



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 07:24 pm BST

PDB ID : 6MPF
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

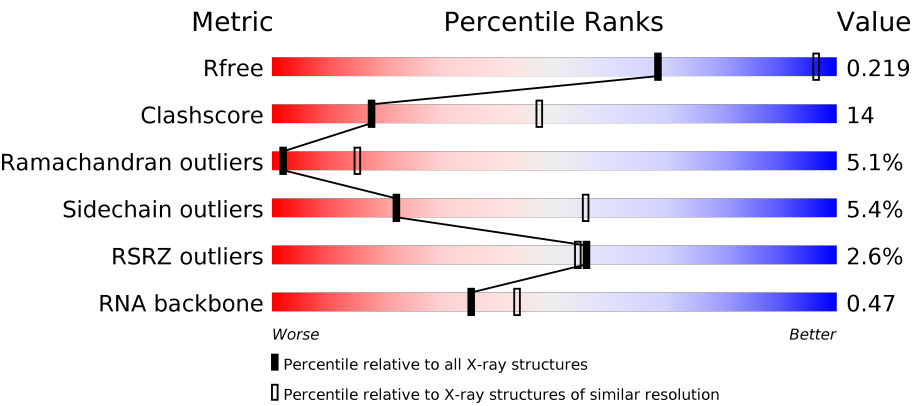
1 Overall quality at a glance i

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.







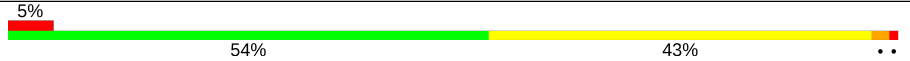
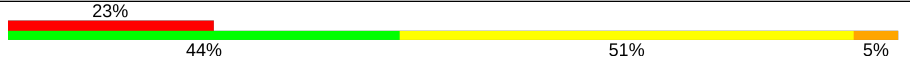
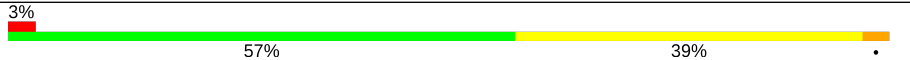
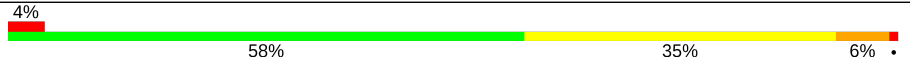
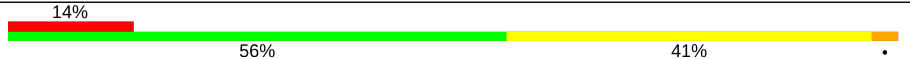
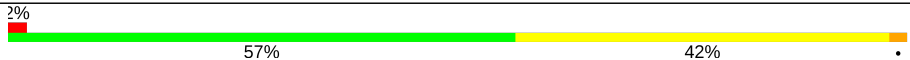
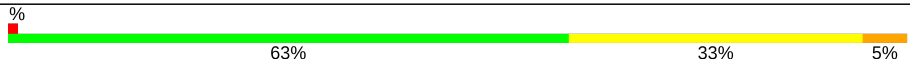
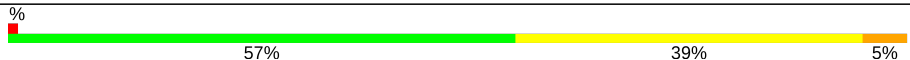
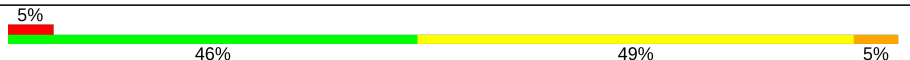
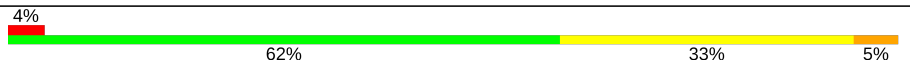
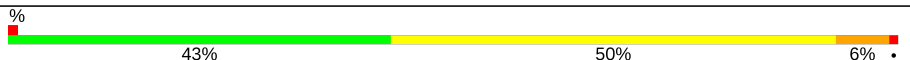

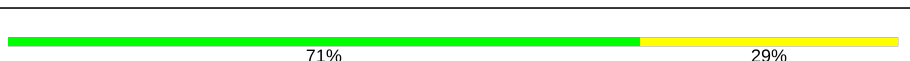
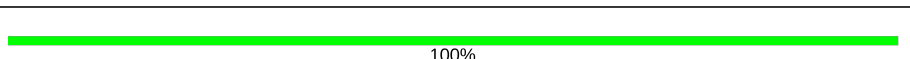
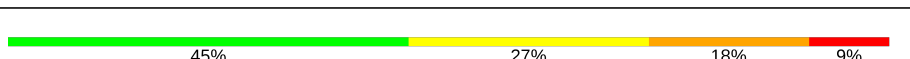
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)
RNA backbone	3102	1129 (3.78-2.90)

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 on 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	<div><div></div><div><div>39%</div><div>39%</div><div>18%</div><div>.</div></div></div>
2	B	234	<div><div>5%</div><div></div><div><div>50%</div><div>43%</div><div>6%</div><div>.</div></div></div>
3	C	206	<div><div>3%</div><div></div><div><div>53%</div><div>38%</div><div>8%</div><div>.</div></div></div>
4	D	208	<div><div>3%</div><div></div><div><div>58%</div><div>39%</div><div>.</div></div></div>

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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	1602	-	-	-	X
25	MG	A	1606	-	-	-	X
25	MG	A	1611	-	-	-	X
25	MG	A	1612	-	-	-	X
25	MG	A	1613	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1617	-	-	-	X
25	MG	A	1628	-	-	-	X
25	MG	A	1634	-	-	-	X
25	MG	A	1648	-	-	-	X
25	MG	A	1653	-	-	-	X
25	MG	A	1664	-	-	-	X
25	MG	A	1675	-	-	-	X
25	MG	A	1676	-	-	-	X
25	MG	A	1679	-	-	-	X
25	MG	A	1683	-	-	-	X
25	MG	A	1685	-	-	-	X
25	MG	A	1686	-	-	-	X
25	MG	A	1687	-	-	-	X
25	MG	A	1691	-	-	-	X
25	MG	A	1692	-	-	-	X
25	MG	A	1698	-	-	-	X
25	MG	A	1699	-	-	-	X

2 Entry composition

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
1	A	1508	Total	C	N	O	P	22	0	0
			32415	14427	6005	10475	1508			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

