf	62	ARG
52	Lf	67	ARG
52	Lf	94	ARG
53	Lg	80	SER
53	Lg	115	LYS
54	Lh	6	LYS
54	Lh	54	LYS
55	Li	93	LYS
55	Li	107	ARG
56	Lj	45	ARG
56	Lj	63	ARG
56	Lj	84	LYS
56	Lj	87	ARG

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Mol	Chain	Res	Type
57	Lk	10	LYS
57	Lk	24	ARG
57	Lk	27	LYS
58	Ll	19	GLN
58	Ll	25	GLN
59	Lq	49	PHE
59	Lq	92	LYS
59	Lq	98	LYS
59	Lq	113	SER
59	Lq	133	LYS
59	Lq	189	TYR
59	Lq	206	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
4	CB	161	ASN
7	CE	525	HIS
10	CH	73	GLN
15	CM	242	ASN
16	CN	106	ASN
20	CR	220	GLN
25	CW	623	ASN
33	LH	118	ASN
35	LL	66	ASN
41	LR	91	GLN
43	LT	146	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2770/3341 (82%)	564 (20%)	21 (0%)
2	C2	254/319 (79%)	54 (21%)	1 (0%)
All	All	3024/3660 (82%)	618 (20%)	22 (0%)

All (618) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	26	A
1	C1	40	A

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Mol	Chain	Res	Type
1	C1	43	A
1	C1	49	A
1	C1	59	G
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	73	A
1	C1	92	G
1	C1	93	C
1	C1	94	G
1	C1	96	G
1	C1	105	C
1	C1	109	A
1	C1	110	G
1	C1	111	C
1	C1	116	A
1	C1	122	A
1	C1	128	G
1	C1	129	C
1	C1	131	U
1	C1	132	C
1	C1	133	G
1	C1	134	G
1	C1	135	C
1	C1	136	C
1	C1	138	G
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	162	U
1	C1	163	U
1	C1	177	U
1	C1	183	U
1	C1	186	C
1	C1	193	C
1	C1	203	C
1	C1	206	A
1	C1	211	G
1	C1	212	A
1	C1	240	U
1	C1	242	U
1	C1	244	U

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Mol	Chain	Res	Type
1	C1	253	U
1	C1	258	C
1	C1	261	G
1	C1	275	G
1	C1	276	A
1	C1	277	A
1	C1	287	A
1	C1	290	U
1	C1	299	A
1	C1	300	A
1	C1	302	U
1	C1	309	A
1	C1	310	A
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	331	C
1	C1	342	C
1	C1	344	A
1	C1	368	G
1	C1	387	A
1	C1	390	U
1	C1	391	A
1	C1	393	C
1	C1	394	A
1	C1	395	C
1	C1	412	G
1	C1	413	G
1	C1	414	A
1	C1	421	U
1	C1	433	U
1	C1	434	G
1	C1	440	G
1	C1	441	G
1	C1	444	G
1	C1	445	A
1	C1	446	U
1	C1	453	G
1	C1	454	U
1	C1	455	G
1	C1	457	U
1	C1	458	C

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Mol	Chain	Res	Type
1	C1	459	U
1	C1	467	G
1	C1	470	C
1	C1	471	U
1	C1	484	G
1	C1	485	G
1	C1	493	C
1	C1	508	G
1	C1	509	A
1	C1	511	A
1	C1	513	A
1	C1	523	A
1	C1	526	G
1	C1	530	C
1	C1	534	U
1	C1	535	C
1	C1	537	G
1	C1	546	A
1	C1	547	U
1	C1	548	A
1	C1	559	U
1	C1	560	A
1	C1	579	A
1	C1	582	A
1	C1	589	U
1	C1	590	C
1	C1	592	G
1	C1	593	C
1	C1	594	A
1	C1	597	G
1	C1	598	A
1	C1	607	U
1	C1	608	A
1	C1	609	A
1	C1	623	C
1	C1	633	A
1	C1	649	U
1	C1	663	G
1	C1	664	A
1	C1	668	U
1	C1	670	U
1	C1	674	U

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Mol	Chain	Res	Type
1	C1	712	A
1	C1	718	U
1	C1	719	C
1	C1	723	G
1	C1	731	G
1	C1	739	C
1	C1	742	A
1	C1	744	G
1	C1	748	U
1	C1	749	C
1	C1	751	G
1	C1	752	A
1	C1	757	U
1	C1	758	U
1	C1	761	A
1	C1	762	G
1	C1	765	G
1	C1	766	G
1	C1	767	A
1	C1	782	A
1	C1	787	A
1	C1	798	A
1	C1	799	C
1	C1	800	U
1	C1	801	A
1	C1	803	G
1	C1	807	G
1	C1	816	G
1	C1	817	A
1	C1	818	A
1	C1	828	A
1	C1	835	G
1	C1	836	U
1	C1	841	G
1	C1	843	U
1	C1	846	C
1	C1	856	G
1	C1	858	C
1	C1	876	A
1	C1	877	A
1	C1	878	U
1	C1	887	G

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Mol	Chain	Res	Type
1	C1	889	G
1	C1	896	A
1	C1	898	A
1	C1	925	A
1	C1	932	A
1	C1	934	G
1	C1	940	C
1	C1	941	U
1	C1	942	C
1	C1	958	A
1	C1	959	C
1	C1	960	C
1	C1	961	U
1	C1	974	G
1	C1	975	G
1	C1	976	U
1	C1	982	G
1	C1	983	A
1	C1	1031	C
1	C1	1033	U
1	C1	1039	A
1	C1	1045	G
1	C1	1046	A
1	C1	1047	A
1	C1	1048	G
1	C1	1049	C
1	C1	1050	C
1	C1	1054	G
1	C1	1063	C
1	C1	1064	U
1	C1	1074	C
1	C1	1075	A
1	C1	1077	U
1	C1	1078	C
1	C1	1079	G
1	C1	1080	A
1	C1	1085	A
1	C1	1086	U
1	C1	1095	G
1	C1	1097	G
1	C1	1098	G
1	C1	1114	C

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Mol	Chain	Res	Type
1	C1	1126	U
1	C1	1134	G
1	C1	1135	A
1	C1	1141	A
1	C1	1157	C
1	C1	1158	C
1	C1	1160	G
1	C1	1164	G
1	C1	1174	C
1	C1	1175	A
1	C1	1178	C
1	C1	1180	C
1	C1	1181	C
1	C1	1186	A
1	C1	1187	A
1	C1	1189	G
1	C1	1190	C
1	C1	1191	G
1	C1	1203	U
1	C1	1204	G
1	C1	1208	G
1	C1	1218	G
1	C1	1227	A
1	C1	1228	G
1	C1	1240	U
1	C1	1245	A
1	C1	1247	U
1	C1	1254	C
1	C1	1268	A
1	C1	1271	G
1	C1	1272	U
1	C1	1277	G
1	C1	1286	A
1	C1	1287	U
1	C1	1289	G
1	C1	1291	U
1	C1	1295	G
1	C1	1312	A
1	C1	1313	U
1	C1	1327	G
1	C1	1330	A
1	C1	1331	G

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Mol	Chain	Res	Type
1	C1	1332	A
1	C1	1333	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G
1	C1	1337	A
1	C1	1338	U
1	C1	1368	A
1	C1	1374	G
1	C1	1381	A
1	C1	1400	A
1	C1	1401	A
1	C1	1416	G
1	C1	1419	C
1	C1	1434	A
1	C1	1437	U
1	C1	1438	A
1	C1	1463	A
1	C1	1465	G
1	C1	1470	G
1	C1	1478	C
1	C1	1490	C
1	C1	1510	G
1	C1	1521	A
1	C1	1535	U
1	C1	1537	U
1	C1	1539	A
1	C1	1541	A
1	C1	1542	G
1	C1	1543	G
1	C1	1548	C
1	C1	1549	U
1	C1	1550	C
1	C1	1553	G
1	C1	1555	C
1	C1	1559	U
1	C1	1560	G
1	C1	1561	U
1	C1	1562	G
1	C1	1566	A
1	C1	1568	A
1	C1	1572	A

