



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 05:04 PM UTC

PDB ID : 7NHN / pdb_00007nhn
EMDB ID : EMD-12334
Title : VgaL, an antibiotic resistance ABCF, in complex with 70S ribosome from *Listeria monocytogenes*
Authors : Crowe-McAuliffe, C.; Turnbull, K.J.; Hauryliuk, V.; Wilson, D.N.
Deposited on : 2021-02-10
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

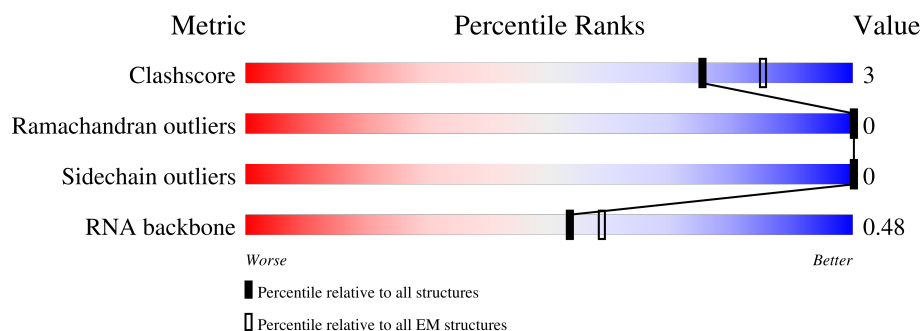
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



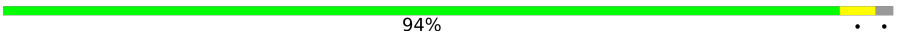
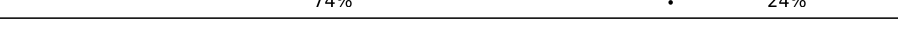
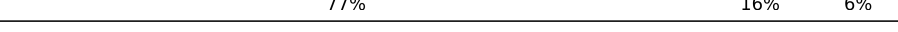
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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

Mol	Chain	Length	Quality of chain
1	0	567	70% (green), 11% (yellow), 19% (grey)
2	D	77	69% (green), 27% (yellow), . (grey)
3	b	14	43% (green), 14% (yellow), 43% (grey)
4	A	2928	71% (green), 25% (yellow), . . (grey)
5	a	1542	70% (green), 26% (yellow), . . (grey)
6	G	277	90% (green), 8% (yellow), . (grey)
7	H	209	86% (green), 12% (yellow), . (grey)

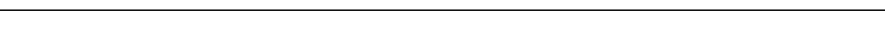
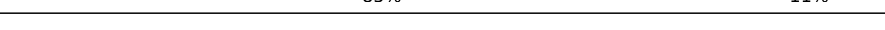
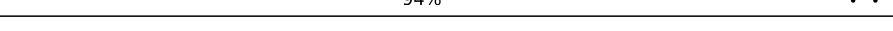
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Mol	Chain	Length	Quality of chain
8	I	207	 94% . .
9	J	179	 84% 13% .
10	K	178	 83% 10% 7%
11	M	145	 86% 12% .
12	N	122	 88% 12%
13	O	146	 92% 7% .
14	P	144	 84% 8% 8%
15	Q	135	 79% 11% 10%
16	R	119	 90% 9% .
17	S	114	 89% 10% .
18	T	119	 90% 8% .
19	U	102	 91% 8% .
20	V	118	 87% 6% 7%
21	W	94	 86% 10% .
22	X	103	 82% 11% 8%
23	Z	96	 74% . 24%
24	1	62	 77% 16% 6%
25	2	63	 83% 11% 6%
26	3	59	 80% 15% 5%
27	5	57	 74% 19% 7%
28	6	49	 90% 6% .
29	7	44	 91% 5% 5%
30	8	66	 77% 18% 5%
31	9	37	 73% 24% .
32	B	114	 71% 26% .

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Mol	Chain	Length	Quality of chain
33	c	249	 76% 10% 15%
34	d	218	 87% 6% 6%
35	e	200	 87% 12%
36	f	167	 90% 7% .
37	g	97	 91% 5% .
38	h	156	 80% 10% 10%
39	i	132	 77% 22% .
40	j	130	 88% 9% .
41	k	102	 84% 10% 6%
42	l	129	 83% 5% 12%
43	m	137	 85% 13% .
44	n	121	 82% 12% 6%
45	o	61	 82% 16% .
46	p	89	 85% 11% .
47	q	90	 94% . .
48	r	87	 83% 9% 8%
49	s	79	 68% 10% 22%
50	t	92	 82% 7% 12%
51	u	84	 90% 5% 5%
52	4	81	 85% 12% .

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 144375 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Lmo0919 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	461	Total	C	N	O	S	0	0
			3647	2298	650	689	10		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	104	GLN	GLU	engineered mutation	UNP Q8Y8I3
0	408	GLN	GLU	engineered mutation	UNP Q8Y8I3
0	524	GLY	-	expression tag	UNP Q8Y8I3
0	525	GLY	-	expression tag	UNP Q8Y8I3
0	526	HIS	-	expression tag	UNP Q8Y8I3
0	527	HIS	-	expression tag	UNP Q8Y8I3
0	528	HIS	-	expression tag	UNP Q8Y8I3
0	529	HIS	-	expression tag	UNP Q8Y8I3
0	530	HIS	-	expression tag	UNP Q8Y8I3
0	531	HIS	-	expression tag	UNP Q8Y8I3
0	532	ALA	-	expression tag	UNP Q8Y8I3
0	533	LYS	-	expression tag	UNP Q8Y8I3
0	534	GLY	-	expression tag	UNP Q8Y8I3
0	535	GLY	-	expression tag	UNP Q8Y8I3
0	536	GLU	-	expression tag	UNP Q8Y8I3
0	537	ASN	-	expression tag	UNP Q8Y8I3
0	538	LEU	-	expression tag	UNP Q8Y8I3
0	539	TYR	-	expression tag	UNP Q8Y8I3
0	540	PHE	-	expression tag	UNP Q8Y8I3
0	541	GLN	-	expression tag	UNP Q8Y8I3
0	542	GLY	-	expression tag	UNP Q8Y8I3
0	543	VAL	-	expression tag	UNP Q8Y8I3
0	544	ALA	-	expression tag	UNP Q8Y8I3
0	545	ASP	-	expression tag	UNP Q8Y8I3
0	546	TYR	-	expression tag	UNP Q8Y8I3
0	547	LYS	-	expression tag	UNP Q8Y8I3
0	548	ASP	-	expression tag	UNP Q8Y8I3
0	549	HIS	-	expression tag	UNP Q8Y8I3

