



wwPDB X-ray Structure Validation Summary Report

Mar 15, 2026 – 01:33 PM UTC

PDB ID : 6MPF / pdb_00006mpf
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a 2-thiocytidine (s2C32) and inosine (I34) modified anticodon stem loop (ASL) of *Escherichia coli* transfer RNA Arginine 1 (TRNAARG1) bound to an mRNA with an CGC-codon in the A-site and paromomycin
Authors : Cantara, W.A.; DeMirci, H.; Agris, P.F.
Deposited on : 2018-10-05
Resolution : 3.33 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

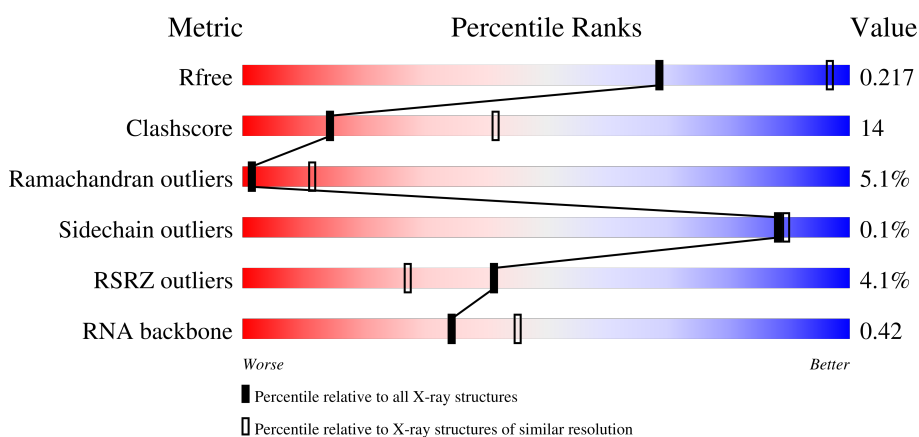
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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.



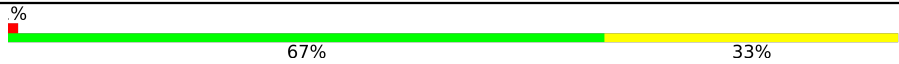

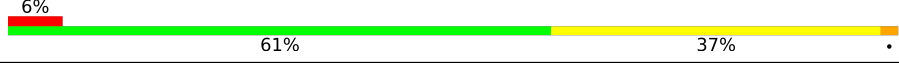
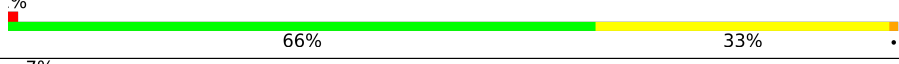

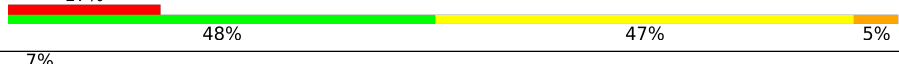


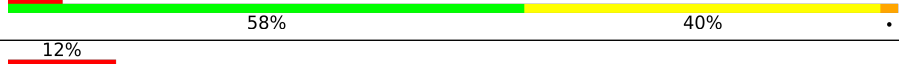




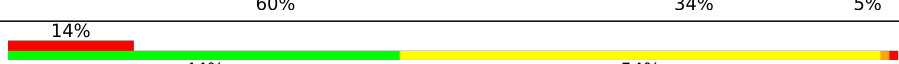
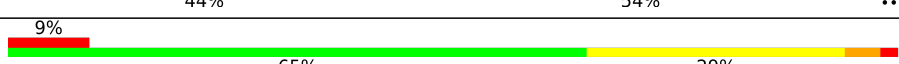
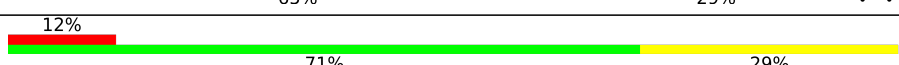
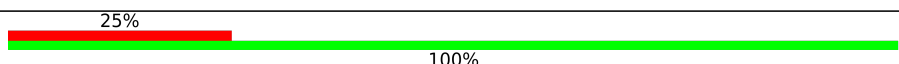
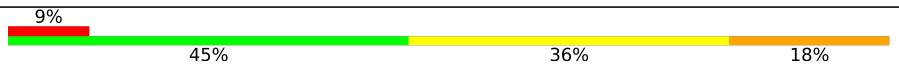

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)
RNA backbone	3983	1083 (3.68-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1508	 8% 52% 38% 9% .
2	B	234	 3% 53% 44% .
3	C	206	 4% 53% 42% 5% .
4	D	208	 8% 61% 38% .

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Mol	Chain	Length	Quality of chain
5	E	150	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	98	
11	K	119	
12	L	124	
13	M	125	
14	N	60	
15	O	88	
16	P	83	
17	Q	104	
18	R	73	
19	S	80	
20	T	99	
21	V	24	
22	W	4	
23	X	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1662	-	-	-	X
25	MG	A	1682	-	-	-	X

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 52108 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1508	32415	14427	6005	10475	1508	22	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1612	1016	314	281	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	101	843	531	155	154	3	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	155	1257	781	252	218	6	0	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	138	1116	705	215	193	3	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	127	1010	639	197	174	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	98	794	499	156	138	1	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	119	885	549	168	165	3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	124	970	611	195	163	1	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	125	997	617	207	171	2	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	60	492	312	104	72	4	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	88	734	459	147	126	2	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	83	700	443	139	117	1	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	104	857	547	160	148	2	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	73	598	381	118	99	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	80	647	414	119	112	2	0	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	T	99	763	470	162	129	2	0	0	0