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Mol	Chain	Res	Type
1	C1	1584	A
1	C1	1598	A
1	C1	1599	U
1	C1	1607	U
1	C1	1608	U
1	C1	1609	G
1	C1	1610	C
1	C1	1618	C
1	C1	1621	A
1	C1	1622	A
1	C1	1623	C
1	C1	1624	U
1	C1	1637	G
1	C1	1662	C
1	C1	1693	A
1	C1	1695	A
1	C1	1696	C
1	C1	1722	G
1	C1	1729	A
1	C1	1730	G
1	C1	1739	A
1	C1	1741	U
1	C1	1744	U
1	C1	1745	G
1	C1	1746	U
1	C1	1750	G
1	C1	1759	G
1	C1	1774	U
1	C1	1775	G
1	C1	1776	A
1	C1	1794	U
1	C1	1795	A
1	C1	1796	A
1	C1	1797	U
1	C1	1798	U
1	C1	1799	C
1	C1	1800	U
1	C1	1819	U
1	C1	1820	A
1	C1	1821	A
1	C1	1825	C
1	C1	1828	C

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Mol	Chain	Res	Type
1	C1	1829	A
1	C1	1842	G
1	C1	1843	A
1	C1	1845	C
1	C1	1846	A
1	C1	1857	G
1	C1	1858	A
1	C1	1859	U
1	C1	1881	G
1	C1	1885	G
1	C1	1886	C
1	C1	1897	C
1	C1	1900	A
1	C1	1901	A
1	C1	1904	U
1	C1	1911	A
1	C1	1920	C
1	C1	1924	A
1	C1	1925	A
1	C1	1927	G
1	C1	1928	G
1	C1	1932	G
1	C1	1942	G
1	C1	1944	U
1	C1	1950	C
1	C1	1952	G
1	C1	1961	G
1	C1	1970	G
1	C1	1971	G
1	C1	1981	G
1	C1	1987	C
1	C1	1994	G
1	C1	1997	G
1	C1	2004	G
1	C1	2006	A
1	C1	2010	G
1	C1	2020	C
1	C1	2021	C
1	C1	2023	U
1	C1	2024	U
1	C1	2043	G
1	C1	2044	G

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Mol	Chain	Res	Type
1	C1	2048	G
1	C1	2049	C
1	C1	2054	A
1	C1	2064	U
1	C1	2065	U
1	C1	2066	A
1	C1	2075	A
1	C1	2297	G
1	C1	2298	U
1	C1	2325	A
1	C1	2335	A
1	C1	2336	C
1	C1	2338	G
1	C1	2339	G
1	C1	2342	U
1	C1	2347	A
1	C1	2350	U
1	C1	2356	G
1	C1	2359	A
1	C1	2361	A
1	C1	2362	G
1	C1	2364	A
1	C1	2384	C
1	C1	2396	U
1	C1	2397	G
1	C1	2407	A
1	C1	2409	A
1	C1	2414	G
1	C1	2421	A
1	C1	2422	U
1	C1	2423	A
1	C1	2424	G
1	C1	2425	G
1	C1	2429	G
1	C1	2430	A
1	C1	2431	G
1	C1	2434	U
1	C1	2435	C
1	C1	2436	G
1	C1	2441	C
1	C1	2449	U
1	C1	2453	A

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Mol	Chain	Res	Type
1	C1	2455	U
1	C1	2456	A
1	C1	2464	U
1	C1	2465	G
1	C1	2467	U
1	C1	2484	G
1	C1	2547	G
1	C1	2551	A
1	C1	2560	G
1	C1	2564	G
1	C1	2723	C
1	C1	2730	C
1	C1	2740	U
1	C1	2749	G
1	C1	2759	A
1	C1	2760	A
1	C1	2761	A
1	C1	2777	A
1	C1	2778	A
1	C1	2782	G
1	C1	2800	U
1	C1	2801	U
1	C1	2802	C
1	C1	2803	A
1	C1	2804	U
1	C1	2815	C
1	C1	2816	U
1	C1	2832	G
1	C1	2833	U
1	C1	2845	A
1	C1	2847	C
1	C1	2856	G
1	C1	2857	C
1	C1	2862	U
1	C1	2869	A
1	C1	2874	U
1	C1	2879	U
1	C1	2881	U
1	C1	2883	C
1	C1	2888	A
1	C1	2893	U
1	C1	2894	A

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Mol	Chain	Res	Type
1	C1	2903	G
1	C1	2906	C
1	C1	2908	G
1	C1	2917	C
1	C1	2929	A
1	C1	2936	U
1	C1	2942	C
1	C1	2943	C
1	C1	2948	G
1	C1	2950	U
1	C1	2955	U
1	C1	2956	C
1	C1	2957	G
1	C1	2960	G
1	C1	2969	A
1	C1	3013	U
1	C1	3016	G
1	C1	3035	G
1	C1	3043	A
1	C1	3049	C
1	C1	3050	C
1	C1	3079	A
1	C1	3084	A
1	C1	3086	A
1	C1	3087	A
1	C1	3088	U
1	C1	3098	A
1	C1	3099	A
1	C1	3100	C
1	C1	3101	G
1	C1	3110	C
1	C1	3111	U
1	C1	3112	A
1	C1	3113	C
1	C1	3118	A
1	C1	3121	U
1	C1	3122	U
1	C1	3125	A
1	C1	3126	G
1	C1	3127	A
1	C1	3130	U
1	C1	3131	A

Continued on next page...

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Mol	Chain	Res	Type
1	C1	3132	U
1	C1	3134	A
1	C1	3140	G
1	C1	3141	G
1	C1	3147	G
1	C1	3153	U
1	C1	3154	A
1	C1	3161	C
1	C1	3162	A
1	C1	3163	G
1	C1	3164	G
1	C1	3171	C
1	C1	3181	C
1	C1	3184	G
1	C1	3185	A
1	C1	3187	G
1	C1	3188	U
1	C1	3189	G
1	C1	3199	A
1	C1	3200	A
1	C1	3205	C
1	C1	3206	G
1	C1	3207	U
1	C1	3210	U
1	C1	3213	A
1	C1	3215	U
1	C1	3217	U
1	C1	3219	G
1	C1	3226	G
1	C1	3227	C
1	C1	3228	G
1	C1	3229	G
1	C1	3230	G
1	C1	3244	C
1	C1	3253	U
1	C1	3256	A
1	C1	3257	U
1	C1	3259	U
1	C1	3260	G
1	C1	3274	U
1	C1	3280	G
1	C1	3281	U

Continued on next page...

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Mol	Chain	Res	Type
1	C1	3282	A
1	C1	3287	A
1	C1	3291	U
1	C1	3293	G
1	C1	3295	U
1	C1	3298	U
1	C1	3303	U
1	C1	3309	G
1	C1	3318	C
1	C1	3322	C
1	C1	3323	C
1	C1	3324	U
1	C1	3325	U
1	C1	3330	U
1	C1	3331	A
1	C1	3333	A
2	C2	34	U
2	C2	35	C
2	C2	38	U
2	C2	51	G
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	79	A
2	C2	81	U
2	C2	82	U
2	C2	83	C
2	C2	84	C
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	103	G
2	C2	104	A
2	C2	106	C
2	C2	110	C
2	C2	111	A
2	C2	112	U
2	C2	113	U
2	C2	120	G
2	C2	125	U
2	C2	151	C
2	C2	152	G

Continued on next page...