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Chain	Residue	Modelled	Actual	Comment	Reference
0	550	ASP	-	expression tag	UNP Q8Y8I3
0	551	GLY	-	expression tag	UNP Q8Y8I3
0	552	ASP	-	expression tag	UNP Q8Y8I3
0	553	TYR	-	expression tag	UNP Q8Y8I3
0	554	LYS	-	expression tag	UNP Q8Y8I3
0	555	ASP	-	expression tag	UNP Q8Y8I3
0	556	HIS	-	expression tag	UNP Q8Y8I3
0	557	ASP	-	expression tag	UNP Q8Y8I3
0	558	ILE	-	expression tag	UNP Q8Y8I3
0	559	ASP	-	expression tag	UNP Q8Y8I3
0	560	TYR	-	expression tag	UNP Q8Y8I3
0	561	LYS	-	expression tag	UNP Q8Y8I3
0	562	ASP	-	expression tag	UNP Q8Y8I3
0	563	ASP	-	expression tag	UNP Q8Y8I3
0	564	ASP	-	expression tag	UNP Q8Y8I3
0	565	ASP	-	expression tag	UNP Q8Y8I3
0	566	LYS	-	expression tag	UNP Q8Y8I3
0	567	GLY	-	expression tag	UNP Q8Y8I3

- Molecule 2 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	74	Total	C	N	O	P	0	0
			1580	704	284	518	74		

- Molecule 3 is a RNA chain called RNA (5'-R(P*GP*AP*GP*GP*UP*NP*NP*NP*NP*NP*AP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	8	Total	C	N	O	P	0	0
			176	78	34	56	8		

- Molecule 4 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2908	Total	C	N	O	P	0	0
			62459	27874	11545	20132	2908		

- Molecule 5 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	1513	Total	C	N	O	P	0	0
			32445	14473	5939	10520	1513		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	273	Total	C	N	O	S	0	0
			2108	1307	415	379	7		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	206	Total	C	N	O	S	0	0
			1582	995	291	292	4		

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	203	Total	C	N	O		0	0
			1563	987	286	290			

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	175	Total	C	N	O	S	0	0
			1365	865	236	258	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	165	Total	C	N	O	S	0	0
			1271	801	232	237	1		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	142	Total	C	N	O	S	0	0
			1117	708	201	205	3		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	122	Total	C	N	O	S	0	0
			925	573	175	172	5		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	144	Total	C	N	O		0	0
			1094	675	214	205			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	133	Total	C	N	O	S	0	0
			1055	675	205	170	5		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	122	Total	C	N	O	S	0	0
			983	619	191	172	1		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	118	Total	C	N	O		0	0
			914	564	176	174			

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	112	Total	C	N	O		0	0
			905	570	181	154			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	116	Total	C	N	O	S	0	0
			939	596	185	154	4		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	101	Total	C	N	O	S	0	0
			786	507	134	144	1		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	110	Total	C	N	O	S	0	0
			848	534	160	154			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	90	Total	C	N	O	S	0	0
			731	462	129	138	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	95	Total	C	N	O	S	0	0
			723	459	134	127	3		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	73	Total	C	N	O	S	0	0
			563	345	111	106	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	58	Total	C	N	O	S	0	0
			457	283	96	76	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	59	Total	C	N	O	S	0	0
			487	298	94	94	1		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	56	Total	C	N	O	S	0	0
			433	272	82	78	1		

- Molecule 27 is a protein called 50S ribosomal protein L32-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	53	Total	C	N	O	S	0	0
			425	259	87	74	5		

- Molecule 28 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	47	Total	C	N	O	S	0	0
			400	243	81	73	3		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	42	Total	C	N	O	S	0	0
			357	217	87	52	1		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	63	Total	C	N	O	S	0	0
			512	317	113	78	4		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	36	Total	C	N	O	S	0	0
			292	183	59	44	6		

- Molecule 32 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B	114	Total	C	N	O	P	0	0
			2428	1082	428	804	114		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	212	Total	C	N	O	S	0	0
			1720	1096	306	312	6		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	204	Total	C	N	O	S	0	0
			1624	1013	311	297	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	199	Total	C	N	O	S	0	0
			1596	999	302	293	2		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	161	Total	C	N	O	S	0	0
			1180	738	217	223	2		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	93	Total	C	N	O	S	0	0
			782	495	136	149	2		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	141	Total	C	N	O	S	0	0
			1114	695	209	202	8		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	130	Total	C	N	O	S	0	0
			1015	646	179	188	2		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	126	Total	C	N	O	S	0	0
			985	618	194	172	1		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	96	Total	C	N	O	S	0	0
			771	485	141	143	2		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	114	Total	C	N	O	S	0	0
			837	516	161	157	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	134	Total	C	N	O	S	0	0
			1040	645	209	184	2		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	114	Total	C	N	O	S	0	0
			906	557	180	168	1		

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	60	Total	C	N	O	S	0	0
			490	313	97	75	5		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	86	Total	C	N	O	S	0	0
			722	448	145	127	2		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	88	Total	C	N	O	S	0	0
			711	451	132	126	2		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	80	Total	C	N	O	S	0	0
			656	413	123	119	1		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	62	Total	C	N	O	S	0	0
			504	325	92	85	2		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	81	Total	C	N	O	S	0	0
			655	418	120	115	2		

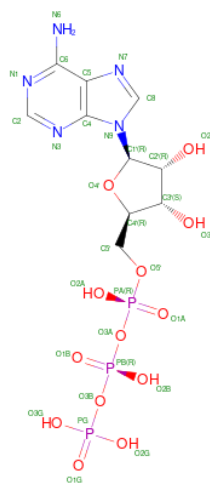
- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	80	Total	C	N	O	S	0	0
			611	369	125	116	1		

- Molecule 52 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	79	Total	C	N	O	S	0	0
			637	403	109	124	1		

- Molecule 53 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

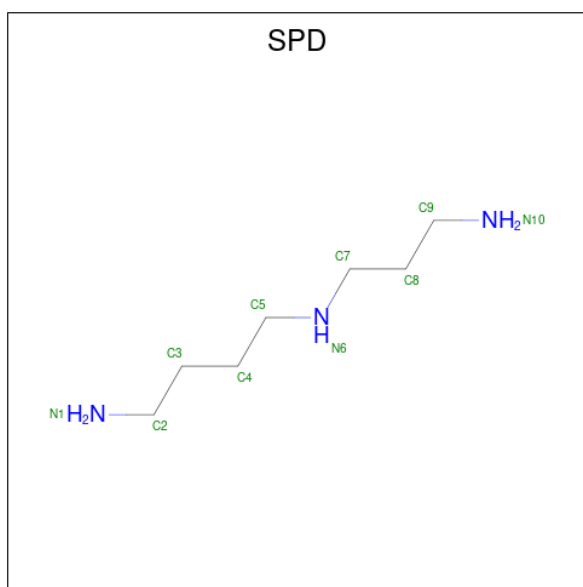


Mol	Chain	Residues	Atoms					AltConf
53	0	1	Total 31	C 10	N 5	O 13	P 3	0
53	0	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
54	0	2	Total Mg 2 2	0
54	D	1	Total Mg 1 1	0
54	b	1	Total Mg 1 1	0
54	A	114	Total Mg 114 114	0
54	a	21	Total Mg 21 21	0
54	G	1	Total Mg 1 1	0
54	H	1	Total Mg 1 1	0
54	O	1	Total Mg 1 1	0
54	o	1	Total Mg 1 1	0

- Molecule 55 is SPERMIDINE (CCD ID: SPD) (formula: $\text{C}_7\text{H}_{19}\text{N}_3$).