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	V	24	208	128	50	30	0	0	0

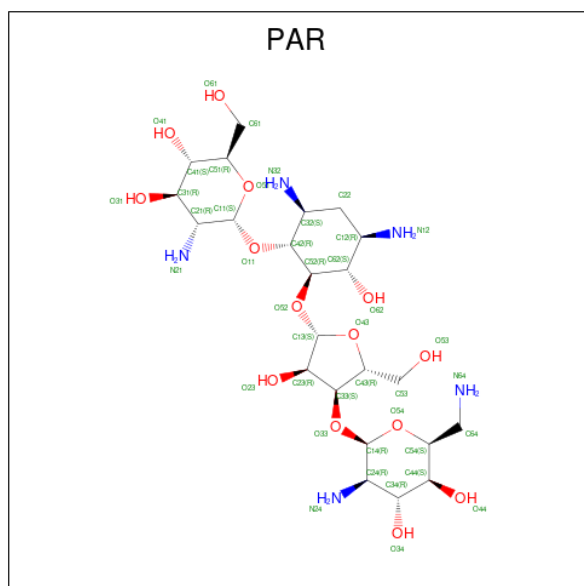
- Molecule 22 is a RNA chain called mRNA A-site fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	W	4	82	38	16	25	3	0	0	0

- Molecule 23 is a RNA chain called tRNA ASL Escherichia coli Arg1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
23	X	11	232	105	43	73	10	1	0	0	0

- Molecule 24 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	42	23	5	14	0	0

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
25	A	98	98	98	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	E	1	Total Mg 1 1	0	0
25	J	2	Total Mg 2 2	0	0
25	W	1	Total Mg 1 1	0	0
25	X	1	Total Mg 1 1	0	0

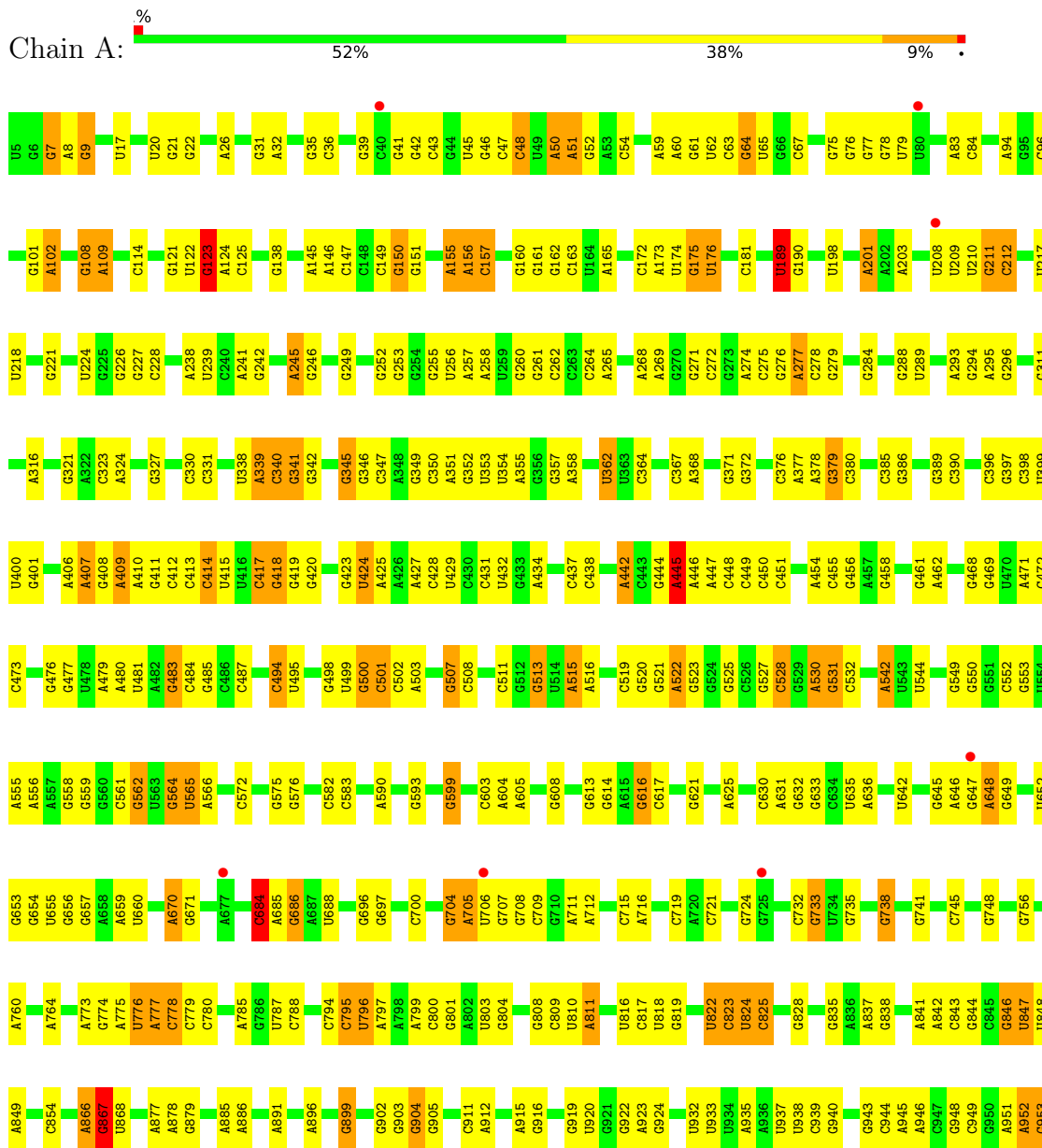
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	D	1	Total Zn 1 1	0	0
26	N	1	Total Zn 1 1	0	0