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Mol	Chain	Res	Type
2	C2	158	U
2	C2	163	C
2	C2	165	U
2	C2	166	C
2	C2	167	A
2	C2	170	C
2	C2	173	U
2	C2	181	U
2	C2	189	A
2	C2	195	G
2	C2	196	G
2	C2	203	G
2	C2	205	G
2	C2	212	G
2	C2	213	A
2	C2	214	A
2	C2	215	A
2	C2	219	A
2	C2	221	U
2	C2	222	G
2	C2	223	G
2	C2	225	G
2	C2	289	G
2	C2	291	G
2	C2	292	C
2	C2	294	A
2	C2	295	G
2	C2	300	A

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	150	G
1	C1	835	G
1	C1	886	U
1	C1	897	G
1	C1	940	C
1	C1	960	C
1	C1	1046	A
1	C1	1063	C
1	C1	1134	G
1	C1	1185	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C1	1924	A
1	C1	1949	G
1	C1	2355	G
1	C1	2831	U
1	C1	3078	U
1	C1	3131	A
1	C1	3162	A
1	C1	3204	G
1	C1	3209	U
1	C1	3229	G
1	C1	3297	U
2	C2	102	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
62	ADP	CW	1001	63	24,29,29	0.69	0	29,45,45	0.78	1 (3%)
60	GTP	CH	701	-	26,34,34	1.18	1 (3%)	32,54,54	1.60	7 (21%)

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
62	ADP	CW	1001	63	-	3/12/32/32	0/3/3/3
60	GTP	CH	701	-	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CH	701	GTP	C5-C6	-4.16	1.39	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CH	701	GTP	PB-O3B-PG	-3.63	120.38	132.83
60	CH	701	GTP	C5-C6-N1	3.20	119.61	113.95
60	CH	701	GTP	C3'-C2'-C1'	3.00	105.49	100.98
60	CH	701	GTP	C8-N7-C5	2.98	108.66	102.99
60	CH	701	GTP	C2-N1-C6	-2.85	119.85	125.10
60	CH	701	GTP	PA-O3A-PB	-2.84	123.07	132.83
62	CW	1001	ADP	C5-C6-N6	2.26	123.79	120.35
60	CH	701	GTP	O6-C6-C5	-2.15	120.18	124.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

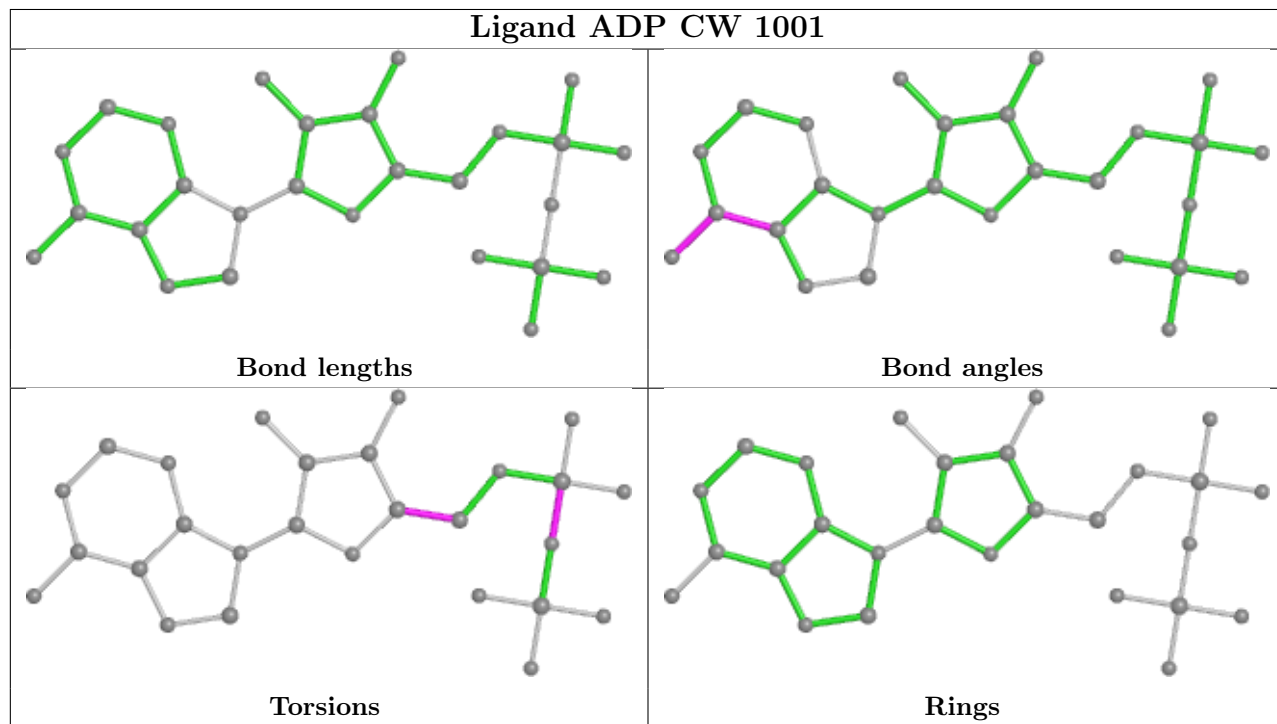
Mol	Chain	Res	Type	Atoms
62	CW	1001	ADP	C3'-C4'-C5'-O5'
62	CW	1001	ADP	O4'-C4'-C5'-O5'
60	CH	701	GTP	PG-O3B-PB-O2B
62	CW	1001	ADP	PB-O3A-PA-O1A
60	CH	701	GTP	PA-O3A-PB-O3B
60	CH	701	GTP	O4'-C4'-C5'-O5'
60	CH	701	GTP	PA-O3A-PB-O1B

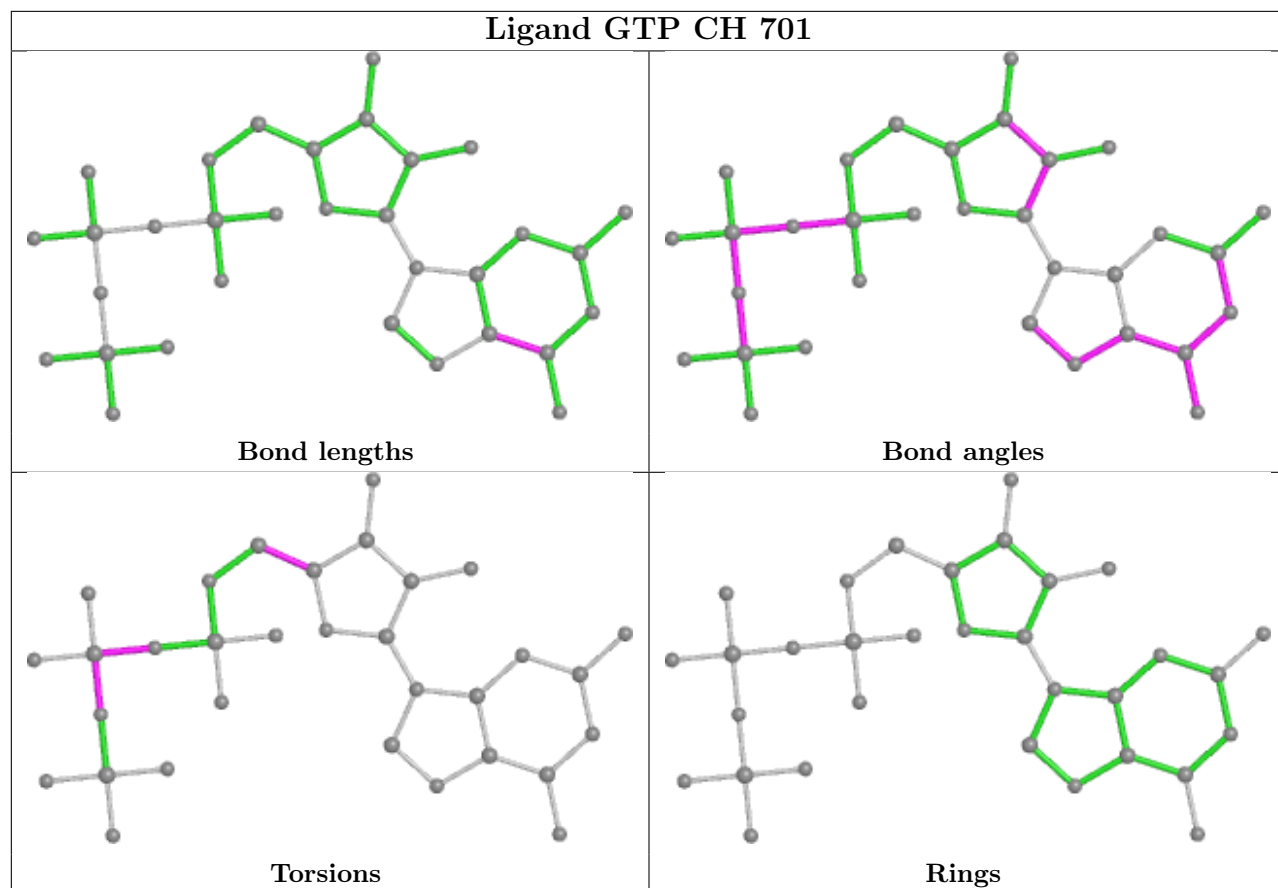
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

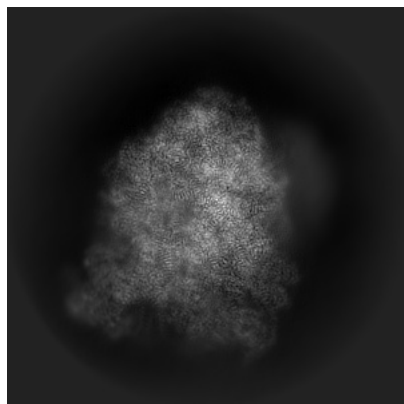
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35289. These allow visual inspection of the internal detail of the map and identification of artifacts.