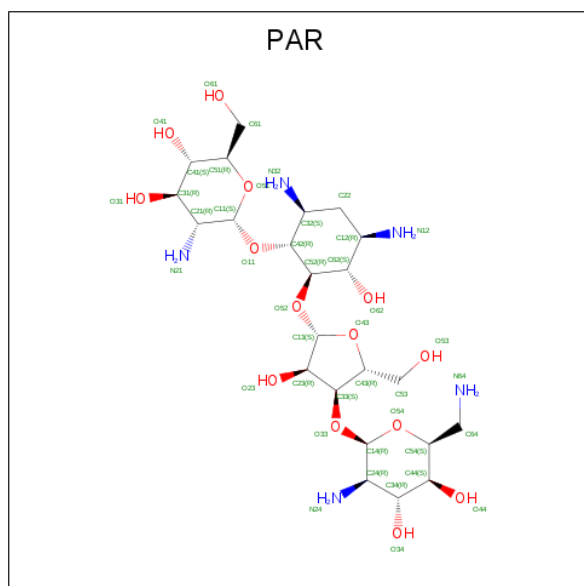
- Molecule 22 is a RNA chain called mRNA A-site fragment.

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

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

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

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	X	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	W	1	Total 1	Mg 1	0	0
25	J	2	Total 2	Mg 2	0	0
25	A	98	Total 98	Mg 98	0	0
25	E	1	Total 1	Mg 1	0	0

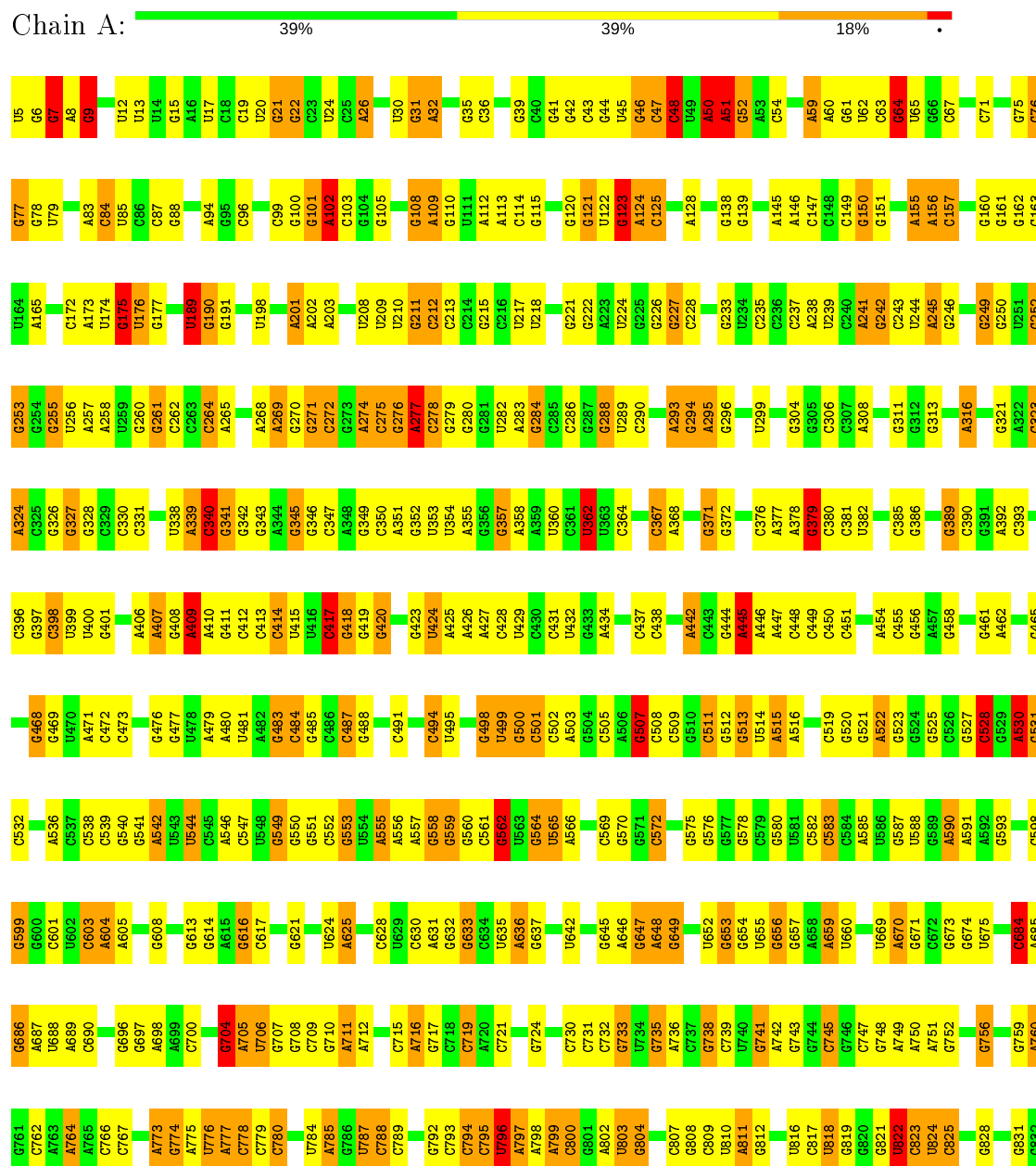
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