3 Residue-property plots [i](#)

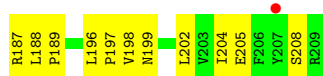
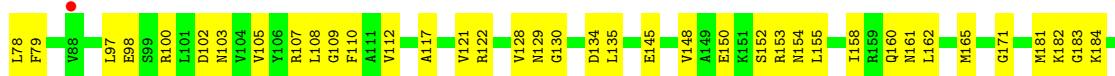
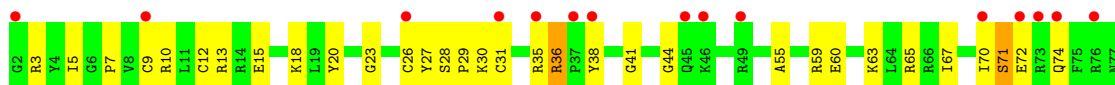
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: 16S rRNA





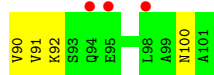
- Molecule 4: 30S ribosomal protein S4



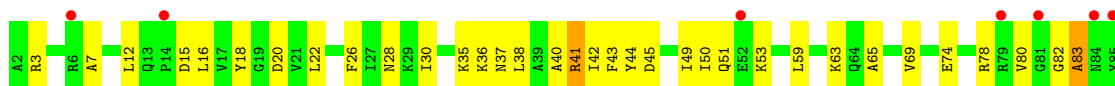
- Molecule 5: 30S ribosomal protein S5



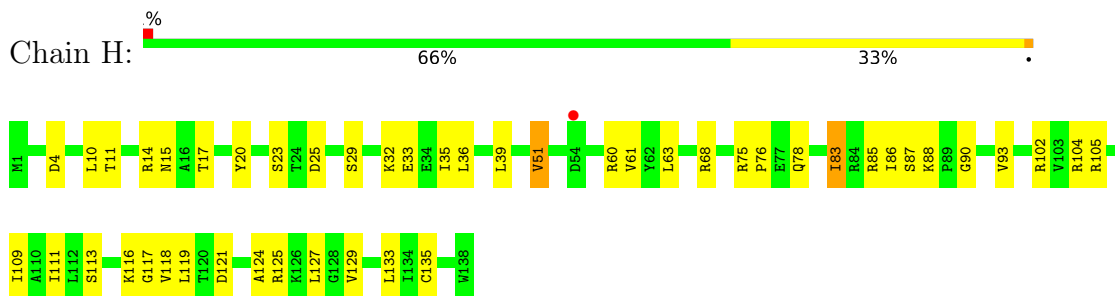
- Molecule 6: 30S ribosomal protein S6



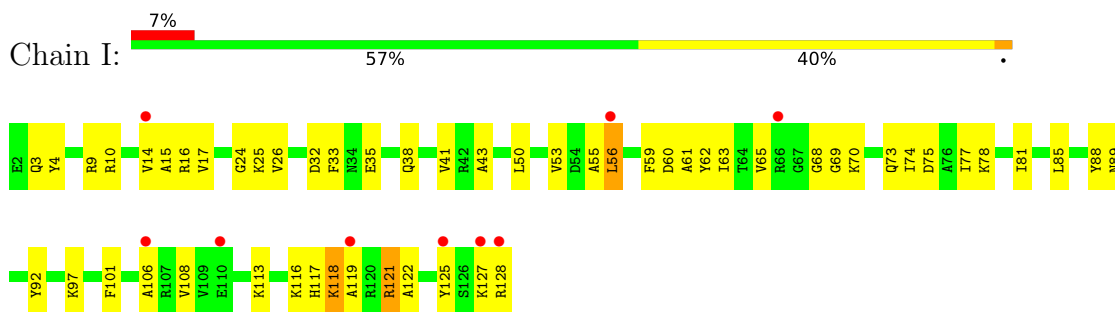
- Molecule 7: 30S ribosomal protein S7



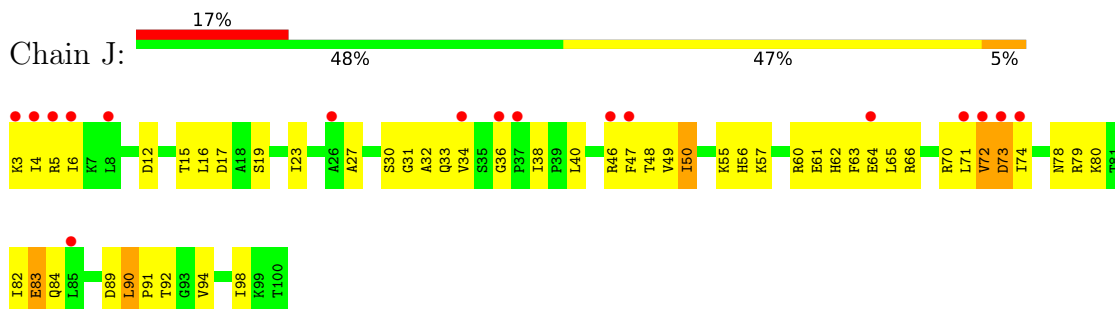
- Molecule 8: 30S ribosomal protein S8



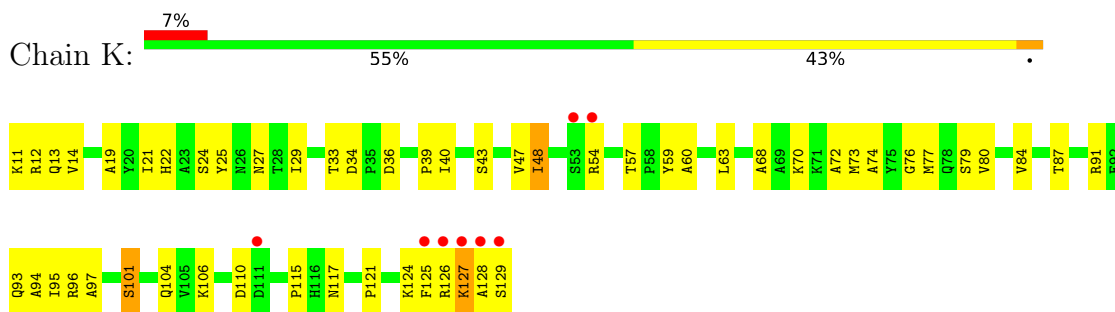
- Molecule 9: 30S ribosomal protein S9



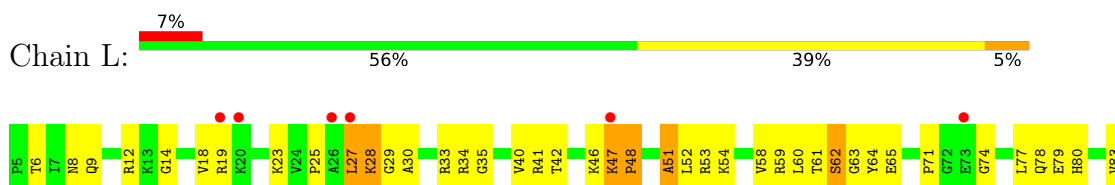
- Molecule 10: 30S ribosomal protein S10