Mol	Chain	Residues	Atoms			AltConf
55	A	1	Total	C	N	0
			10	7	3	
55	a	1	Total	C	N	0
			10	7	3	

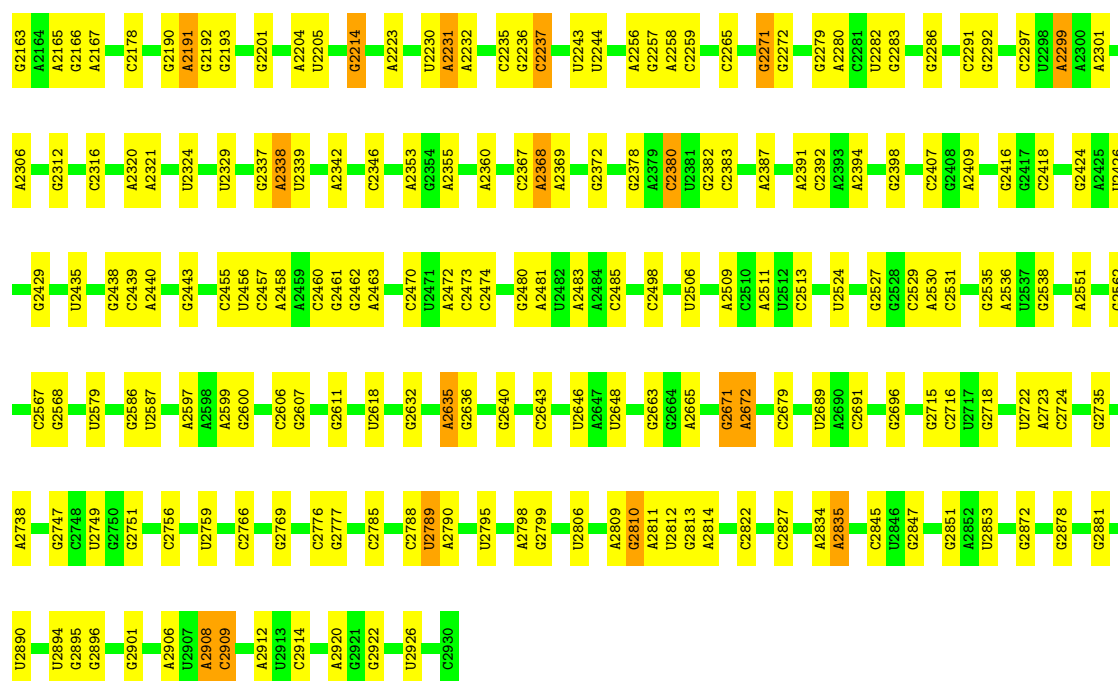
- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
56	A	17	Total	K	0
			17	17	
56	a	3	Total	K	0
			3	3	
56	P	1	Total	K	0
			1	1	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

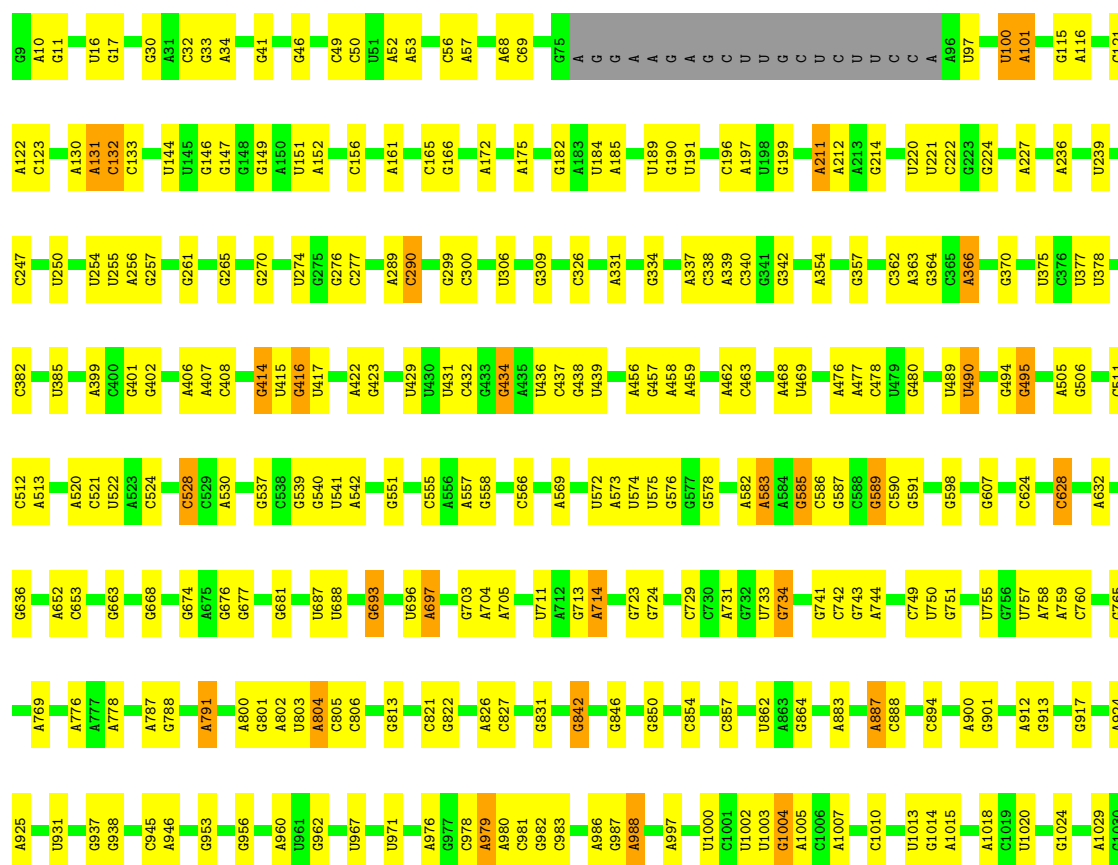
Mol	Chain	Residues	Atoms		AltConf
57	5	1	Total	Zn	0
			1	1	
57	9	1	Total	Zn	0
			1	1	
57	o	1	Total	Zn	0
			1	1	