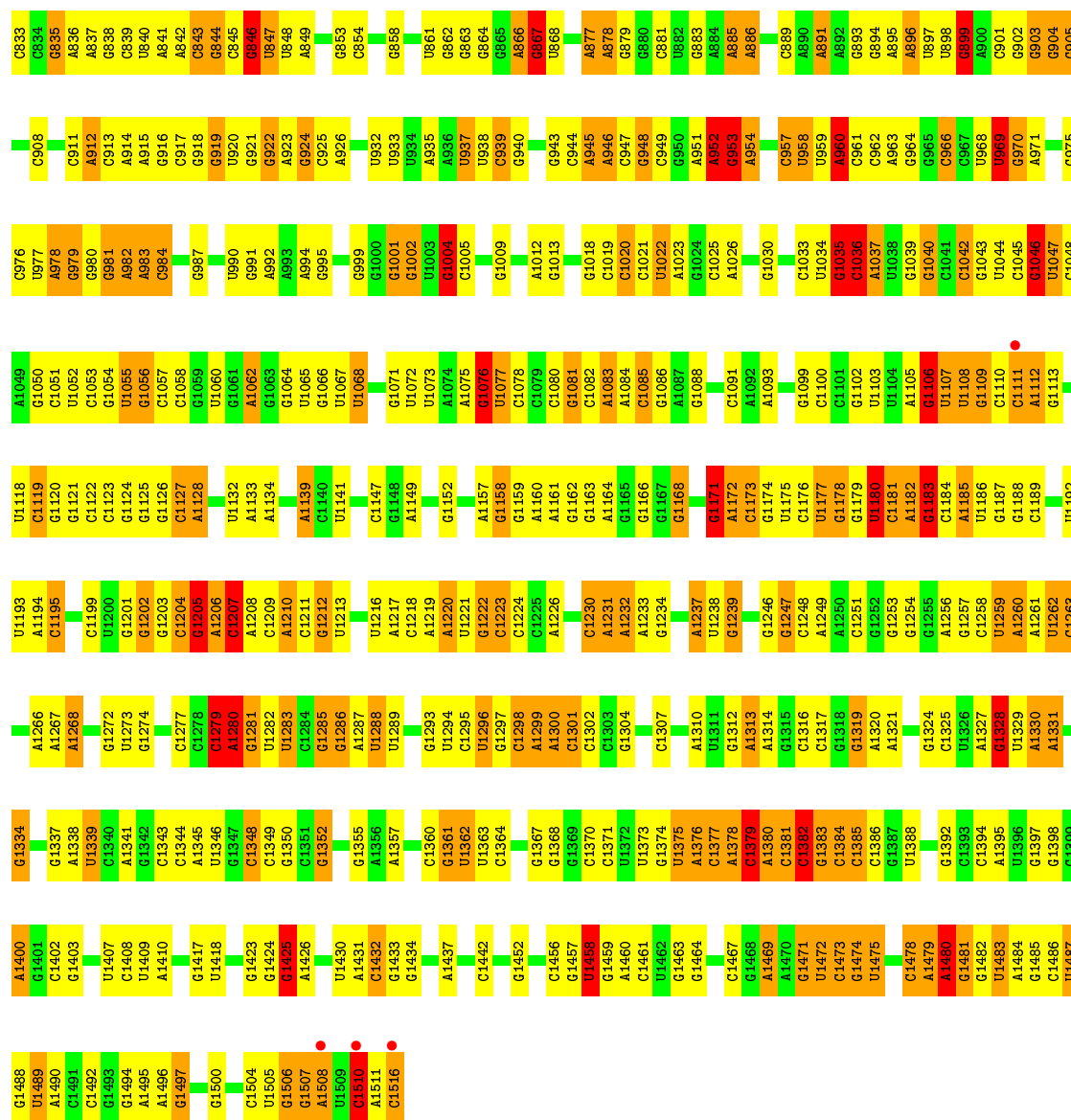
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total 1	Zn 1	0	0
26	N	1	Total 1	Zn 1	0	0

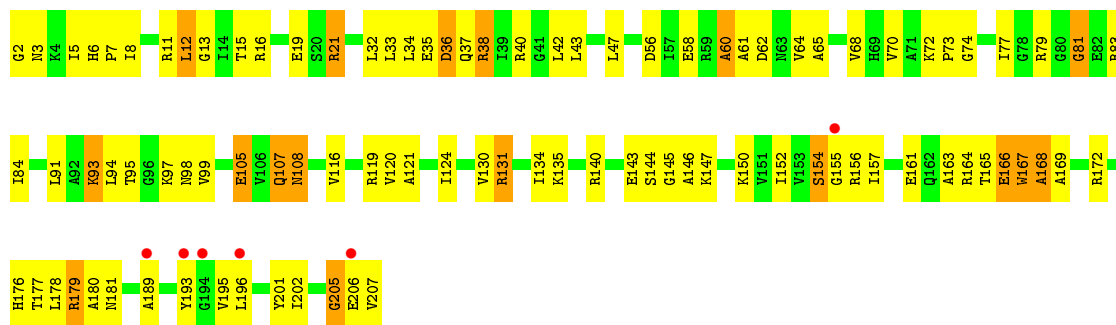
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

