



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 12:15 am BST

PDB ID : 1XMQ  
Title : Crystal Structure of t6A37-ASLLysUUU AAA-mRNA Bound to the Decoding Center  
Authors : Murphy, F.V.; Ramakrishnan, V.; Malkiewicz, A.; Agris, P.F.  
Deposited on : 2004-10-04  
Resolution : 3.00 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](mailto: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

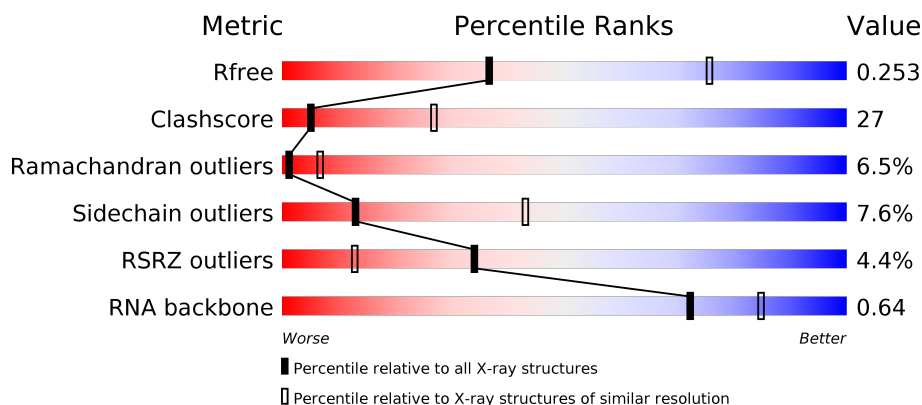
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


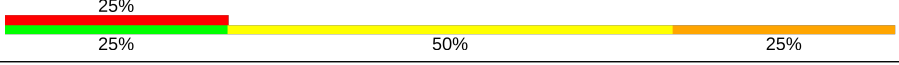
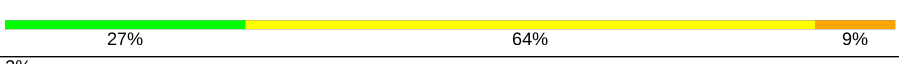

The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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  $\geq 3$ , 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	1522	
2	W	4	
3	X	11	
4	B	256	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	239	
6	D	209	
7	E	162	
8	F	101	
9	G	156	
10	H	138	
11	I	128	
12	J	105	
13	K	129	
14	L	135	
15	M	126	
16	N	61	
17	O	89	
18	P	88	
19	Q	105	
20	R	88	
21	S	93	
22	T	106	
23	V	27	

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	1608	-	-	-	X
25	MG	A	1613	-	-	-	X
25	MG	A	1627	-	-	-	X
25	MG	A	493	-	-	-	X
3	T6A	X	37	X	-	-	-

## 2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 52081 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	22	0	0
			32380	14414	5990	10470	1506			

- Molecule 2 is a RNA chain called A-Site Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	4	Total	C	N	O	P	0	0	0
			85	40	20	22	3			

- Molecule 3 is a RNA chain called Anticodon RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	11	Total	C	N	O	P	0	0	0
			236	108	37	81	10			

- Molecule 4 is a protein called 30S Ribosomal Protein S2.

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

- Molecule 5 is a protein called 30S Ribosomal Protein S3.

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

- Molecule 6 is a protein called 30S Ribosomal Protein S4.

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

- Molecule 7 is a protein called 30S Ribosomal Protein S5.

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

- Molecule 8 is a protein called 30S Ribosomal Protein S6.

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

- Molecule 9 is a protein called 30S Ribosomal Protein S7.

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

- Molecule 10 is a protein called 30S Ribosomal Protein S8.

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

- Molecule 11 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 12 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 13 is a protein called 30S Ribosomal Protein S11.

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

- Molecule 14 is a protein called 30S Ribosomal Protein S12.

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

- Molecule 15 is a protein called 30S Ribosomal Protein S13.

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

- Molecule 16 is a protein called 30S Ribosomal Protein S14.

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

- Molecule 17 is a protein called 30S Ribosomal Protein S15.

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

- Molecule 18 is a protein called 30S Ribosomal Protein S16.

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

- Molecule 19 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 21 is a protein called 30S Ribosomal Protein S19.