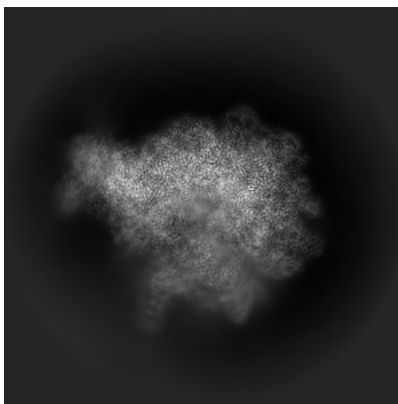
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

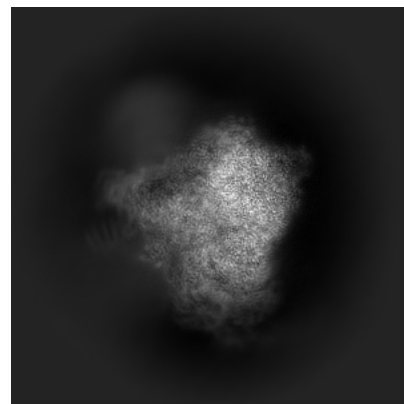
6.1.1 Primary map



X

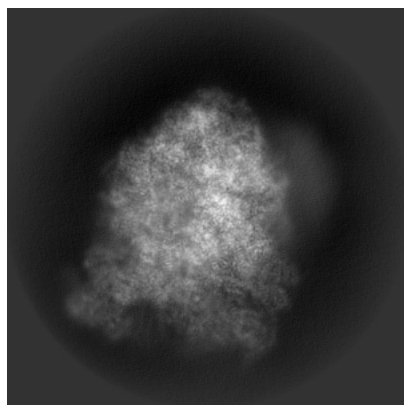


Y

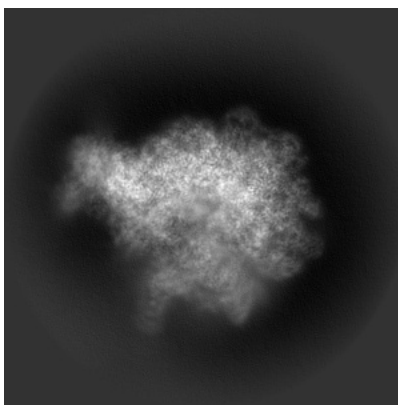


Z

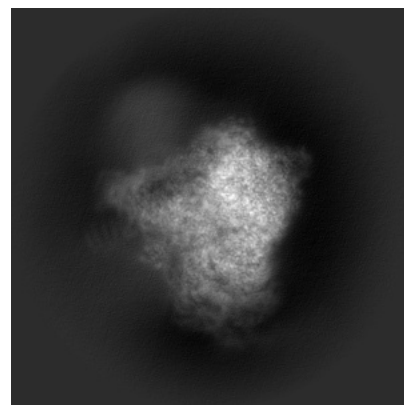
6.1.2 Raw map



X



Y

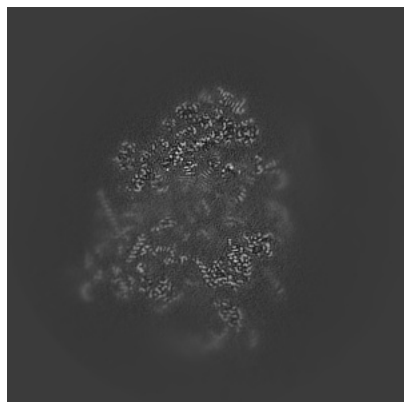


Z

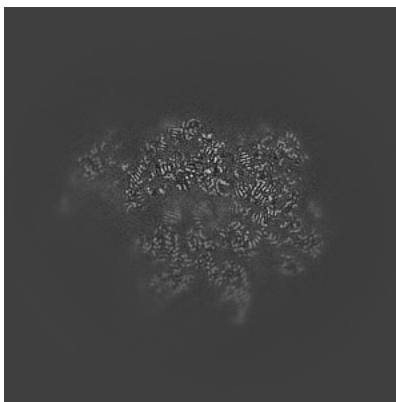
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

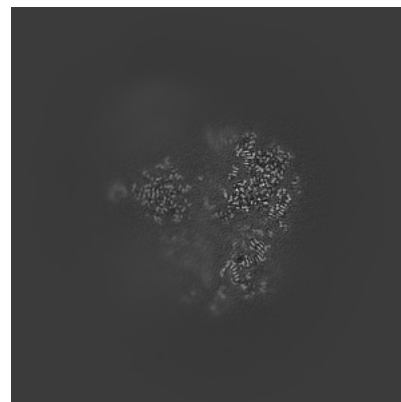
6.2.1 Primary map



X Index: 210

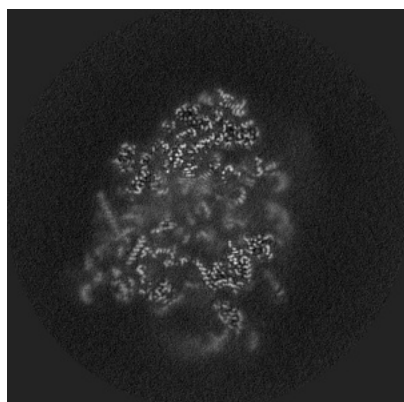


Y Index: 210

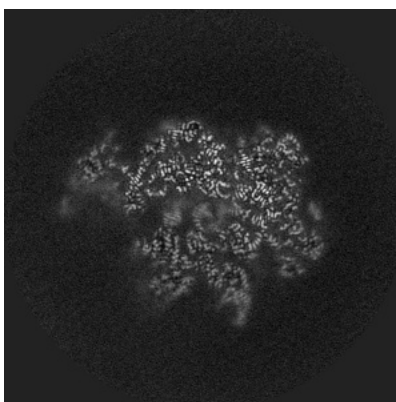


Z Index: 210

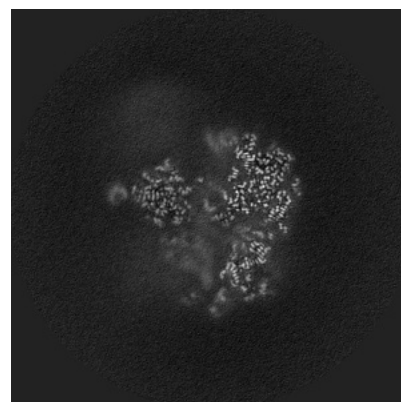
6.2.2 Raw map



X Index: 210



Y Index: 210

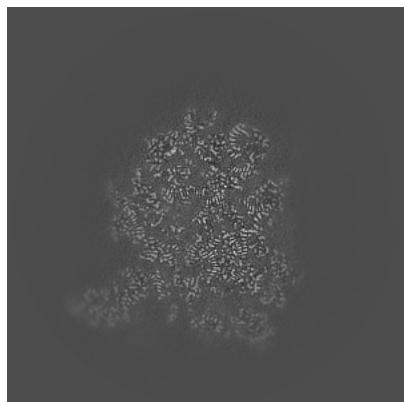


Z Index: 210

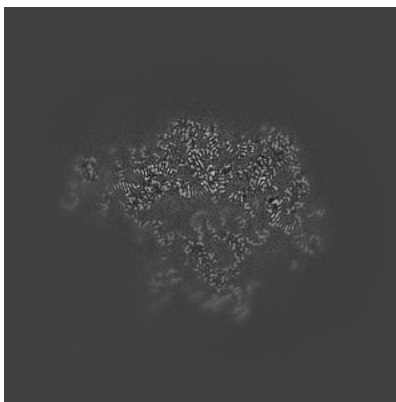
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