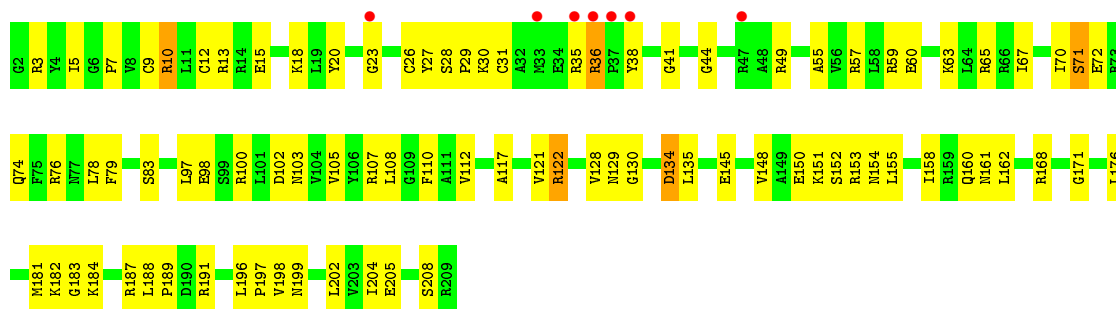
• Molecule 1: 16S rRNA



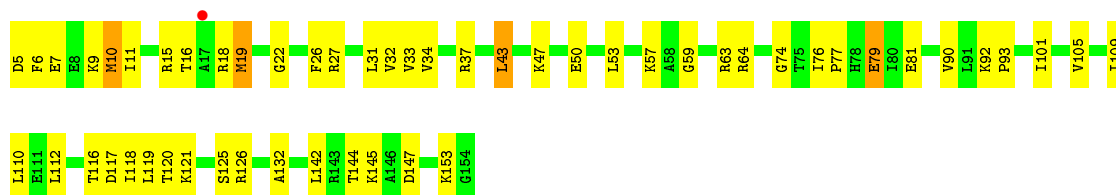




• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

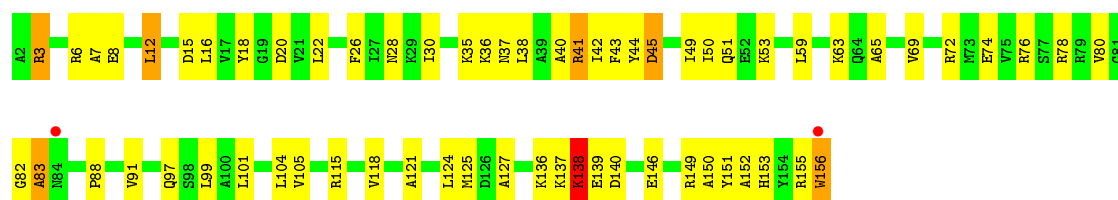


• Molecule 6: 30S ribosomal protein S6

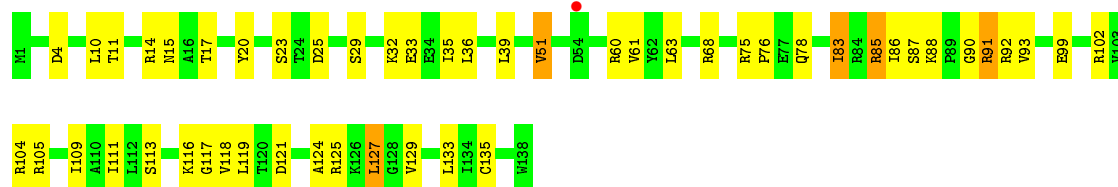


• Molecule 7: 30S ribosomal protein S7

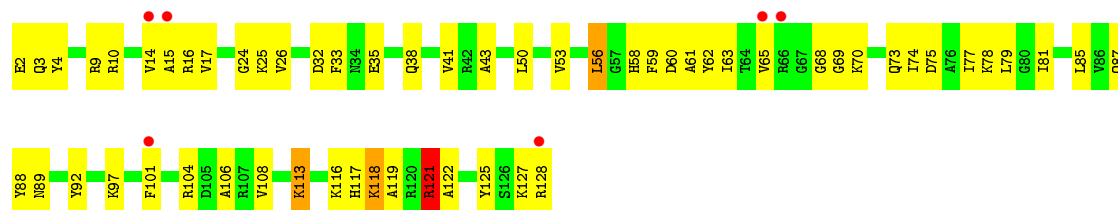




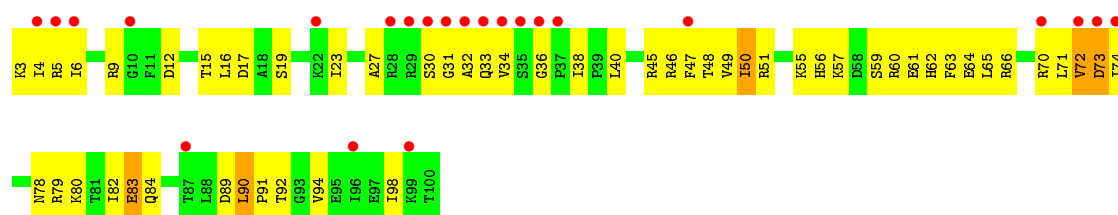
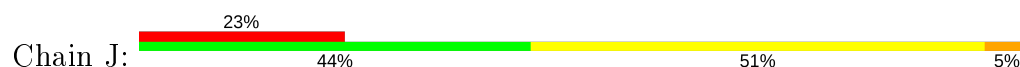
• Molecule 8: 30S ribosomal protein S8



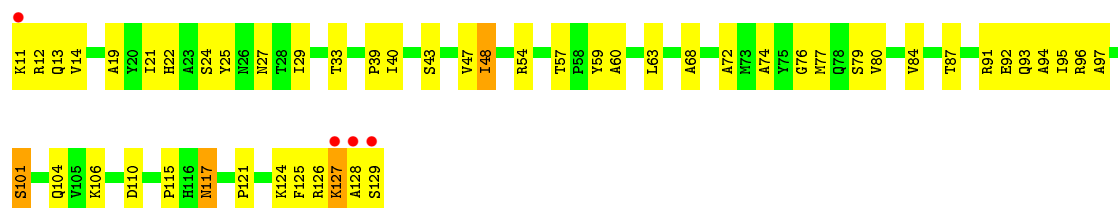
• Molecule 9: 30S ribosomal protein S9



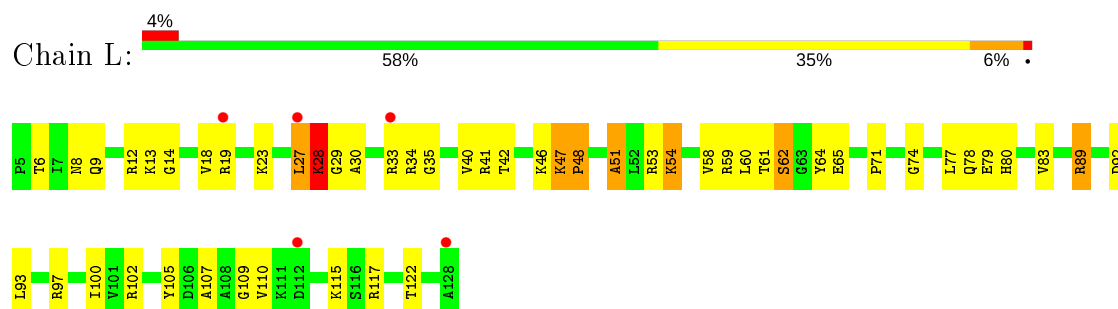
• Molecule 10: 30S ribosomal protein S10



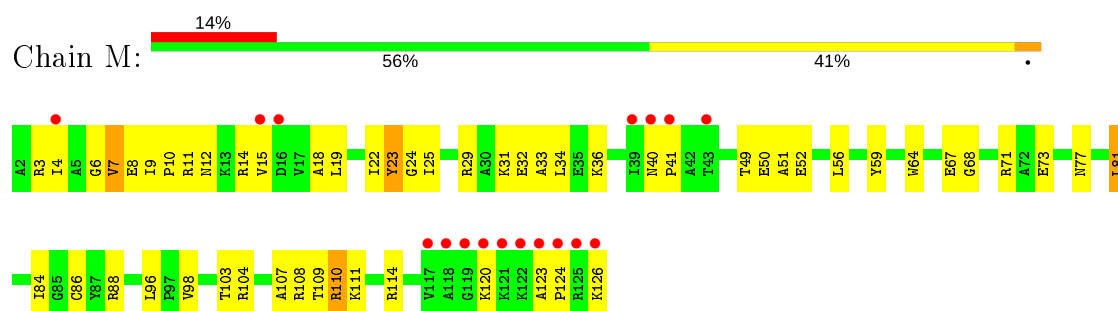
• Molecule 11: 30S ribosomal protein S11



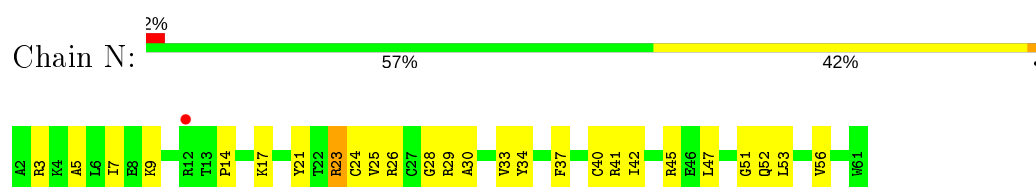
- Molecule 12: 30S ribosomal protein S12