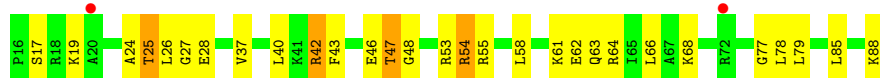


- Molecule 11: 30S ribosomal protein S11

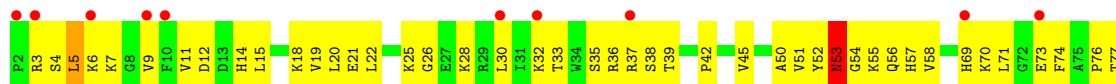
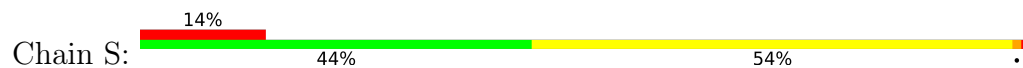


- Molecule 12: 30S ribosomal protein S12





- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



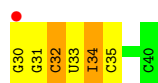
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA A-site fragment



- Molecule 23: tRNA ASL Escherichia coli Arg1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.33Å 402.33Å 176.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 3.33 49.56 – 3.33	Depositor EDS
% Data completeness (in resolution range)	92.9 (49.56-3.33) 92.1 (49.56-3.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.178 , 0.219 0.179 , 0.217	Depositor DCC
R_{free} test set	2000 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	118.3	Xtrriage
Anisotropy	0.110	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 90.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52108	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: PAR, MG, RSP, 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	A	0.54	2/36285 (0.0%)	0.77	29/56631 (0.1%)
2	B	0.41	0/1935	0.68	0/2609
3	C	0.45	0/1636	0.75	0/2205
4	D	0.46	0/1733	0.73	0/2318
5	E	0.61	0/1162	0.83	0/1564
6	F	0.40	0/856	0.64	0/1154
7	G	0.43	0/1276	0.68	0/1709
8	H	0.60	0/1136	0.83	0/1527
9	I	0.42	0/1029	0.70	0/1379
10	J	0.49	0/807	0.78	0/1085
11	K	0.49	0/900	0.77	0/1213
12	L	0.65	0/986	0.93	0/1320
13	M	0.44	0/1008	0.74	0/1347
14	N	0.46	0/501	0.70	0/664
15	O	0.49	0/745	0.73	0/992
16	P	0.56	0/716	0.85	0/963
17	Q	0.62	0/870	0.84	0/1159
18	R	0.46	0/604	0.68	0/801
19	S	0.40	0/661	0.70	0/890
20	T	0.56	0/765	0.97	2/1007 (0.2%)
21	V	0.43	0/212	0.77	0/277
22	W	0.52	0/91	0.76	0/140
23	X	0.72	0/235	0.79	0/360
All	All	0.53	2/56149 (0.0%)	0.77	31/83314 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
8	H	0	1
9	I	0	1
12	L	0	1
14	N	0	1
17	Q	0	1
18	R	0	1
19	S	0	1
20	T	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	G	C5-C6	-7.63	1.27	1.42
1	A	564	G	N1-C2	7.18	1.52	1.37

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	74	LYS	CA-C-N	9.89	142.09	122.31
20	T	74	LYS	C-N-CA	9.89	142.09	122.31
1	A	564	G	N1-C6-O6	8.44	145.22	119.90
1	A	795	C	C2'-C3'-O3'	8.04	121.56	109.50
1	A	500	G	C2'-C3'-O3'	6.71	119.56	109.50

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	15	THR	Peptide
3	C	166	GLU	Peptide
8	H	90	GLY	Peptide
9	I	117	HIS	Peptide
12	L	14	GLY	Peptide

5.2 Too-close contacts [i](#)

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	A	32415	0	16360	507	0
2	B	1900	0	1951	92	0
3	C	1612	0	1677	95	0
4	D	1703	0	1763	63	0
5	E	1146	0	1207	37	0
6	F	843	0	857	34	0
7	G	1257	0	1296	42	0
8	H	1116	0	1177	40	0
9	I	1010	0	1037	43	0
10	J	794	0	840	51	1
11	K	885	0	904	38	0
12	L	970	0	1057	43	0
13	M	997	0	1072	42	0
14	N	492	0	529	32	0
15	O	734	0	771	30	0
16	P	700	0	720	26	0
17	Q	857	0	928	43	0
18	R	598	0	670	32	0
19	S	647	0	673	43	0
20	T	763	0	861	33	0
21	V	208	0	221	7	0
22	W	82	0	46	0	0
23	X	232	0	121	6	0
24	A	42	0	45	1	0
25	A	98	0	0	0	0
25	E	1	0	0	0	0
25	J	2	0	0	0	0
25	W	1	0	0	0	0
25	X	1	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52108	0	36783	1219	1

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 14.