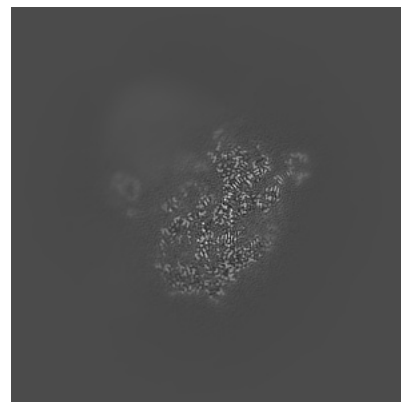
6.3.1 Primary map



X Index: 246

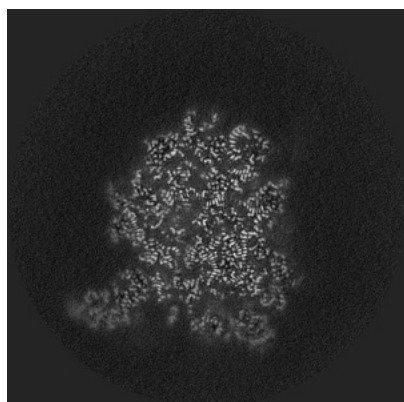


Y Index: 219

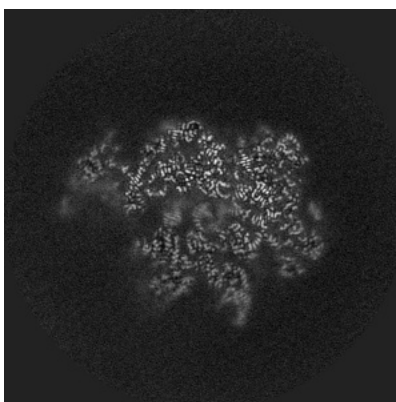


Z Index: 261

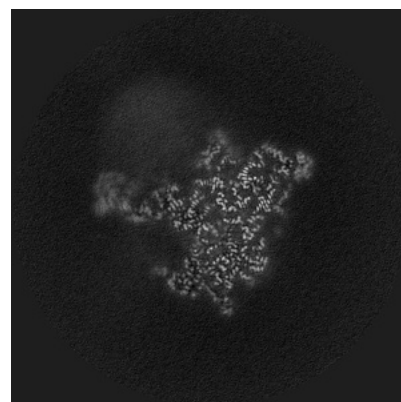
6.3.2 Raw map



X Index: 246



Y Index: 210

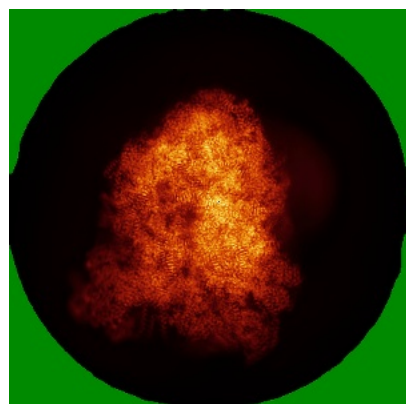


Z Index: 249

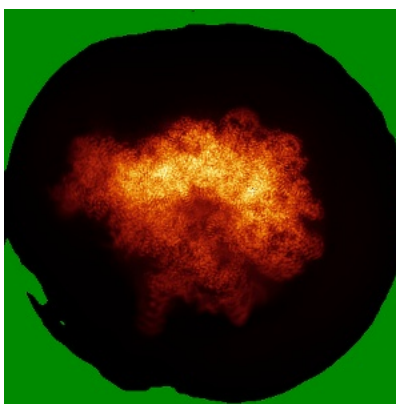
The images above show the largest variance slices of the map in three orthogonal directions.

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

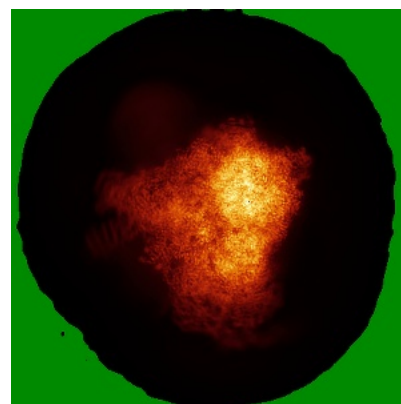
6.4.1 Primary map



X

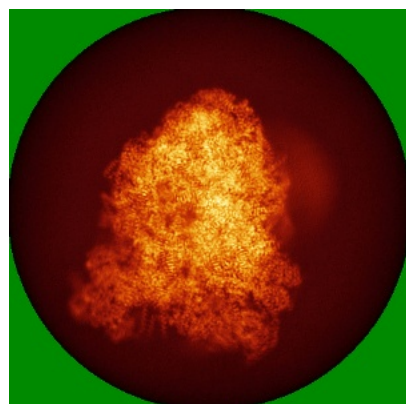


Y

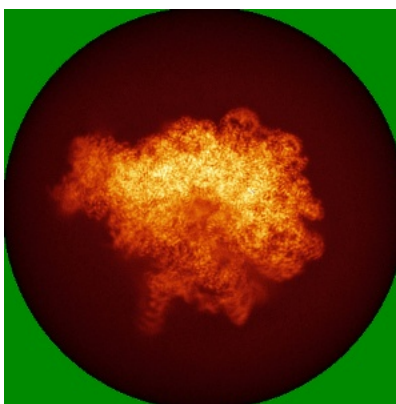


Z

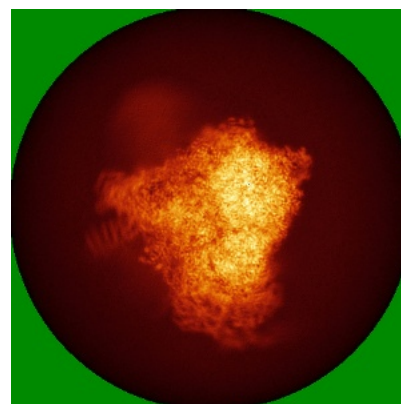
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



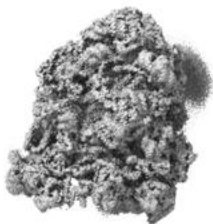
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

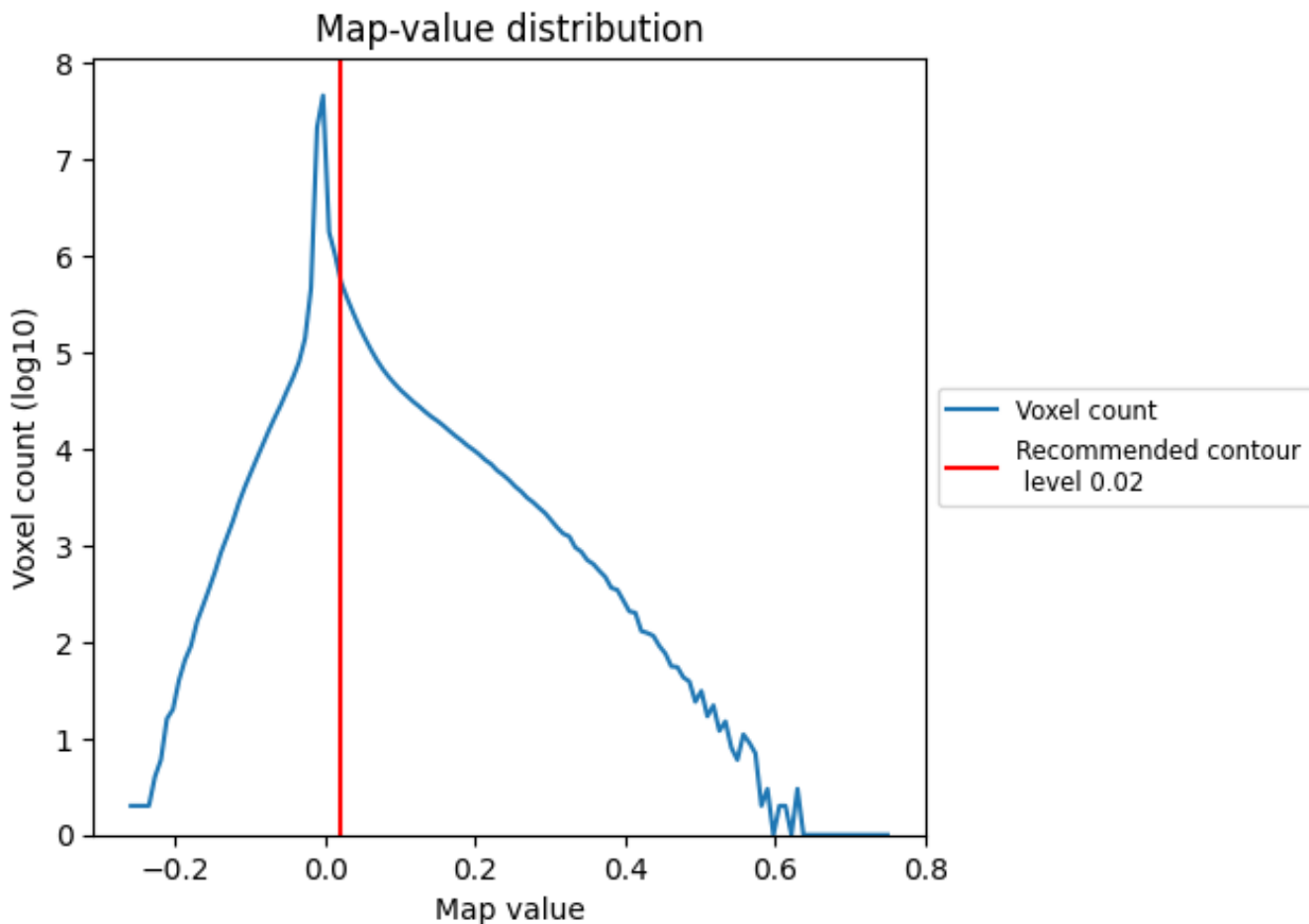
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