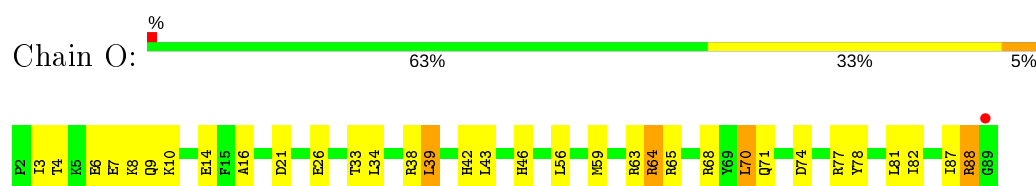
- Molecule 13: 30S ribosomal protein S13



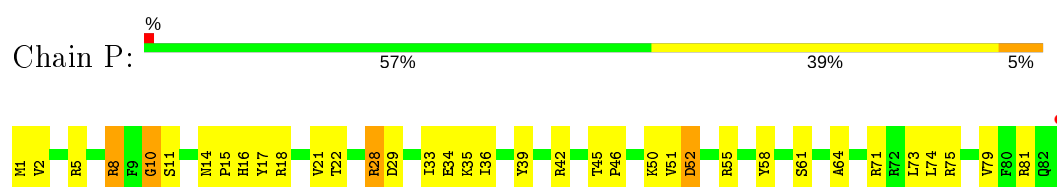
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

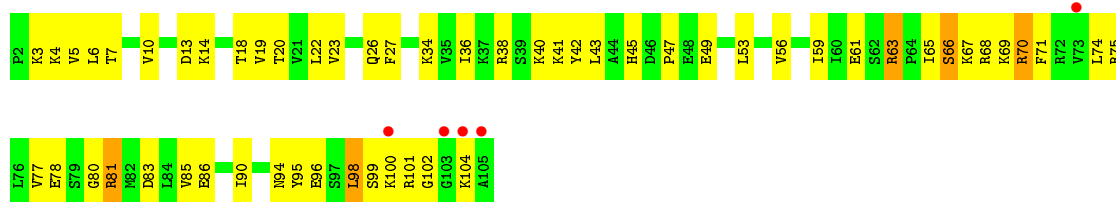


- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17





- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



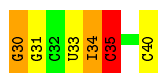
- Molecule 22: mRNA A-site fragment



There are no outlier residues recorded for this chain.

- Molecule 23: tRNA ASL Escherichia coli Arg1

Chain X: 45% 27% 18% 9%



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)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.178 , 0.219 0.178 , 0.219	Depositor DCC
R_{free} test set	1895 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	118.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 101.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, RSP, PAR

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	1.05	59/36285 (0.2%)	1.70	908/56631 (1.6%)
2	B	0.46	0/1935	0.66	0/2609
3	C	0.50	0/1636	0.69	0/2205
4	D	0.49	0/1733	0.70	0/2318
5	E	0.64	0/1162	0.81	1/1564 (0.1%)
6	F	0.46	0/856	0.65	0/1154
7	G	0.47	0/1276	0.65	1/1709 (0.1%)
8	H	0.67	0/1136	0.82	2/1527 (0.1%)
9	I	0.48	0/1029	0.70	1/1379 (0.1%)
10	J	0.48	0/807	0.70	0/1085
11	K	0.52	0/900	0.72	0/1213
12	L	0.68	0/986	0.90	1/1320 (0.1%)
13	M	0.47	0/1008	0.68	0/1347
14	N	0.50	0/501	0.68	0/664
15	O	0.50	0/745	0.75	1/992 (0.1%)
16	P	0.62	0/716	0.81	0/963
17	Q	0.72	0/870	0.81	1/1159 (0.1%)
18	R	0.54	0/604	0.67	0/801
19	S	0.43	0/661	0.66	0/890
20	T	0.56	0/765	0.87	3/1007 (0.3%)
21	V	0.47	0/212	0.68	0/277
22	W	0.97	0/91	1.62	0/140
23	X	0.95	0/235	1.52	4/360 (1.1%)
All	All	0.90	59/56149 (0.1%)	1.47	923/83314 (1.1%)

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
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

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	G	N1-C2	17.96	1.52	1.37
1	A	564	G	C5-C6	-15.25	1.27	1.42
1	A	564	G	C6-N1	12.96	1.48	1.39
1	A	564	G	N9-C8	11.08	1.45	1.37
1	A	564	G	N7-C5	-10.97	1.32	1.39

The worst 5 of 923 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	564	G	N1-C6-O6	42.19	145.22	119.90
1	A	564	G	C5-C6-O6	-33.26	108.64	128.60
1	A	564	G	C4-C5-N7	27.13	121.65	110.80
1	A	564	G	N3-C2-N2	-25.32	102.17	119.90
1	A	564	G	C5-N7-C8	-23.55	92.52	104.30

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 ⓘ

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	502	0
2	B	1900	0	1951	89	0
3	C	1612	0	1677	90	0
4	D	1703	0	1763	60	0
5	E	1146	0	1207	35	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	42	0
10	J	794	0	840	51	1
11	K	885	0	904	33	0
12	L	970	0	1057	39	0
13	M	997	0	1072	41	0
14	N	492	0	529	31	0
15	O	734	0	771	29	0
16	P	700	0	720	25	0
17	Q	857	0	928	39	0
18	R	598	0	670	31	0
19	S	647	0	673	43	0
20	T	763	0	860	32	0
21	V	208	0	221	6	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	36782	1183	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 1183 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)
18:R:54:ARG:HH12	18:R:55:ARG:CG	1.67	1.07
2:B:178:ARG:HH21	2:B:196:LEU:C	1.56	1.06
18:R:54:ARG:NH1	18:R:55:ARG:HG2	1.70	1.05
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	9
3	C	204/206 (99%)	150 (74%)	39 (19%)	15 (7%)	1	8
4	D	206/208 (99%)	179 (87%)	20 (10%)	7 (3%)	3	24
5	E	148/150 (99%)	133 (90%)	12 (8%)	3 (2%)	7	34
6	F	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	49
7	G	153/155 (99%)	129 (84%)	16 (10%)	8 (5%)	2	14
8	H	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	10	40
9	I	125/127 (98%)	106 (85%)	15 (12%)	4 (3%)	4	25
10	J	96/98 (98%)	66 (69%)	18 (19%)	12 (12%)	0	2
11	K	117/119 (98%)	98 (84%)	12 (10%)	7 (6%)	1	12
12	L	122/124 (98%)	94 (77%)	16 (13%)	12 (10%)	0	4
13	M	123/125 (98%)	98 (80%)	22 (18%)	3 (2%)	6	31
14	N	58/60 (97%)	45 (78%)	11 (19%)	2 (3%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	13	45
16	P	81/83 (98%)	69 (85%)	10 (12%)	2 (2%)	5	30
17	Q	102/104 (98%)	87 (85%)	8 (8%)	7 (7%)	1	9
18	R	71/73 (97%)	59 (83%)	9 (13%)	3 (4%)	3	19
19	S	78/80 (98%)	62 (80%)	10 (13%)	6 (8%)	1	7
20	T	97/99 (98%)	70 (72%)	18 (19%)	9 (9%)	0	4
21	V	22/24 (92%)	18 (82%)	4 (18%)	0	100	100
All	All	2356/2396 (98%)	1935 (82%)	301 (13%)	120 (5%)	2	15