The worst 5 of 1219 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)
2:B:178:ARG:HH21	2:B:196:LEU:C	1.56	1.11
18:R:54:ARG:HH12	18:R:55:ARG:CG	1.67	1.07
18:R:54:ARG:NH1	18:R:55:ARG:HG2	1.70	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:ARG:NH2	2:B:196:LEU:O	1.88	1.05
3:C:107:GLN:OE1	3:C:108:ASN:HB2	1.55	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:79:ARG:CB	10:J:79:ARG:NE[8_665]	1.89	0.31

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/234 (99%)	179 (77%)	37 (16%)	16 (7%)	1	7
3	C	204/206 (99%)	150 (74%)	39 (19%)	15 (7%)	1	6
4	D	206/208 (99%)	179 (87%)	20 (10%)	7 (3%)	3	19
5	E	148/150 (99%)	133 (90%)	12 (8%)	3 (2%)	6	28
6	F	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	41
7	G	153/155 (99%)	129 (84%)	16 (10%)	8 (5%)	1	11
8	H	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	8	33
9	I	125/127 (98%)	106 (85%)	15 (12%)	4 (3%)	3	19
10	J	96/98 (98%)	66 (69%)	18 (19%)	12 (12%)	0	1
11	K	117/119 (98%)	98 (84%)	12 (10%)	7 (6%)	1	9
12	L	122/124 (98%)	94 (77%)	16 (13%)	12 (10%)	0	3
13	M	123/125 (98%)	98 (80%)	22 (18%)	3 (2%)	4	24
14	N	58/60 (97%)	45 (78%)	11 (19%)	2 (3%)	3	19
15	O	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	10	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	81/83 (98%)	69 (85%)	10 (12%)	2 (2%)	4	24
17	Q	102/104 (98%)	87 (85%)	8 (8%)	7 (7%)	1	7
18	R	71/73 (97%)	59 (83%)	9 (13%)	3 (4%)	2	15
19	S	78/80 (98%)	62 (80%)	10 (13%)	6 (8%)	1	5
20	T	97/99 (98%)	70 (72%)	18 (19%)	9 (9%)	0	3
21	V	22/24 (92%)	18 (82%)	4 (18%)	0	100	100
All	All	2356/2396 (98%)	1935 (82%)	301 (13%)	120 (5%)	1	11

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	234	PRO
3	C	5	ILE
3	C	61	ALA
3	C	144	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/202 (100%)	202 (100%)	0	100	100
3	C	160/160 (100%)	160 (100%)	0	100	100
4	D	180/180 (100%)	180 (100%)	0	100	100
5	E	115/115 (100%)	115 (100%)	0	100	100
6	F	90/90 (100%)	90 (100%)	0	100	100
7	G	126/126 (100%)	126 (100%)	0	100	100
8	H	119/119 (100%)	119 (100%)	0	100	100
9	I	98/98 (100%)	98 (100%)	0	100	100
10	J	88/88 (100%)	88 (100%)	0	100	100
11	K	90/90 (100%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	104/104 (100%)	104 (100%)	0	100	100
13	M	100/100 (100%)	100 (100%)	0	100	100
14	N	49/49 (100%)	49 (100%)	0	100	100
15	O	79/79 (100%)	78 (99%)	1 (1%)	61	73
16	P	72/72 (100%)	72 (100%)	0	100	100
17	Q	96/96 (100%)	96 (100%)	0	100	100
18	R	64/64 (100%)	63 (98%)	1 (2%)	55	71
19	S	71/71 (100%)	71 (100%)	0	100	100
20	T	76/76 (100%)	76 (100%)	0	100	100
21	V	19/19 (100%)	19 (100%)	0	100	100
All	All	1998/1998 (100%)	1996 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	39	LEU
18	R	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	46	HIS
17	Q	93	GLN
3	C	170	GLN
4	D	74	GLN
4	D	161	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1508 (99%)	308 (20%)	51 (3%)
22	W	3/4 (75%)	0	0
23	X	9/11 (81%)	2 (22%)	1 (11%)
All	All	1519/1523 (99%)	310 (20%)	52 (3%)

5 of 310 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	20	U
1	A	26	A
1	A	32	A

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	968	U
1	A	1163	G
1	A	1379	C
1	A	969	U
1	A	1046	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	RSP	X	32	23	17,21,22	0.97	1 (5%)	21,30,33	1.12	2 (9%)

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
23	RSP	X	32	23	-	7/7/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	X	32	RSP	C2-N3	2.75	1.38	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	32	RSP	S2-C2-N3	-2.81	116.72	121.27
23	X	32	RSP	C1'-N1-C2	2.40	123.71	118.45

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	X	32	RSP	O4'-C4'-C5'-O5'
23	X	32	RSP	C3'-C4'-C5'-O5'
23	X	32	RSP	C2'-C1'-N1-C6
23	X	32	RSP	O4'-C1'-N1-C6
23	X	32	RSP	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 106 ligands modelled in this entry, 105 are monoatomic - leaving 1 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
24	PAR	A	1601	-	44,45,45	1.38	6 (13%)	63,67,67	1.68	13 (20%)

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
24	PAR	A	1601	-	-	2/18/94/94	1/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	C52-C42	4.35	1.61	1.52
24	A	1601	PAR	O54-C14	2.93	1.49	1.41
24	A	1601	PAR	C22-C12	-2.60	1.48	1.53
24	A	1601	PAR	C11-C21	2.56	1.57	1.52
24	A	1601	PAR	C14-C24	2.36	1.57	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1601	PAR	O33-C14-C24	6.73	119.08	108.08
24	A	1601	PAR	O34-C34-C44	-3.42	102.31	110.38
24	A	1601	PAR	C34-C24-N24	-3.13	104.63	111.05
24	A	1601	PAR	O43-C13-C23	-3.01	101.15	104.98
24	A	1601	PAR	O11-C11-O51	2.99	118.57	110.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	O51-C11-O11-C42
24	A	1601	PAR	C41-C51-C61-O61