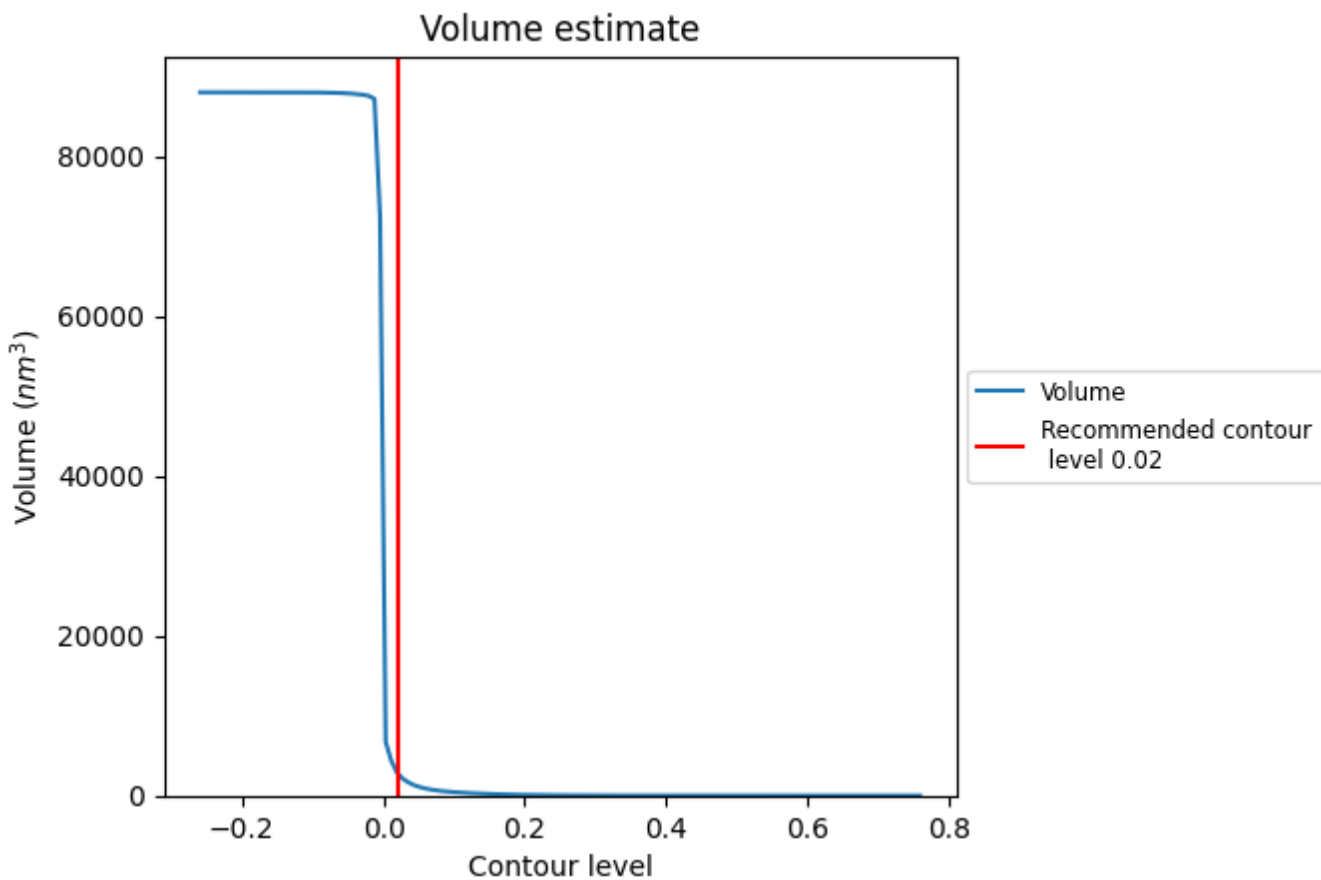
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

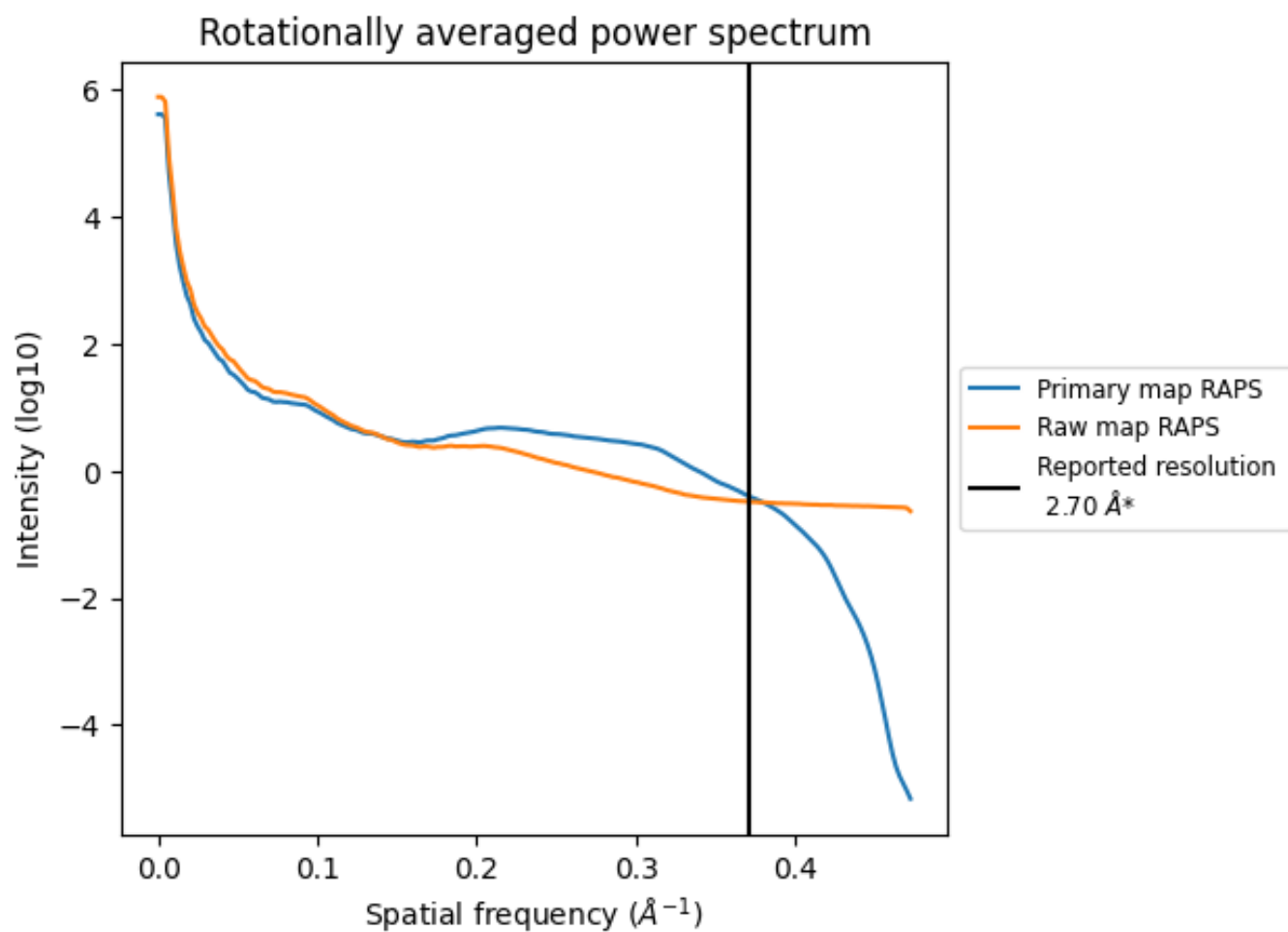
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2816 nm³; this corresponds to an approximate mass of 2544 kDa.