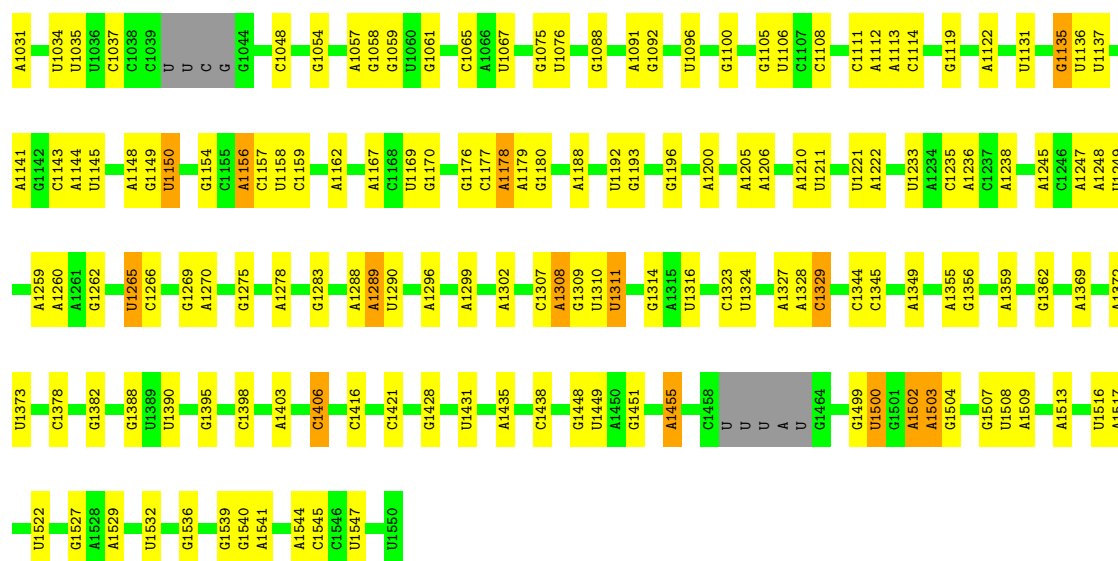
C2023	A1899	A1637	G1530	C1407	G1293	A1172	A1056	G940	G809	G675	U553	A373	G250
U2024	G1900	G1638	U1531	C1408	G1294	A1173	A1057	U941	A810	A676	C554	C374	G251
G2025	C1901	C1656	A1532	G1409	G1295	A1174	A1058	U942	U815	G679	C555	A375	C252
U2026	U1902	A1657	A1533	A1408	A1059	A1175	A1059	A943	Q816	C680	C562	A404	G256
C2029	U1903	C1658	G1534	C1414	G1296	U1176	U1065	C945	G821	G681	U564	G410	A257
A2030	C1904	A1659	A1535	A1422	G1297	U1177	A1066	G946	A828	G682	G565	A411	A267
A2031	G1908	C1660	A1536	U1423	A1298	U1178	A1067	A947	U829	G683	U566	A417	
C2032	A1929	C1661	A1539	U1424	G1301	A1179	G1068	U948	U830	U684	G567	U419	
G2037	U1933	A1665	C1542	A1429	U1308	C1180	G1070	A957	U831	A688	C572	U420	
A2038	A1934	A1671	A1543	U1434	G1309	C1181	G1071	A958	U836	A573	A574	A274	
C2039	C1938	A1681	U1546	A1435	A1310	G1182	A1072	C959	U837	U699	G283	C283	
G2043	G1939	U1688	G1558	U1440	G1311	G1183	A1073	C962	C837	A700	U575	C429	
U2049	U1945	U1689	A1559	U1447	U1312	C1186		G963	U851	G688	G576	U284	
U2052	A1946	G1692	C1562	A1452	G1313	A1187	U1079	G964	U853	A701	U577	U285	
C2058	C1947	G1694	A1563	U1462	G1320	A1188	G1080	A964	U856	G432	U578	G286	
A2064	U1948	A1695	C1567	U1463	A1318	A1189	U1081	A965	U857	U443	C287	C287	
G2065	A1949	G1696	U1569	U1464	G1324	A1190	G1084	U966	C858	U711	G582	U288	
A2066	A1952	C1697	C1570	A1477	G1327	C1216	U1092	C976	U859	C718	A583	U289	
C2069	U1956	G1698	U1571	A1485	G1330	U	G1093	C975	U861	U732	U590	U297	
G2072	C1957	A1701	G1572	C1466	A1337	C	A1097	C974	U862	G746	A591	U298	
U1959	U1959	C1487	A1573	U1468	U1338	U	U1106	U979	U865	U749	A592	G289	
A1960	A1960	G1486	U1574	C1469	C1338	A	U1107	A980	U866	U750	U593	U300	
A1961	A1961	U1470	G1575	U1470	A1344	G	G1108	G985	U867	G598	G594	A304	
G1962	G1962	A1704	A1580	A1477	A1345	A	G1109	G986	U874	U760	U597	A307	
U1963	U1963	C1705	G	C1478	A1351	G1225	C1110	U987	A875	A761	G606	U309	
A1971	A1971	U1708	G	A1479	A1351	G1230	G1114	G992	U891	U762	U611	C482	
U1972	U1972	U1711	A	A1485	G1364	G1233	A1115	A892	U892	A763	U616	A313	
C1974	C1974	G1716	A	G1486	A1365	G1236	A1116	A893	A893	A764	G616	C490	
G1975	G1975	A1717	U	U1487	A1366	G1237	G1117	G1007	G897	A768	A617	C491	
U1976	U1976	U1851	A	A1494	A1369	A1248	C1125	A1008	U898	G772	A618	G492	
U1977	U1977	A1852	A	A1498	C1369	A1249	G1129	G905	G905	G775	A622	A493	
U1988	U1988	U1853	G	C1498	U1373	G1250	A1132	G906	G906	U776	A629	C501	
A1993	A1993	G1856	C1593	A1502	C1374	G1253	G1133	A1017	A913	C782	G630	C502	
C1996	C1996	A1862	C1611	A1503	C1377	G1254	A1025	A1019	A916	G787	U631	A503	
G1997	G1997	G1743	G1612	U1504	U1378	U1255	G1135	A1020	G916	G788	U632	A526	
C1998	C1998	G1752	G1612	U1505	C1379	U1256	U1136	A1026	A925	A789	G635	C528	
A1999	A1999	A1738	A1618	A1508	A1386	G1257	G1137	G1030	A925	C790	A646	A536	
C2000	C2000	A1747	A1619	U1509	G1387	G1284	A1142	G1031	G929	G791	A657	G540	
A2003	A2003	U1762	G1620	U1510	U1388	G1288	U1143	C1041	C930	U792	A658	G541	
A2004	A2004	U1763	A1621	G1511	U1388	G1288	A1157	A1042	C931	U793	A659	A542	
G2005	G2005	A1764	U1516	U1516	G1392	G1289	U1158	G1043	C932	G794	A666	A548	
A2013	A2013	G1765	A1630	C1517	A1393	G1290	U1159	U934	U934	A798	A666	C549	
G2014	G2014	G1766	A1631	C1518	C1394	G1291	G1160	C1052	C935	G799	A666	A550	
A2150	A2150	G1773	G1632	A1519	G1395	A1282	A1161	C1053	U936	U800	G673	G551	
A2159	A2159	A1778	A1635	G1528	U1396	C1283	A1161	C1054	C937		A674	U552	
			G1636	U1529	G1404	G1285	G1171	A1055					



• Molecule 5: 16S rRNA

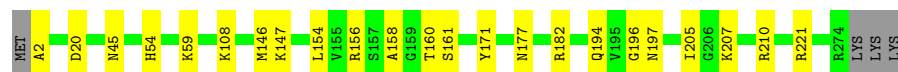
Chain a: 70% 26%





• Molecule 6: 50S ribosomal protein L2

Chain G: 90% 8% .



• Molecule 7: 50S ribosomal protein L3

Chain H: 86% 12% .



• Molecule 8: 50S ribosomal protein L4

Chain I: 94% 2% .