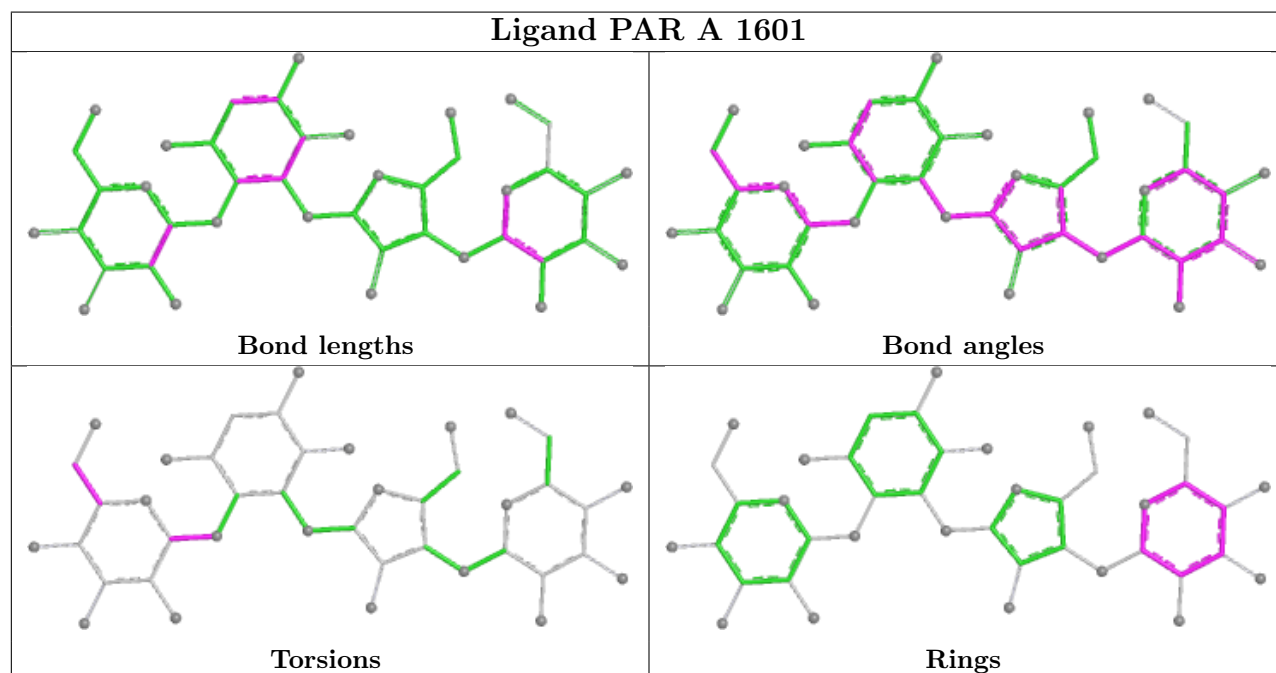
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C14-C24-C34-C44-C54-O54

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1601	PAR	1	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.