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

7.3 Rotationally averaged power spectrum i

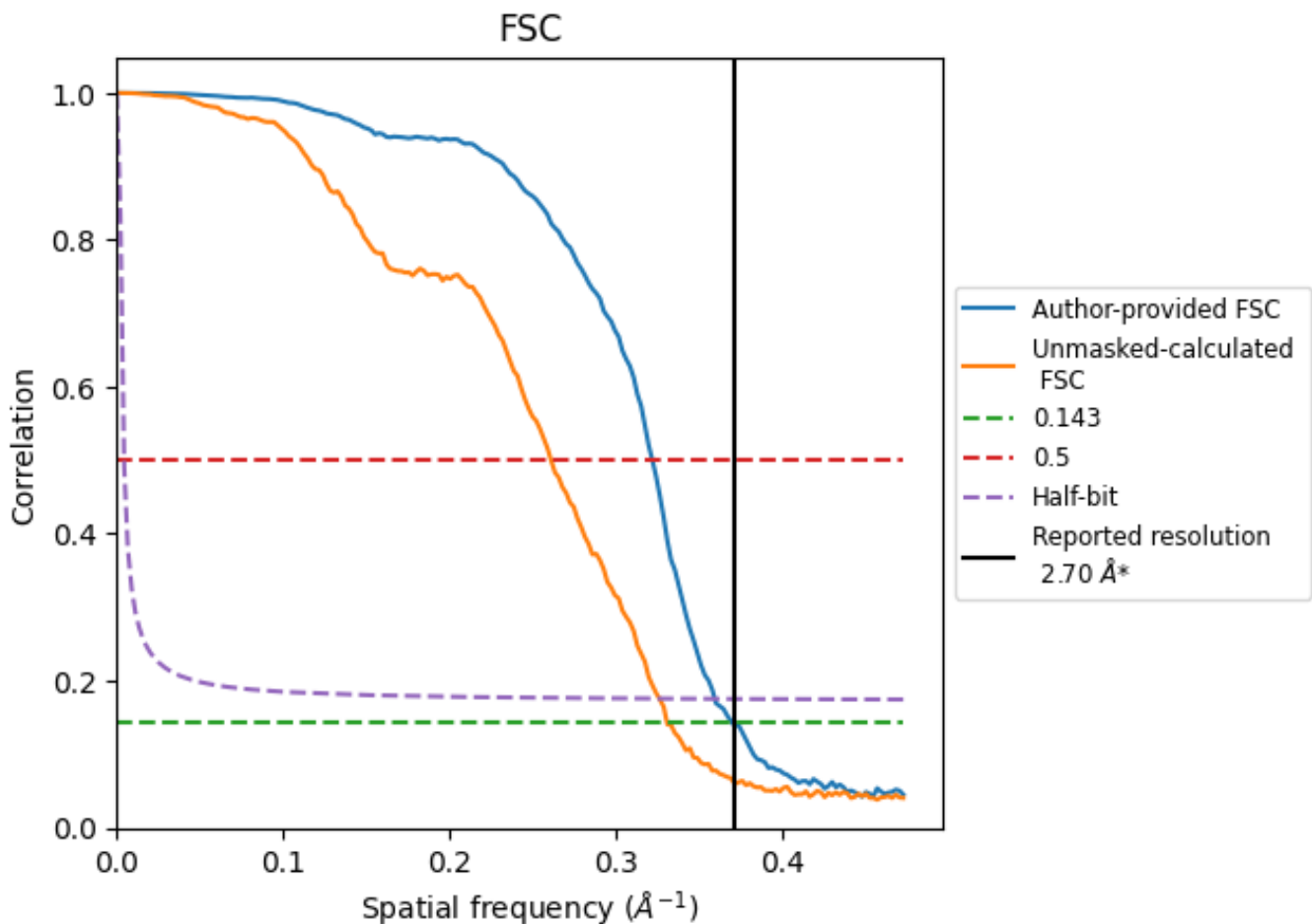


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

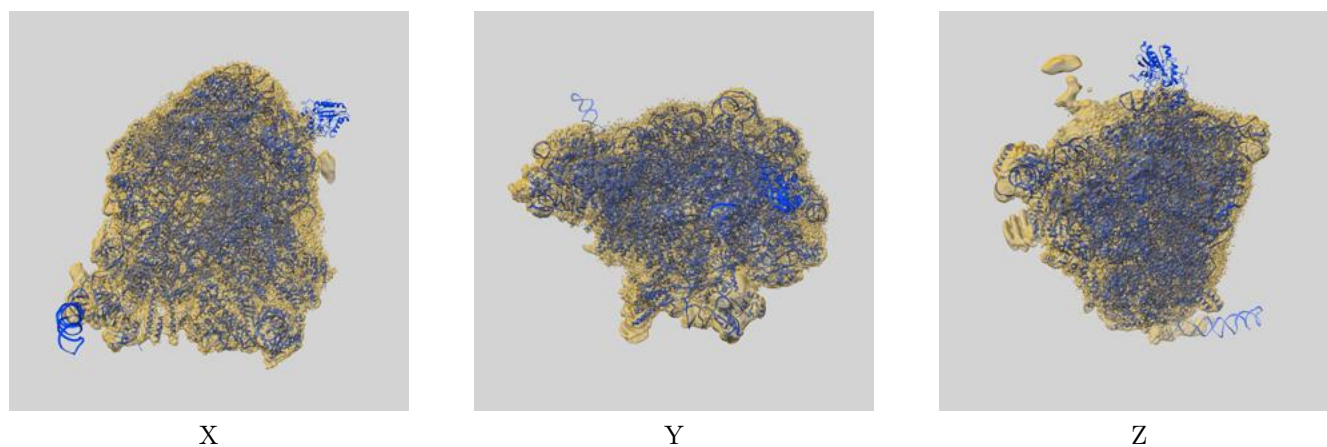
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.11	2.79
Unmasked-calculated*	3.03	3.84	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.03 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

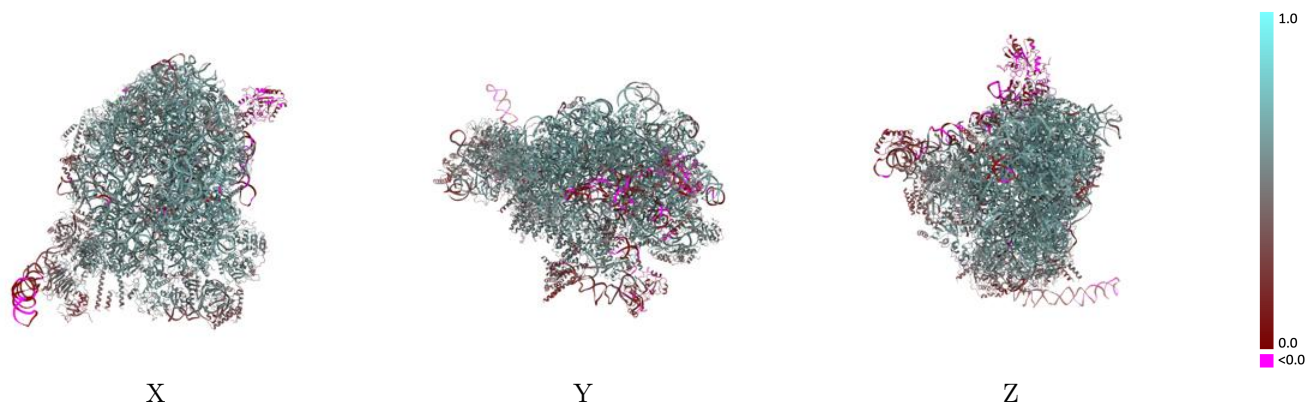
This section contains information regarding the fit between EMDB map EMD-35289 and PDB model 8I9Z. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