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 ⓘ

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%)	185 (92%)	17 (8%)	11	38
3	C	160/160 (100%)	152 (95%)	8 (5%)	24	57
4	D	180/180 (100%)	169 (94%)	11 (6%)	18	51
5	E	115/115 (100%)	106 (92%)	9 (8%)	12	41
6	F	90/90 (100%)	86 (96%)	4 (4%)	28	61
7	G	126/126 (100%)	118 (94%)	8 (6%)	18	49
8	H	119/119 (100%)	115 (97%)	4 (3%)	37	67
9	I	98/98 (100%)	91 (93%)	7 (7%)	14	45
10	J	88/88 (100%)	84 (96%)	4 (4%)	27	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	90/90 (100%)	88 (98%)	2 (2%)	52	76
12	L	104/104 (100%)	100 (96%)	4 (4%)	33	64
13	M	100/100 (100%)	94 (94%)	6 (6%)	19	51
14	N	49/49 (100%)	48 (98%)	1 (2%)	55	78
15	O	79/79 (100%)	76 (96%)	3 (4%)	33	64
16	P	72/72 (100%)	67 (93%)	5 (7%)	15	47
17	Q	96/96 (100%)	92 (96%)	4 (4%)	30	62
18	R	64/64 (100%)	63 (98%)	1 (2%)	62	81
19	S	71/71 (100%)	66 (93%)	5 (7%)	15	46
20	T	76/76 (100%)	73 (96%)	3 (4%)	32	63
21	V	19/19 (100%)	18 (95%)	1 (5%)	22	56
All	All	1998/1998 (100%)	1891 (95%)	107 (5%)	22	55

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	92	LYS
8	H	92	ARG
19	S	6	LYS
7	G	3	ARG
7	G	76	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	161	ASN
15	O	46	HIS
6	F	73	ASN
3	C	6	HIS
9	I	38	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1508 (99%)	303 (20%)	51 (3%)
22	W	3/4 (75%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	X	9/11 (81%)	3 (33%)	1 (11%)
All	All	1519/1523 (99%)	306 (20%)	52 (3%)

5 of 306 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	795	C
1	A	969	U
1	A	1378	A
1	A	847	U
1	A	867	G

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

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	15,21,22	1.21	1 (6%)	16,30,33	1.57	1 (6%)

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	-	5/5/25/26	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	C6-N1	3.80	1.40	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	32	RSP	C2-N3-C4	5.30	121.41	115.51

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	X	32	RSP	C2'-C1'-N1-C6
23	X	32	RSP	O4'-C1'-N1-C6
23	X	32	RSP	C3'-C4'-C5'-O5'
23	X	32	RSP	O4'-C4'-C5'-O5'
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 carbohydrates 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	-	45,45,45	1.42	7 (15%)	64,67,67	1.70	15 (23%)

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 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	C52-C42	4.32	1.61	1.52
24	A	1601	PAR	O54-C14	2.96	1.49	1.41
24	A	1601	PAR	C64-C54	2.91	1.56	1.52
24	A	1601	PAR	C11-C21	2.55	1.57	1.52
24	A	1601	PAR	C22-C12	-2.52	1.48	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1601	PAR	O33-C14-C24	6.31	119.08	108.22
24	A	1601	PAR	O52-C13-C23	3.86	115.95	107.96
24	A	1601	PAR	O34-C34-C44	-3.48	102.31	110.35
24	A	1601	PAR	C34-C24-N24	-3.13	104.63	111.05
24	A	1601	PAR	O43-C13-C23	-2.97	101.15	104.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

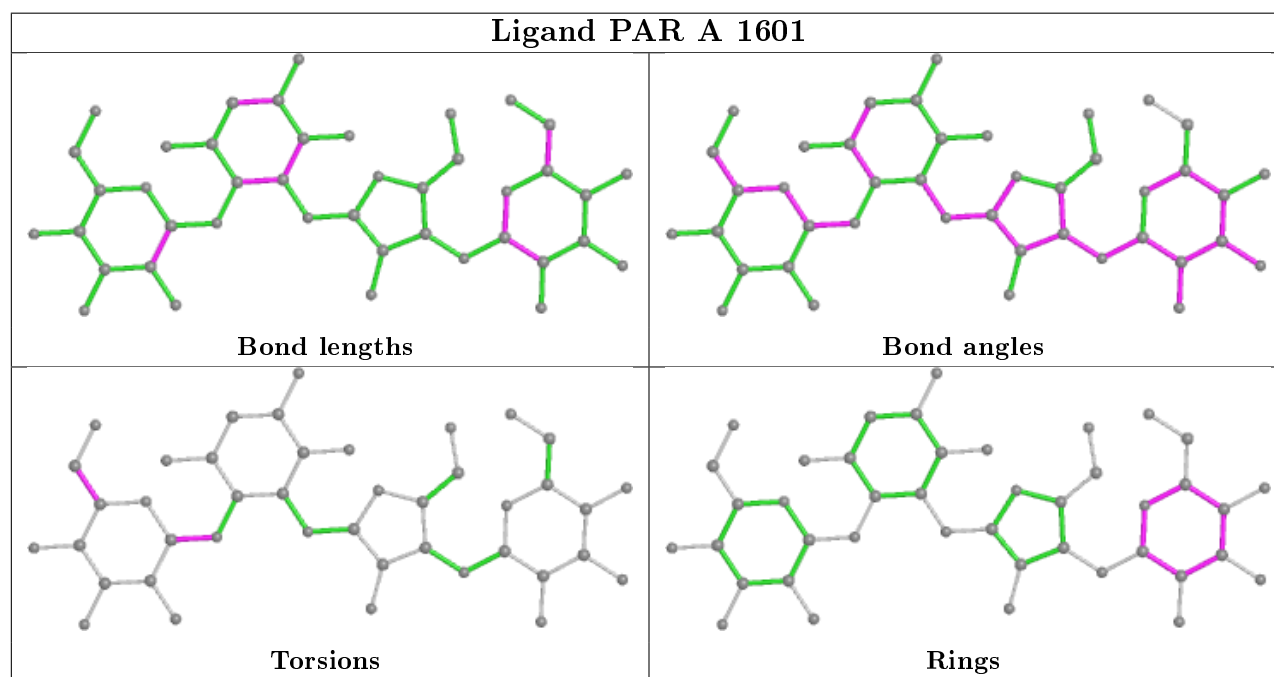
All (1) ring outliers are listed below:

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.11	4 (0%) 94 95	66, 105, 180, 256	0
2	B	234/234 (100%)	0.31	12 (5%) 28 28	105, 149, 202, 218	0
3	C	206/206 (100%)	-0.06	6 (2%) 51 51	103, 141, 182, 195	0
4	D	208/208 (100%)	0.08	7 (3%) 45 44	91, 122, 158, 177	0
5	E	150/150 (100%)	-0.15	1 (0%) 87 90	75, 99, 125, 148	0
6	F	101/101 (100%)	-0.18	1 (0%) 82 83	100, 135, 158, 171	0
7	G	155/155 (100%)	-0.20	2 (1%) 77 78	102, 130, 176, 199	0
8	H	138/138 (100%)	-0.14	1 (0%) 87 90	74, 94, 124, 151	0
9	I	127/127 (100%)	0.30	6 (4%) 31 32	91, 146, 179, 196	0
10	J	98/98 (100%)	1.00	23 (23%) 0 0	100, 170, 236, 255	0
11	K	119/119 (100%)	0.04	4 (3%) 45 44	77, 108, 141, 171	0
12	L	124/124 (100%)	0.05	5 (4%) 38 37	66, 104, 143, 174	0
13	M	125/125 (100%)	0.70	17 (13%) 3 2	99, 139, 170, 217	0
14	N	60/60 (100%)	0.23	1 (1%) 70 69	110, 128, 163, 199	0
15	O	88/88 (100%)	0.03	1 (1%) 80 81	83, 108, 146, 186	0
16	P	83/83 (100%)	0.20	1 (1%) 79 79	78, 95, 120, 165	0
17	Q	104/104 (100%)	0.35	5 (4%) 30 31	71, 97, 141, 210	0
18	R	73/73 (100%)	0.29	3 (4%) 37 36	98, 118, 179, 216	0
19	S	80/80 (100%)	0.06	1 (1%) 77 78	123, 163, 195, 205	0
20	T	99/99 (100%)	0.15	1 (1%) 82 83	67, 101, 141, 148	0
21	V	24/24 (100%)	0.28	0 100 100	109, 129, 151, 173	0
22	W	4/4 (100%)	1.21	0 100 100	107, 109, 110, 138	0
23	X	9/11 (81%)	0.23	0 100 100	117, 131, 190, 193	0
All	All	3916/3919 (99%)	0.04	102 (2%) 56 54	66, 116, 183, 256	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	124	PRO	8.5
17	Q	105	ALA	7.3
11	K	128	ALA	7.1
13	M	126	LYS	7.1
10	J	28	ARG	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	0.73	0.25	191,199,203,206	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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	A	1613	1/1	0.38	0.72	103,103,103,103	0
25	MG	A	1611	1/1	0.51	0.49	101,101,101,101	0
25	MG	A	1686	1/1	0.56	0.81	93,93,93,93	0
25	MG	A	1606	1/1	0.60	1.37	79,79,79,79	0
25	MG	A	1612	1/1	0.62	0.94	97,97,97,97	0
25	MG	A	1643	1/1	0.62	0.28	113,113,113,113	0
25	MG	A	1674	1/1	0.63	0.38	82,82,82,82	0
25	MG	A	1617	1/1	0.63	1.49	101,101,101,101	0
25	MG	A	1676	1/1	0.64	0.50	133,133,133,133	0
25	MG	A	1648	1/1	0.64	0.61	81,81,81,81	0
25	MG	A	1698	1/1	0.65	1.26	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1609	1/1	0.66	0.31	119,119,119,119	0
25	MG	A	1691	1/1	0.68	0.50	93,93,93,93	0
25	MG	A	1687	1/1	0.68	0.70	105,105,105,105	0
25	MG	A	1664	1/1	0.69	0.47	98,98,98,98	0
25	MG	A	1634	1/1	0.70	1.29	97,97,97,97	0
25	MG	A	1699	1/1	0.70	1.02	94,94,94,94	0
25	MG	A	1675	1/1	0.71	0.69	97,97,97,97	0
25	MG	A	1683	1/1	0.72	1.04	121,121,121,121	0
25	MG	A	1602	1/1	0.75	0.75	92,92,92,92	0
25	MG	A	1679	1/1	0.75	0.52	85,85,85,85	0
25	MG	A	1692	1/1	0.77	1.31	86,86,86,86	0
25	MG	A	1628	1/1	0.79	0.69	84,84,84,84	0
25	MG	A	1685	1/1	0.79	0.69	86,86,86,86	0
25	MG	A	1607	1/1	0.79	0.34	104,104,104,104	0
25	MG	A	1697	1/1	0.79	0.38	94,94,94,94	0
25	MG	A	1605	1/1	0.80	0.13	94,94,94,94	0
25	MG	A	1653	1/1	0.80	0.60	88,88,88,88	0
25	MG	X	101	1/1	0.81	0.47	137,137,137,137	0
25	MG	A	1662	1/1	0.82	1.03	115,115,115,115	0
25	MG	A	1614	1/1	0.82	0.50	111,111,111,111	0
25	MG	A	1633	1/1	0.82	0.62	99,99,99,99	0
25	MG	A	1677	1/1	0.83	0.37	91,91,91,91	0
25	MG	A	1671	1/1	0.83	1.22	74,74,74,74	0
25	MG	W	101	1/1	0.84	0.70	84,84,84,84	0
25	MG	A	1608	1/1	0.85	0.21	108,108,108,108	0
25	MG	A	1681	1/1	0.85	0.78	91,91,91,91	0
25	MG	A	1610	1/1	0.85	0.37	88,88,88,88	0
25	MG	A	1663	1/1	0.85	0.59	98,98,98,98	0
25	MG	A	1646	1/1	0.86	0.31	88,88,88,88	0
25	MG	J	202	1/1	0.86	0.39	95,95,95,95	0
25	MG	A	1632	1/1	0.87	0.61	75,75,75,75	0
25	MG	A	1668	1/1	0.87	0.13	112,112,112,112	0
25	MG	A	1678	1/1	0.87	0.35	92,92,92,92	0
25	MG	A	1635	1/1	0.87	0.88	79,79,79,79	0
25	MG	A	1618	1/1	0.88	0.96	70,70,70,70	0
25	MG	E	201	1/1	0.88	0.94	66,66,66,66	0
25	MG	A	1649	1/1	0.89	0.85	78,78,78,78	0
25	MG	A	1665	1/1	0.89	0.12	61,61,61,61	0
25	MG	A	1623	1/1	0.90	0.46	81,81,81,81	0
25	MG	A	1673	1/1	0.90	0.24	115,115,115,115	0
25	MG	A	1680	1/1	0.91	0.46	95,95,95,95	0
25	MG	A	1654	1/1	0.91	0.33	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1604	1/1	0.91	0.39	86,86,86,86	0
25	MG	A	1672	1/1	0.92	0.99	89,89,89,89	0
25	MG	A	1696	1/1	0.92	0.40	96,96,96,96	0
25	MG	A	1619	1/1	0.92	0.29	94,94,94,94	0
25	MG	A	1636	1/1	0.92	0.63	86,86,86,86	0
25	MG	A	1637	1/1	0.93	1.01	107,107,107,107	0
25	MG	A	1615	1/1	0.93	0.32	84,84,84,84	0
25	MG	A	1647	1/1	0.93	0.42	88,88,88,88	0
25	MG	A	1657	1/1	0.93	0.76	60,60,60,60	0
25	MG	A	1640	1/1	0.93	0.29	90,90,90,90	0
25	MG	A	1684	1/1	0.93	0.10	82,82,82,82	0
25	MG	A	1627	1/1	0.93	0.63	66,66,66,66	0
25	MG	A	1694	1/1	0.94	0.58	72,72,72,72	0
25	MG	A	1638	1/1	0.94	0.39	84,84,84,84	0
25	MG	A	1645	1/1	0.94	0.14	67,67,67,67	0
25	MG	A	1630	1/1	0.94	0.10	81,81,81,81	0
25	MG	A	1625	1/1	0.94	0.35	65,65,65,65	0
25	MG	A	1682	1/1	0.94	0.45	121,121,121,121	0
25	MG	A	1655	1/1	0.95	0.27	71,71,71,71	0
25	MG	A	1666	1/1	0.95	0.41	84,84,84,84	0
25	MG	A	1670	1/1	0.95	0.67	85,85,85,85	0
25	MG	A	1669	1/1	0.96	0.29	90,90,90,90	0
25	MG	A	1693	1/1	0.96	0.60	83,83,83,83	0
25	MG	A	1629	1/1	0.96	0.51	59,59,59,59	0
25	MG	A	1660	1/1	0.96	0.24	68,68,68,68	0
25	MG	A	1659	1/1	0.96	0.59	100,100,100,100	0
24	PAR	A	1601	42/42	0.96	0.19	76,88,98,105	0
25	MG	A	1603	1/1	0.96	0.51	76,76,76,76	0
25	MG	A	1620	1/1	0.96	0.47	56,56,56,56	0
25	MG	A	1656	1/1	0.96	0.54	71,71,71,71	0
25	MG	A	1622	1/1	0.96	0.33	65,65,65,65	0
25	MG	A	1689	1/1	0.97	0.34	83,83,83,83	0
25	MG	A	1690	1/1	0.97	0.28	87,87,87,87	0
25	MG	A	1642	1/1	0.97	0.27	63,63,63,63	0
25	MG	A	1644	1/1	0.97	0.51	86,86,86,86	0
25	MG	A	1631	1/1	0.97	0.45	64,64,64,64	0
25	MG	A	1641	1/1	0.97	0.86	63,63,63,63	0
25	MG	A	1624	1/1	0.97	0.67	56,56,56,56	0
25	MG	A	1639	1/1	0.97	0.30	81,81,81,81	0
25	MG	A	1661	1/1	0.97	1.00	83,83,83,83	0
25	MG	A	1658	1/1	0.97	0.24	76,76,76,76	0
25	MG	J	201	1/1	0.97	0.54	90,90,90,90	0