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 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1507/1508 (99%)	-0.39	14 (0%) 81 67	66, 105, 180, 256	0
2	B	234/234 (100%)	0.11	8 (3%) 48 32	105, 149, 202, 218	0
3	C	206/206 (100%)	0.20	8 (3%) 43 29	103, 141, 182, 195	0
4	D	208/208 (100%)	0.23	17 (8%) 17 14	91, 122, 158, 177	0
5	E	150/150 (100%)	-0.16	2 (1%) 75 57	75, 99, 125, 148	0
6	F	101/101 (100%)	0.15	3 (2%) 52 35	100, 135, 158, 171	0
7	G	155/155 (100%)	0.27	10 (6%) 25 17	102, 130, 176, 199	0
8	H	138/138 (100%)	-0.27	1 (0%) 84 71	74, 94, 124, 151	0
9	I	127/127 (100%)	0.47	9 (7%) 22 15	91, 146, 179, 196	0
10	J	98/98 (100%)	1.19	17 (17%) 4 4	100, 170, 236, 255	0
11	K	119/119 (100%)	0.24	8 (6%) 24 16	77, 108, 141, 171	0
12	L	124/124 (100%)	0.47	9 (7%) 21 15	66, 104, 143, 174	0
13	M	125/125 (100%)	0.43	8 (6%) 25 17	99, 139, 170, 217	0
14	N	60/60 (100%)	0.63	7 (11%) 9 9	110, 128, 163, 199	0
15	O	88/88 (100%)	0.25	7 (7%) 18 14	83, 108, 146, 186	0
16	P	83/83 (100%)	-0.06	0 100 100	78, 95, 120, 165	0
17	Q	104/104 (100%)	0.42	4 (3%) 44 30	71, 97, 141, 210	0
18	R	73/73 (100%)	0.26	2 (2%) 56 38	98, 118, 179, 216	0
19	S	80/80 (100%)	0.84	11 (13%) 6 6	123, 163, 195, 205	0
20	T	99/99 (100%)	0.46	9 (9%) 15 12	67, 101, 141, 148	0
21	V	24/24 (100%)	0.85	3 (12%) 8 7	109, 129, 151, 173	0
22	W	4/4 (100%)	1.98	1 (25%) 2 2	107, 109, 110, 138	0
23	X	9/11 (81%)	0.67	1 (11%) 10 10	117, 131, 190, 193	0
All	All	3916/3919 (99%)	0.03	159 (4%) 41 27	66, 116, 183, 256	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	3	ARG	11.9
9	I	128	ARG	9.3
11	K	128	ALA	7.2
10	J	73	ASP	6.6
11	K	129	SER	6.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	RSP	X	32	20/21	0.65	0.12	191,199,203,206	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	X	101	1/1	0.49	0.27	137,137,137,137	0
25	MG	A	1662	1/1	0.66	0.42	115,115,115,115	0
25	MG	A	1608	1/1	0.69	0.35	108,108,108,108	0
25	MG	A	1643	1/1	0.69	0.27	113,113,113,113	0
25	MG	A	1674	1/1	0.70	0.24	82,82,82,82	0
25	MG	A	1678	1/1	0.74	0.31	92,92,92,92	0
25	MG	A	1683	1/1	0.75	0.35	121,121,121,121	0
25	MG	A	1682	1/1	0.75	0.43	121,121,121,121	0
25	MG	A	1602	1/1	0.77	0.29	92,92,92,92	0
25	MG	A	1668	1/1	0.78	0.24	112,112,112,112	0
25	MG	A	1640	1/1	0.79	0.22	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1646	1/1	0.80	0.27	88,88,88,88	0
25	MG	A	1688	1/1	0.81	0.32	65,65,65,65	0
25	MG	A	1659	1/1	0.81	0.34	100,100,100,100	0
25	MG	A	1696	1/1	0.82	0.24	96,96,96,96	0
25	MG	A	1613	1/1	0.83	0.42	103,103,103,103	0
25	MG	A	1663	1/1	0.84	0.41	98,98,98,98	0
25	MG	A	1680	1/1	0.85	0.41	95,95,95,95	0
25	MG	A	1667	1/1	0.85	0.50	101,101,101,101	0
25	MG	A	1619	1/1	0.85	0.30	94,94,94,94	0
25	MG	A	1625	1/1	0.86	0.33	65,65,65,65	0
25	MG	A	1693	1/1	0.86	0.53	83,83,83,83	0
25	MG	A	1656	1/1	0.86	0.36	71,71,71,71	0
25	MG	A	1636	1/1	0.86	0.28	86,86,86,86	0
25	MG	A	1695	1/1	0.87	0.17	105,105,105,105	0
25	MG	A	1690	1/1	0.87	0.30	87,87,87,87	0
25	MG	A	1637	1/1	0.87	0.43	107,107,107,107	0
25	MG	A	1673	1/1	0.88	0.17	115,115,115,115	0
25	MG	A	1634	1/1	0.88	0.58	97,97,97,97	0
25	MG	A	1609	1/1	0.88	0.25	119,119,119,119	0
25	MG	A	1604	1/1	0.88	0.36	86,86,86,86	0
25	MG	A	1652	1/1	0.88	0.26	70,70,70,70	0
25	MG	A	1638	1/1	0.88	0.28	84,84,84,84	0
25	MG	A	1677	1/1	0.89	0.19	91,91,91,91	0
25	MG	A	1611	1/1	0.89	0.27	101,101,101,101	0
25	MG	A	1685	1/1	0.89	0.26	86,86,86,86	0
25	MG	A	1686	1/1	0.89	0.34	93,93,93,93	0
25	MG	A	1664	1/1	0.89	0.09	98,98,98,98	0
25	MG	A	1666	1/1	0.90	0.23	84,84,84,84	0
25	MG	A	1641	1/1	0.90	0.23	63,63,63,63	0
25	MG	A	1631	1/1	0.90	0.35	64,64,64,64	0
25	MG	A	1624	1/1	0.90	0.34	56,56,56,56	0
25	MG	A	1610	1/1	0.90	0.18	88,88,88,88	0
25	MG	A	1654	1/1	0.90	0.33	82,82,82,82	0
25	MG	A	1626	1/1	0.91	0.24	76,76,76,76	0
25	MG	A	1605	1/1	0.91	0.12	94,94,94,94	0
25	MG	A	1689	1/1	0.91	0.50	83,83,83,83	0
25	MG	A	1658	1/1	0.91	0.26	76,76,76,76	0
25	MG	A	1681	1/1	0.91	0.44	91,91,91,91	0
25	MG	A	1645	1/1	0.91	0.12	67,67,67,67	0
25	MG	A	1633	1/1	0.91	0.32	99,99,99,99	0
25	MG	J	201	1/1	0.91	0.25	90,90,90,90	0
25	MG	A	1620	1/1	0.91	0.32	56,56,56,56	0