• Molecule 9: 50S ribosomal protein L5

Chain J: 84% 13% .



• Molecule 10: 50S ribosomal protein L6

Chain K: 83% 10% 7%



- Molecule 11: 50S ribosomal protein L13

Chain M: 86% 12%



- Molecule 12: 50S ribosomal protein L14

Chain N: 88% 12%



- Molecule 13: 50S ribosomal protein L15

Chain O: 92% 7%



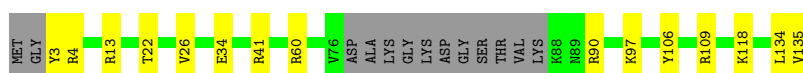
- Molecule 14: 50S ribosomal protein L16

Chain P: 84% 8% 8%



- Molecule 15: 50S ribosomal protein L17

Chain Q: 79% 11% 10%



- Molecule 16: 50S ribosomal protein L18

Chain R: 90% 9%

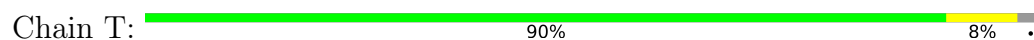


- Molecule 17: 50S ribosomal protein L19

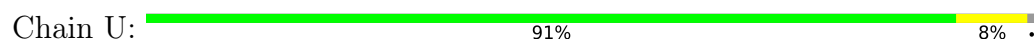
Chain S: 89% 10%



- Molecule 18: 50S ribosomal protein L20



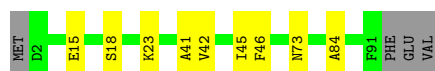
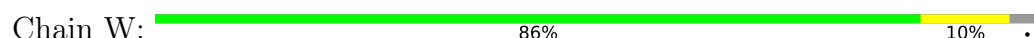
- Molecule 19: 50S ribosomal protein L21



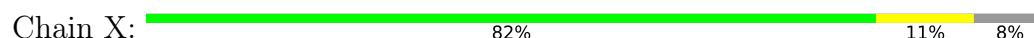
- Molecule 20: 50S ribosomal protein L22



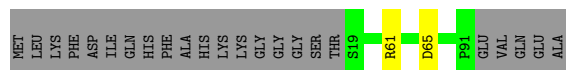
- Molecule 21: 50S ribosomal protein L23



- Molecule 22: 50S ribosomal protein L24



- Molecule 23: 50S ribosomal protein L27

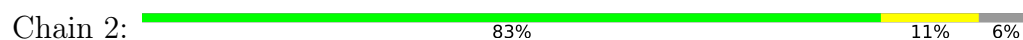


- Molecule 24: 50S ribosomal protein L28

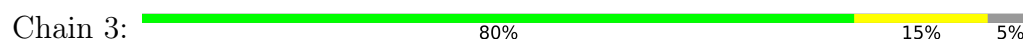




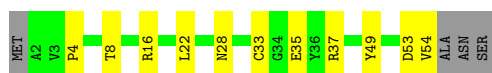
- Molecule 25: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L30



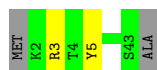
- Molecule 27: 50S ribosomal protein L32-2



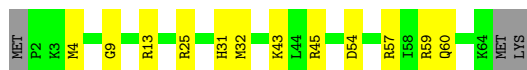
- Molecule 28: 50S ribosomal protein L33 1



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



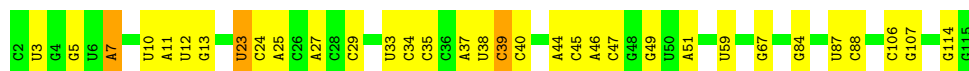
- Molecule 31: 50S ribosomal protein L36





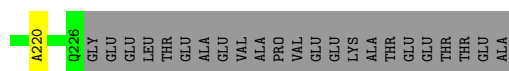
- Molecule 32: 5S rRNA

Chain B: 71% 26% .



- Molecule 33: 30S ribosomal protein S2

Chain c: 76% 10% 15%



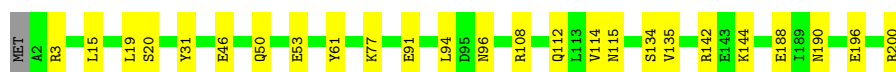
- Molecule 34: 30S ribosomal protein S3

Chain d: 87% 6% 6%



- Molecule 35: 30S ribosomal protein S4

Chain e: 87% 12%



- Molecule 36: 30S ribosomal protein S5

Chain f: 90% 7% .



- Molecule 37: 30S ribosomal protein S6

Chain g: 91% 5% .



- Molecule 38: 30S ribosomal protein S7

Chain h:  80% 10% 10%



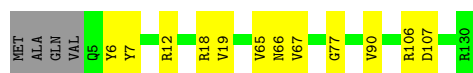
- Molecule 39: 30S ribosomal protein S8

Chain i:  77% 22% .



- Molecule 40: 30S ribosomal protein S9

Chain j:  88% 9% .



- Molecule 41: 30S ribosomal protein S10

Chain k:  84% 10% 6%



- Molecule 42: 30S ribosomal protein S11

Chain l:  83% 5% 12%



- Molecule 43: 30S ribosomal protein S12

Chain m:  85% 13% .



- Molecule 44: 30S ribosomal protein S13

Chain n:  82% 12% 6%



- Molecule 45: 30S ribosomal protein S14 type Z

Chain o:  82% 16%

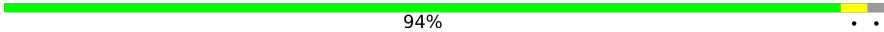


- Molecule 46: 30S ribosomal protein S15

Chain p:  85% 11%



- Molecule 47: 30S ribosomal protein S16

Chain q:  94%



- Molecule 48: 30S ribosomal protein S17

Chain r:  83% 9% 8%



- Molecule 49: 30S ribosomal protein S18

Chain s:  68% 10% 22%



- Molecule 50: 30S ribosomal protein S19

Chain t:  82% 7% 12%



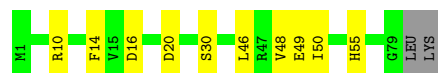
- Molecule 51: 30S ribosomal protein S20

Chain u:  90% 5% 5%



- Molecule 52: 50S ribosomal protein L31 type B

85% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45548	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 ($e^-/\text{\AA}^2$)	26.3	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-1900	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, MG, K, SPD