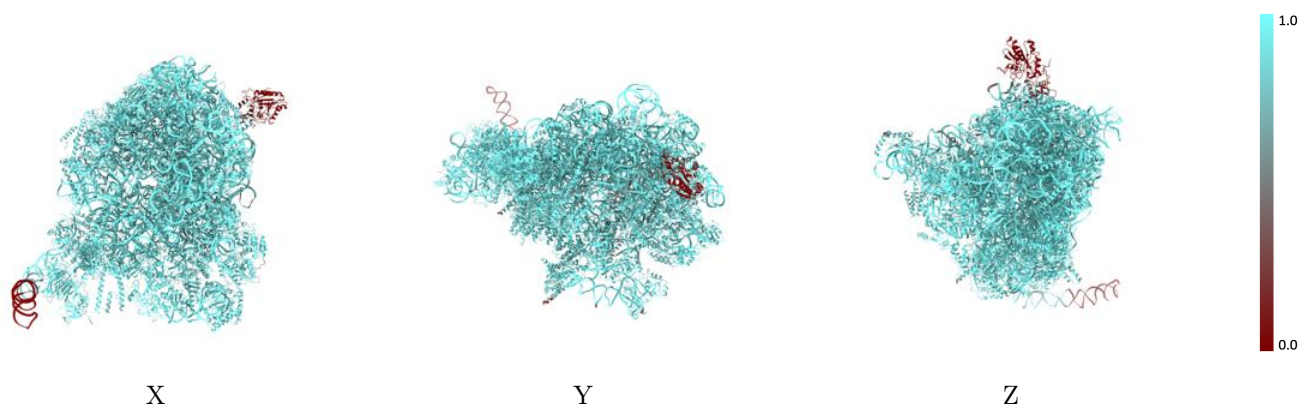
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



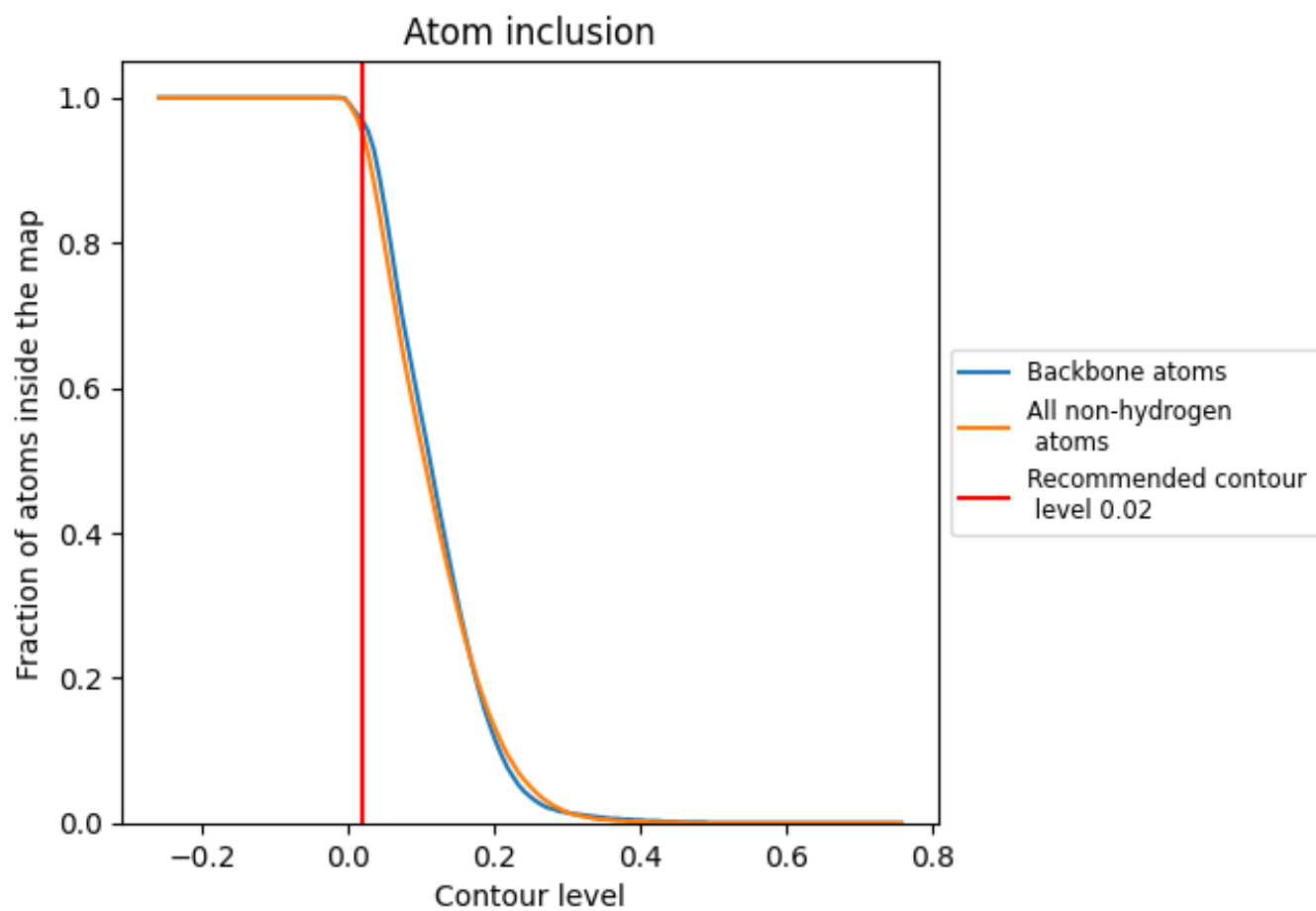
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9510	 0.5240
C1	 0.9610	 0.5300
C2	 0.9790	 0.5420
CA	 0.9810	 0.5940
CB	 0.9340	 0.4530
CC	 0.9670	 0.5520
CD	 0.9330	 0.3950
CE	 0.9450	 0.5220
CF	 0.9540	 0.5110
CG	 0.9690	 0.5750
CH	 0.9640	 0.5440
CI	 0.9280	 0.4660
CJ	 0.9510	 0.5260
CK	 0.9660	 0.5600
CL	 0.3380	 0.2040
CM	 0.9450	 0.4760
CN	 0.9630	 0.5610
CO	 0.9540	 0.5600
CP	 0.9720	 0.5530
CQ	 0.9490	 0.5230
CR	 0.9650	 0.5790
CS	 0.9240	 0.4080
CT	 0.9660	 0.5230
CU	 0.9650	 0.5490
CV	 0.9790	 0.6210
CW	 0.9330	 0.3830
CX	 0.9240	 0.4990
CY	 0.9060	 0.3620
Cz	 0.9060	 0.3840
LB	 0.9800	 0.6080
LC	 0.9790	 0.6320
LE	 0.9670	 0.5790
LF	 0.9710	 0.6050
LG	 0.9760	 0.6100
LH	 0.9730	 0.5960



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Chain	Atom inclusion	Q-score
LK	 0.9390	 0.4380
LL	 0.9850	 0.6300
LM	 0.9760	 0.6110
LN	 0.9980	 0.6700
LO	 0.9860	 0.6440
LP	 0.9730	 0.5830
LQ	 0.9800	 0.5950
LR	 0.9520	 0.5090
LS	 0.9830	 0.6110
LT	 0.9320	 0.3910
LU	 0.9610	 0.5410
LV	 0.9820	 0.5820
LX	 0.9670	 0.5730
LY	 0.9720	 0.6020
LZ	 0.9750	 0.5790
Lc	 0.9620	 0.5250
Ld	 0.9620	 0.6020
Le	 0.9830	 0.6420
Lf	 0.9870	 0.6500
Lg	 0.9610	 0.5850
Lh	 0.9580	 0.5680
Li	 0.9570	 0.5740
Lj	 0.9880	 0.6440
Lk	 0.9420	 0.5120
Ll	 0.9810	 0.5260
Lq	 0.8570	 0.1750