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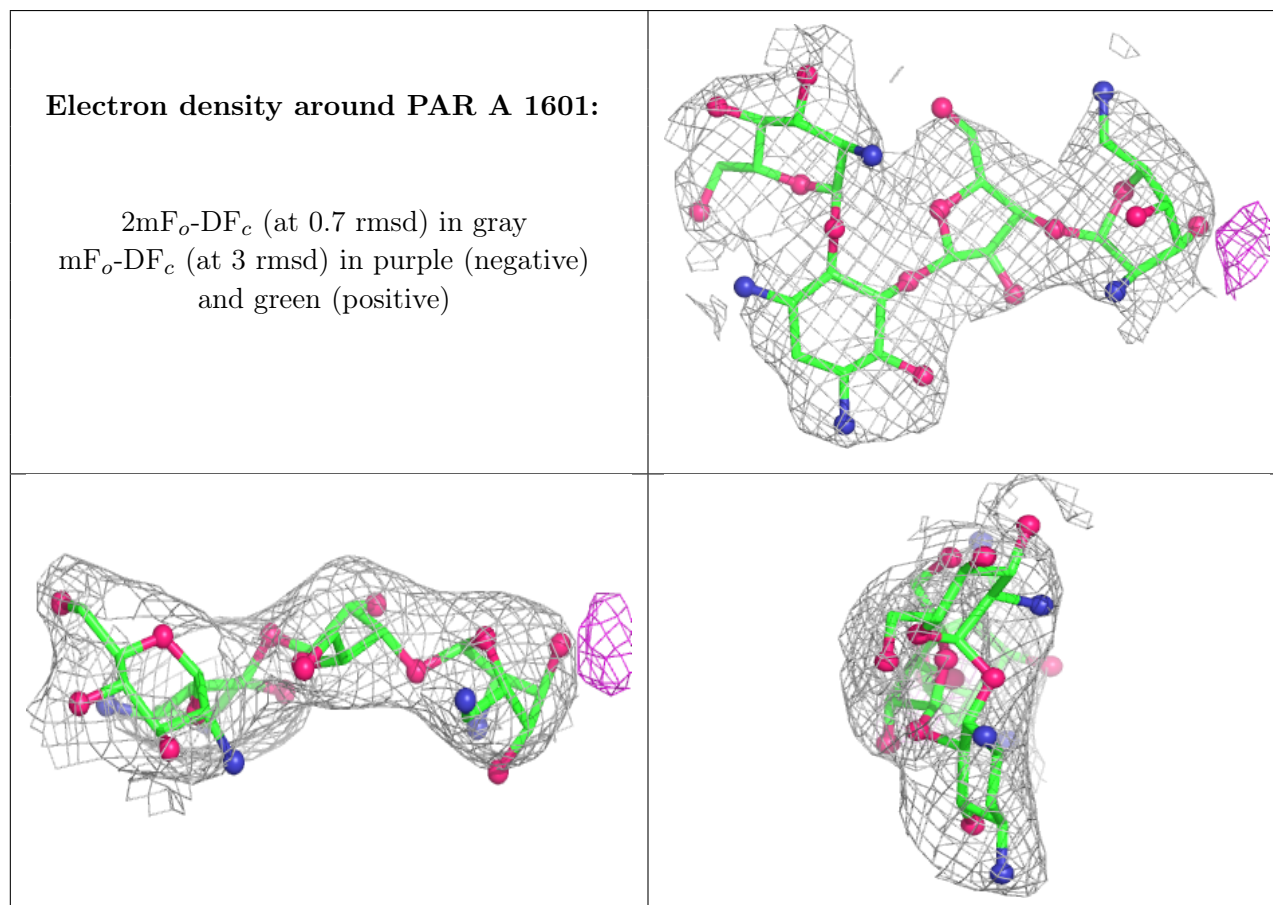
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1623	1/1	0.92	0.39	81,81,81,81	0
25	MG	A	1672	1/1	0.92	0.29	89,89,89,89	0
25	MG	A	1630	1/1	0.92	0.14	81,81,81,81	0
25	MG	A	1603	1/1	0.92	0.19	76,76,76,76	0
25	MG	A	1661	1/1	0.92	0.68	83,83,83,83	0
25	MG	A	1691	1/1	0.92	0.36	93,93,93,93	0
25	MG	A	1692	1/1	0.92	0.43	86,86,86,86	0
25	MG	A	1632	1/1	0.92	0.30	75,75,75,75	0
25	MG	A	1639	1/1	0.92	0.21	81,81,81,81	0
25	MG	A	1653	1/1	0.92	0.46	88,88,88,88	0
25	MG	A	1699	1/1	0.92	0.20	94,94,94,94	0
25	MG	A	1617	1/1	0.92	0.18	101,101,101,101	0
25	MG	A	1655	1/1	0.92	0.27	71,71,71,71	0
25	MG	A	1649	1/1	0.93	0.39	78,78,78,78	0
25	MG	A	1687	1/1	0.93	0.41	105,105,105,105	0
25	MG	A	1676	1/1	0.93	0.41	133,133,133,133	0
25	MG	A	1671	1/1	0.93	0.54	74,74,74,74	0
25	MG	A	1694	1/1	0.93	0.39	72,72,72,72	0
25	MG	A	1684	1/1	0.94	0.10	82,82,82,82	0
25	MG	A	1697	1/1	0.94	0.14	94,94,94,94	0
25	MG	A	1621	1/1	0.94	0.34	62,62,62,62	0
25	MG	A	1627	1/1	0.94	0.29	66,66,66,66	0
25	MG	W	101	1/1	0.94	0.20	84,84,84,84	0
25	MG	A	1615	1/1	0.94	0.29	84,84,84,84	0
24	PAR	A	1601	42/42	0.95	0.10	76,88,98,105	0
25	MG	A	1642	1/1	0.95	0.20	63,63,63,63	0
25	MG	A	1616	1/1	0.95	0.37	91,91,91,91	0
25	MG	A	1644	1/1	0.95	0.23	86,86,86,86	0
25	MG	A	1614	1/1	0.95	0.16	111,111,111,111	0
25	MG	A	1698	1/1	0.95	0.48	100,100,100,100	0
25	MG	A	1618	1/1	0.95	0.29	70,70,70,70	0
25	MG	A	1669	1/1	0.95	0.21	90,90,90,90	0
25	MG	J	202	1/1	0.95	0.18	95,95,95,95	0
25	MG	A	1629	1/1	0.95	0.26	59,59,59,59	0
25	MG	A	1650	1/1	0.95	0.19	67,67,67,67	0
25	MG	A	1647	1/1	0.96	0.16	88,88,88,88	0
25	MG	E	201	1/1	0.96	0.40	66,66,66,66	0
25	MG	A	1670	1/1	0.96	0.27	85,85,85,85	0
25	MG	A	1675	1/1	0.96	0.31	97,97,97,97	0
25	MG	A	1648	1/1	0.96	0.34	81,81,81,81	0
25	MG	A	1635	1/1	0.96	0.34	79,79,79,79	0
26	ZN	D	301	1/1	0.96	0.23	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1622	1/1	0.97	0.27	65,65,65,65	0
25	MG	A	1612	1/1	0.97	0.40	97,97,97,97	0
25	MG	A	1606	1/1	0.97	0.61	79,79,79,79	0
25	MG	A	1679	1/1	0.97	0.28	85,85,85,85	0
25	MG	A	1657	1/1	0.97	0.29	60,60,60,60	0
25	MG	A	1628	1/1	0.97	0.38	84,84,84,84	0
25	MG	A	1660	1/1	0.98	0.10	68,68,68,68	0
25	MG	A	1607	1/1	0.98	0.16	104,104,104,104	0
25	MG	A	1651	1/1	0.98	0.08	67,67,67,67	0
25	MG	A	1665	1/1	0.99	0.04	61,61,61,61	0
26	ZN	N	101	1/1	1.00	0.03	125,125,125,125	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.