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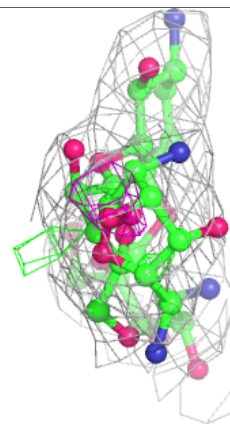
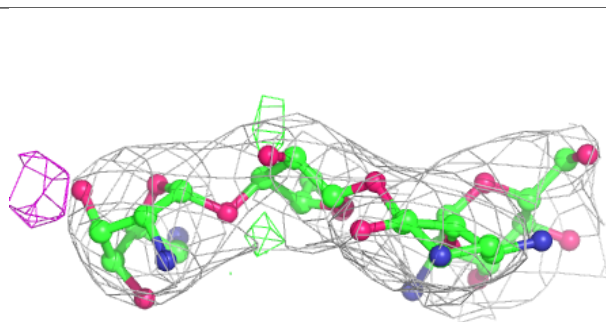
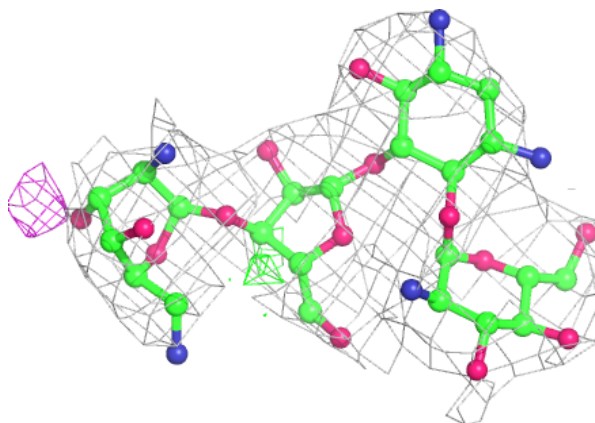
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1667	1/1	0.98	0.63	101,101,101,101	0
25	MG	A	1621	1/1	0.98	0.56	62,62,62,62	0
25	MG	A	1650	1/1	0.98	0.20	67,67,67,67	0
25	MG	A	1616	1/1	0.98	0.64	91,91,91,91	0
25	MG	A	1688	1/1	0.98	0.44	65,65,65,65	0
25	MG	A	1695	1/1	0.98	0.06	105,105,105,105	0
25	MG	A	1626	1/1	0.99	0.41	76,76,76,76	0
25	MG	A	1651	1/1	0.99	0.14	67,67,67,67	0
26	ZN	N	101	1/1	0.99	0.18	125,125,125,125	0
25	MG	A	1652	1/1	0.99	0.19	70,70,70,70	0
26	ZN	D	301	1/1	1.00	0.31	131,131,131,131	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.

Electron density around PAR A 1601:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.