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	0	0.54	0/3699	0.67	1/4976 (0.0%)
2	D	0.44	0/1765	0.46	0/2750
3	b	0.33	0/196	0.57	0/302
4	A	0.62	0/69974	0.53	0/109160
5	a	0.39	0/36323	0.45	0/56652
6	G	0.81	0/2144	0.75	1/2875 (0.0%)
7	H	0.85	0/1604	0.69	1/2156 (0.0%)
8	I	0.79	0/1583	0.70	0/2133
9	J	0.45	1/1383 (0.1%)	0.61	0/1863
10	K	0.39	0/1293	0.53	0/1749
11	M	0.80	0/1140	0.68	0/1533
12	N	0.79	0/932	0.71	0/1248
13	O	0.74	0/1105	0.69	0/1470
14	P	0.74	0/1077	0.64	0/1439
15	Q	0.77	0/994	0.68	0/1329
16	R	0.46	0/923	0.68	0/1232
17	S	0.76	0/917	0.70	0/1230
18	T	0.85	0/952	0.73	0/1266
19	U	0.82	0/799	0.63	0/1072
20	V	0.85	0/858	0.82	0/1160
21	W	0.71	0/739	0.66	0/990
22	X	0.61	0/733	0.65	0/980
23	Z	0.79	0/570	0.79	0/758
24	1	0.75	0/462	0.84	0/612
25	2	0.56	0/488	0.66	0/651
26	3	0.71	0/436	0.77	0/585
27	5	0.89	0/433	0.88	0/577
28	6	0.61	0/404	0.65	0/541
29	7	0.95	0/360	0.72	0/469
30	8	0.86	0/519	0.77	0/675
31	9	0.77	0/295	0.69	0/387
32	B	0.38	0/2711	0.42	0/4224

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.34	0/1749	0.63	0/2351
34	d	0.43	0/1649	0.59	0/2218
35	e	0.38	0/1624	0.62	0/2179
36	f	0.48	0/1192	0.60	0/1609
37	g	0.33	0/794	0.58	0/1063
38	h	0.38	0/1128	0.57	0/1514
39	i	0.47	0/1028	0.64	0/1382
40	j	0.47	0/1003	0.67	0/1349
41	k	0.43	0/783	0.64	0/1056
42	l	0.37	0/851	0.54	0/1148
43	m	0.53	0/1056	0.70	0/1418
44	n	0.43	0/912	0.68	0/1220
45	o	0.54	0/500	0.64	0/664
46	p	0.39	0/732	0.57	0/980
47	q	0.41	0/724	0.68	0/971
48	r	0.39	0/665	0.61	0/889
49	s	0.37	0/512	0.60	0/686
50	t	0.41	0/671	0.56	0/902
51	u	0.43	0/614	0.63	0/817
52	4	0.34	0/654	0.64	0/881
All	All	0.57	1/156652 (0.0%)	0.55	3/234341 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	13	VAL	CA-CB	-5.39	1.51	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	131	GLY	CA-C-O	-5.72	116.91	122.46
6	G	221	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	0	148	ILE	CA-C-O	-5.12	118.18	122.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	3647	0	3757	79	0
2	D	1580	0	801	4	0
3	b	176	0	88	1	0
4	A	62459	0	31404	218	0
5	a	32445	0	16335	139	0
6	G	2108	0	2184	17	0
7	H	1582	0	1646	18	0
8	I	1563	0	1655	5	0
9	J	1365	0	1417	20	0
10	K	1271	0	1308	10	0
11	M	1117	0	1140	15	0
12	N	925	0	982	9	0
13	O	1094	0	1137	11	0
14	P	1055	0	1125	6	0
15	Q	983	0	1045	12	0
16	R	914	0	941	9	0
17	S	905	0	973	8	0
18	T	939	0	1011	8	0
19	U	786	0	825	6	0
20	V	848	0	905	8	0
21	W	731	0	763	6	0
22	X	723	0	794	11	0
23	Z	563	0	568	1	0
24	1	457	0	502	9	0
25	2	487	0	504	4	0
26	3	433	0	479	7	0
27	5	425	0	423	11	0
28	6	400	0	413	2	0
29	7	357	0	405	2	0
30	8	512	0	562	11	0
31	9	292	0	334	6	0
32	B	2428	0	1229	16	0
33	c	1720	0	1769	13	0
34	d	1624	0	1650	9	0
35	e	1596	0	1620	18	0
36	f	1180	0	1241	7	0
37	g	782	0	777	4	0
38	h	1114	0	1154	10	0
39	i	1015	0	1069	22	0
40	j	985	0	1021	9	0
41	k	771	0	808	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	l	837	0	853	5	0
43	m	1040	0	1108	15	0
44	n	906	0	960	10	0
45	o	490	0	525	7	0
46	p	722	0	747	11	0
47	q	711	0	742	3	0
48	r	656	0	687	7	0
49	s	504	0	542	7	0
50	t	655	0	663	6	0
51	u	611	0	643	3	0
52	4	637	0	614	6	0
53	0	62	0	24	6	0
54	0	2	0	0	0	0
54	A	114	0	0	0	0
54	D	1	0	0	0	0
54	G	1	0	0	0	0
54	H	1	0	0	0	0
54	O	1	0	0	0	0
54	a	21	0	0	0	0
54	b	1	0	0	0	0
54	o	1	0	0	0	0
55	A	10	0	19	0	0
55	a	10	0	19	0	0
56	A	17	0	0	0	0
56	P	1	0	0	0	0
56	a	3	0	0	0	0
57	5	1	0	0	0	0
57	9	1	0	0	0	0
57	o	1	0	0	0	0
All	All	144375	0	96910	710	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 710 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:334:PHE:CD1	1:0:392:LEU:HD23	1.35	1.58
20:V:69:LEU:HD22	20:V:114:GLU:OE2	1.08	1.23
1:0:334:PHE:HD1	1:0:392:LEU:CD2	1.50	1.22
1:0:392:LEU:HA	1:0:395:MET:CE	1.76	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:334:PHE:CD1	1:0:392:LEU:CD2	2.29	1.13

There are no symmetry-related clashes.

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	
1	0	459/567 (81%)	430 (94%)	29 (6%)	0	100	100
6	G	271/277 (98%)	256 (94%)	15 (6%)	0	100	100
7	H	204/209 (98%)	191 (94%)	13 (6%)	0	100	100
8	I	201/207 (97%)	190 (94%)	11 (6%)	0	100	100
9	J	173/179 (97%)	163 (94%)	10 (6%)	0	100	100
10	K	163/178 (92%)	155 (95%)	8 (5%)	0	100	100
11	M	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
12	N	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
13	O	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
14	P	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
15	Q	118/135 (87%)	113 (96%)	5 (4%)	0	100	100
16	R	116/119 (98%)	106 (91%)	10 (9%)	0	100	100
17	S	110/114 (96%)	103 (94%)	7 (6%)	0	100	100
18	T	114/119 (96%)	107 (94%)	7 (6%)	0	100	100
19	U	99/102 (97%)	93 (94%)	6 (6%)	0	100	100
20	V	108/118 (92%)	106 (98%)	2 (2%)	0	100	100
21	W	88/94 (94%)	82 (93%)	6 (7%)	0	100	100
22	X	93/103 (90%)	91 (98%)	2 (2%)	0	100	100
23	Z	71/96 (74%)	67 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	1	56/62 (90%)	51 (91%)	5 (9%)	0	100	100
25	2	57/63 (90%)	54 (95%)	3 (5%)	0	100	100
26	3	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
27	5	51/57 (90%)	49 (96%)	2 (4%)	0	100	100
28	6	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
29	7	40/44 (91%)	39 (98%)	1 (2%)	0	100	100
30	8	61/66 (92%)	53 (87%)	8 (13%)	0	100	100
31	9	34/37 (92%)	30 (88%)	4 (12%)	0	100	100
33	c	210/249 (84%)	188 (90%)	22 (10%)	0	100	100
34	d	202/218 (93%)	185 (92%)	17 (8%)	0	100	100
35	e	197/200 (98%)	182 (92%)	15 (8%)	0	100	100
36	f	159/167 (95%)	149 (94%)	10 (6%)	0	100	100
37	g	91/97 (94%)	83 (91%)	8 (9%)	0	100	100
38	h	139/156 (89%)	130 (94%)	9 (6%)	0	100	100
39	i	128/132 (97%)	116 (91%)	12 (9%)	0	100	100
40	j	124/130 (95%)	114 (92%)	10 (8%)	0	100	100
41	k	94/102 (92%)	87 (93%)	7 (7%)	0	100	100
42	l	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
43	m	132/137 (96%)	120 (91%)	12 (9%)	0	100	100
44	n	112/121 (93%)	103 (92%)	9 (8%)	0	100	100
45	o	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	p	84/89 (94%)	81 (96%)	3 (4%)	0	100	100
47	q	86/90 (96%)	81 (94%)	5 (6%)	0	100	100
48	r	78/87 (90%)	73 (94%)	5 (6%)	0	100	100
49	s	60/79 (76%)	59 (98%)	1 (2%)	0	100	100
50	t	79/92 (86%)	75 (95%)	4 (5%)	0	100	100
51	u	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
52	4	77/81 (95%)	59 (77%)	18 (23%)	0	100	100
All	All	5619/6112 (92%)	5249 (93%)	370 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	
1	O	400/492 (81%)	400 (100%)	0	100	100
6	G	221/225 (98%)	221 (100%)	0	100	100
7	H	169/171 (99%)	169 (100%)	0	100	100
8	I	171/174 (98%)	171 (100%)	0	100	100
9	J	151/155 (97%)	151 (100%)	0	100	100
10	K	137/147 (93%)	137 (100%)	0	100	100
11	M	119/121 (98%)	119 (100%)	0	100	100
12	N	101/101 (100%)	101 (100%)	0	100	100
13	O	113/115 (98%)	113 (100%)	0	100	100
14	P	105/113 (93%)	105 (100%)	0	100	100
15	Q	102/111 (92%)	102 (100%)	0	100	100
16	R	96/97 (99%)	96 (100%)	0	100	100
17	S	98/100 (98%)	98 (100%)	0	100	100
18	T	95/97 (98%)	95 (100%)	0	100	100
19	U	82/82 (100%)	82 (100%)	0	100	100
20	V	91/97 (94%)	91 (100%)	0	100	100
21	W	80/84 (95%)	80 (100%)	0	100	100
22	X	81/88 (92%)	81 (100%)	0	100	100
23	Z	58/76 (76%)	58 (100%)	0	100	100
24	1	50/53 (94%)	50 (100%)	0	100	100
25	2	52/55 (94%)	52 (100%)	0	100	100
26	3	50/52 (96%)	50 (100%)	0	100	100
27	5	47/50 (94%)	47 (100%)	0	100	100
28	6	46/48 (96%)	46 (100%)	0	100	100
29	7	38/39 (97%)	38 (100%)	0	100	100
30	8	53/56 (95%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	9	35/35 (100%)	35 (100%)	0	100	100
33	c	185/215 (86%)	185 (100%)	0	100	100
34	d	165/177 (93%)	165 (100%)	0	100	100
35	e	169/170 (99%)	169 (100%)	0	100	100
36	f	126/131 (96%)	126 (100%)	0	100	100
37	g	83/85 (98%)	83 (100%)	0	100	100
38	h	117/130 (90%)	117 (100%)	0	100	100
39	i	108/110 (98%)	108 (100%)	0	100	100
40	j	99/102 (97%)	99 (100%)	0	100	100
41	k	88/93 (95%)	88 (100%)	0	100	100
42	l	86/100 (86%)	86 (100%)	0	100	100
43	m	115/118 (98%)	115 (100%)	0	100	100
44	n	97/102 (95%)	97 (100%)	0	100	100
45	o	51/52 (98%)	51 (100%)	0	100	100
46	p	79/81 (98%)	79 (100%)	0	100	100
47	q	78/80 (98%)	78 (100%)	0	100	100
48	r	73/78 (94%)	73 (100%)	0	100	100
49	s	56/67 (84%)	56 (100%)	0	100	100
50	t	70/78 (90%)	70 (100%)	0	100	100
51	u	63/66 (96%)	63 (100%)	0	100	100
52	4	71/73 (97%)	71 (100%)	0	100	100
All	All	4820/5142 (94%)	4820 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
20	V	66	ASN
46	p	37	ASN
28	6	16	ASN
49	s	24	HIS
41	k	15	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	73/77 (94%)	16 (21%)	0
3	b	6/14 (42%)	1 (16%)	0
32	B	113/114 (99%)	18 (15%)	1 (0%)
4	A	2905/2928 (99%)	575 (19%)	48 (1%)
5	a	1509/1542 (97%)	296 (19%)	0
All	All	4606/4675 (98%)	906 (19%)	49 (1%)

5 of 906 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	5	G
2	D	6	G
2	D	8	U
2	D	9	G
2	D	13	C

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	1533	A
4	A	1946	A
4	A	1569	U
4	A	1880	A
4	A	2320	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 171 ligands modelled in this entry, 167 are monoatomic - leaving 4 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
53	ATP	0	602	54	32,33,33	0.77	1 (3%)	48,52,52	0.31	0
55	SPD	A	3001	-	9,9,9	0.49	0	8,8,8	1.35	2 (25%)
53	ATP	0	601	54	32,33,33	0.54	0	48,52,52	0.29	0
55	SPD	a	1601	-	9,9,9	0.28	0	8,8,8	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	ATP	0	602	54	-	7/22/38/38	0/3/3/3
55	SPD	A	3001	-	-	4/7/7/7	-
53	ATP	0	601	54	-	6/22/38/38	0/3/3/3
55	SPD	a	1601	-	-	2/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	0	602	ATP	PB-O3B	-2.90	1.56	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A	3001	SPD	C4-C5-N6	-2.75	104.68	112.07
55	A	3001	SPD	C8-C7-N6	-2.37	105.71	112.07

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	0	601	ATP	C5'-O5'-PA-O1A
53	0	601	ATP	C5'-O5'-PA-O2A
53	0	601	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
53	0	602	ATP	C5'-O5'-PA-O2A
53	0	602	ATP	C3'-C4'-C5'-O5'

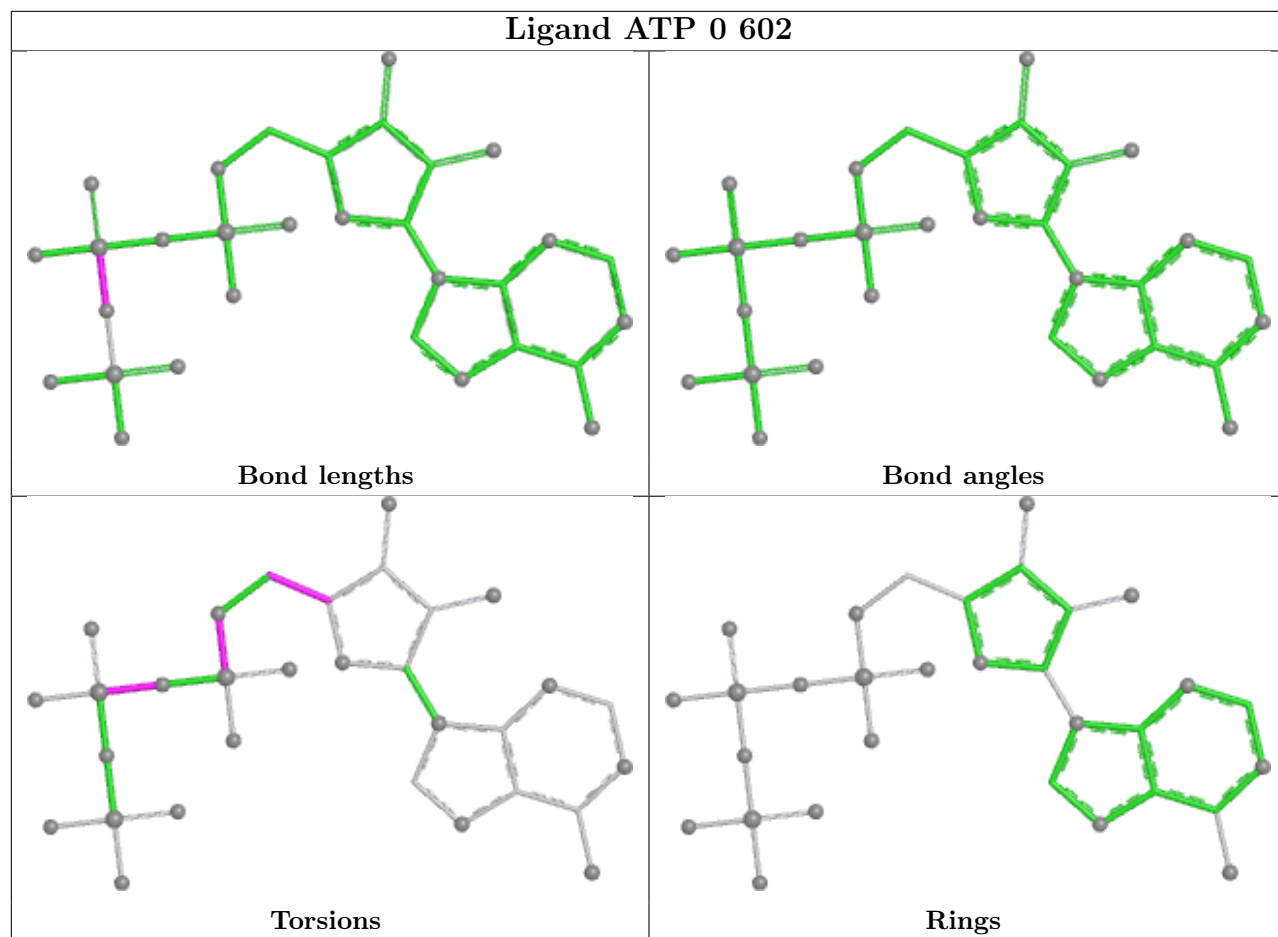
There are no ring outliers.

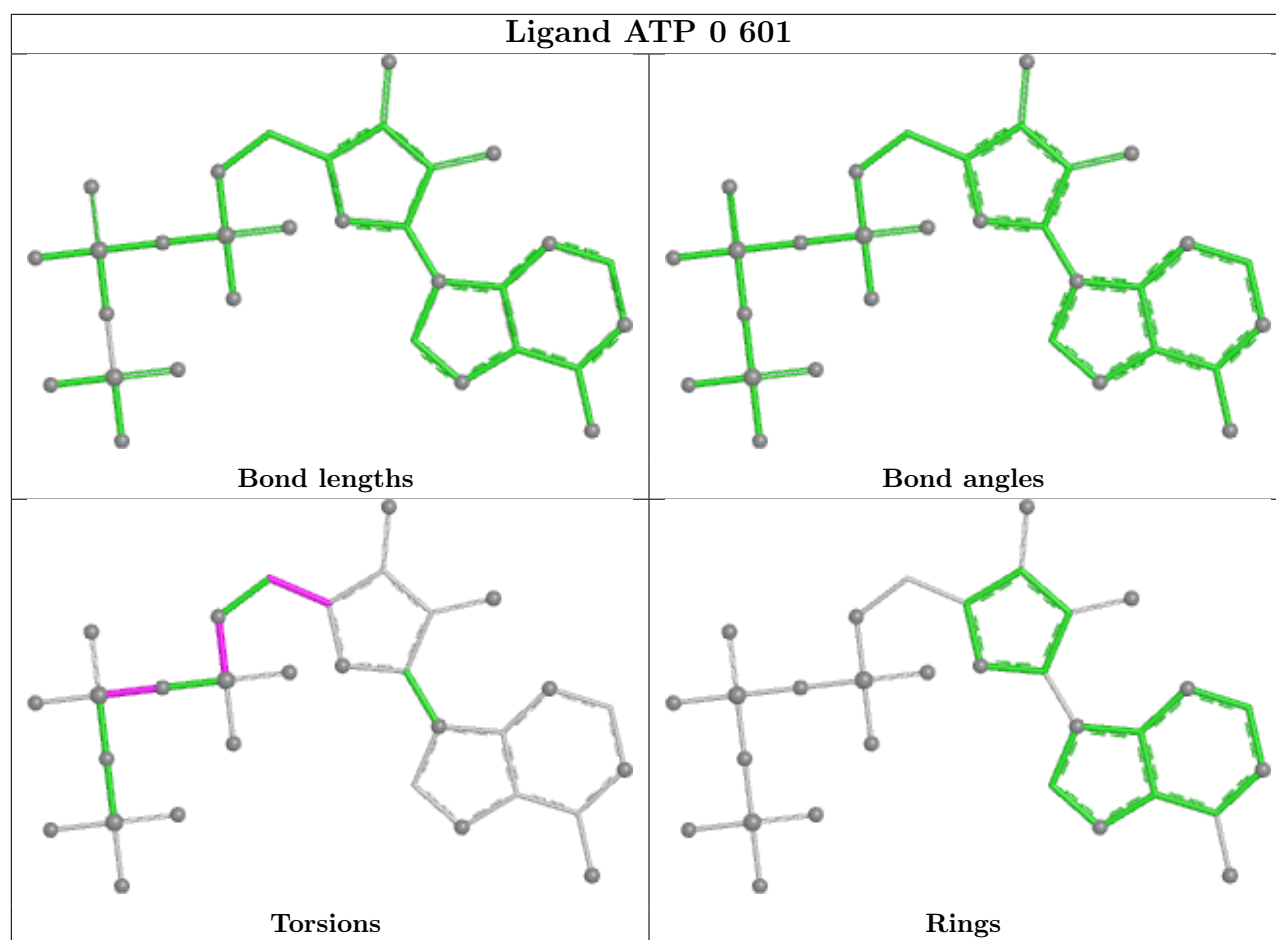
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	0	602	ATP	4	0
53	0	601	ATP	2	0

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.

Ligand ATP 0 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12334. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.