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

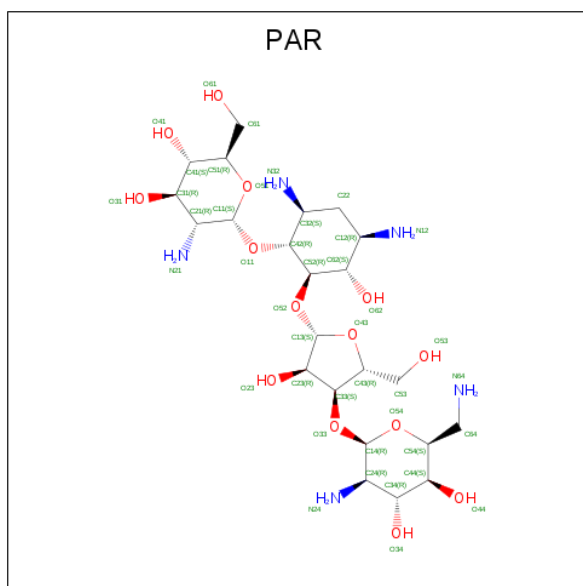
- Molecule 22 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 23 is a protein called 30S Ribosomal Protein Thx.

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

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



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	2	Total	Mg	0	0
			2	2		

*Continued on next page...*

*Continued from previous page...*

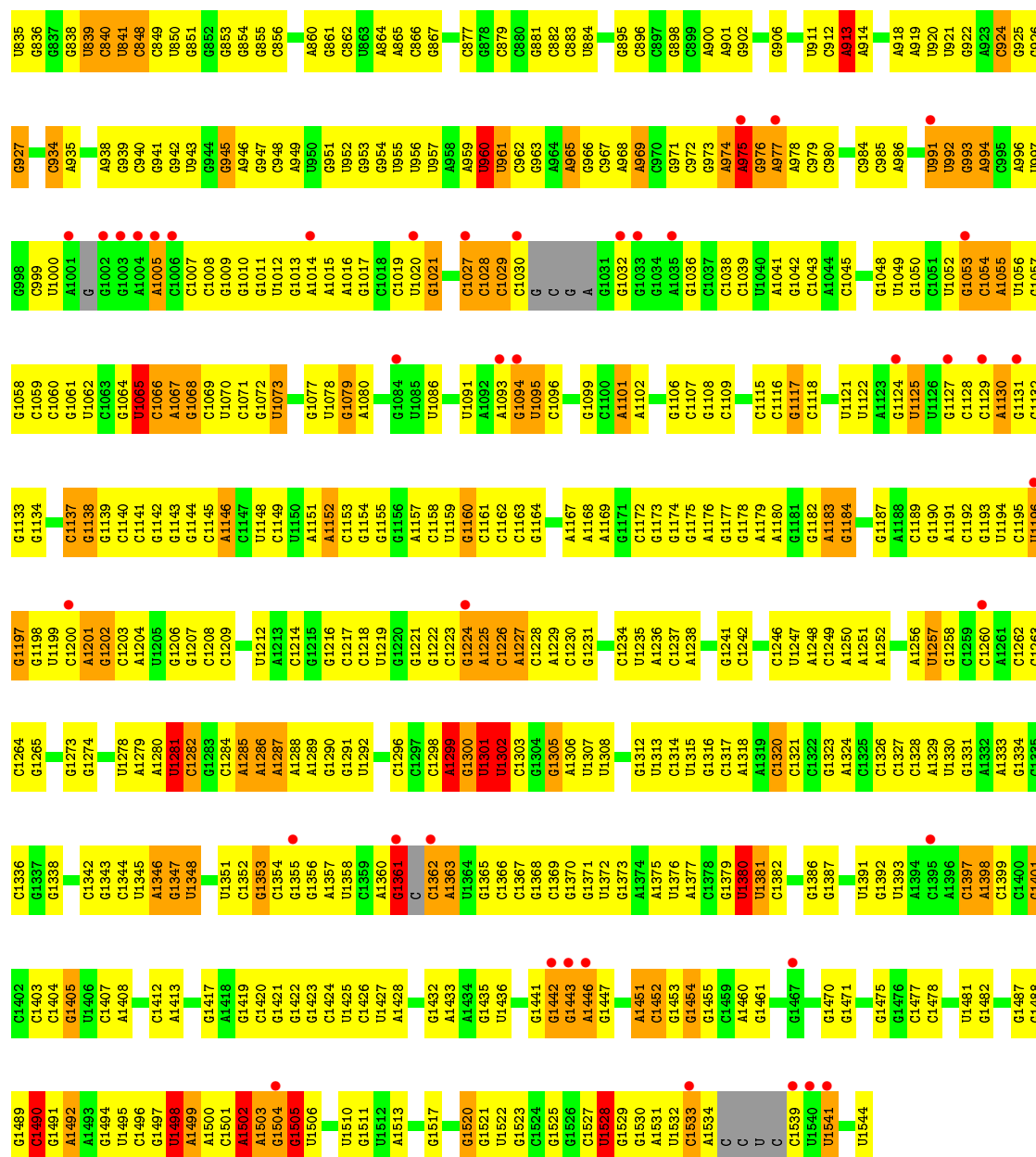
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	104	Total 104	Mg 104	0	0
25	N	1	Total 1	Mg 1	0	0

- 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







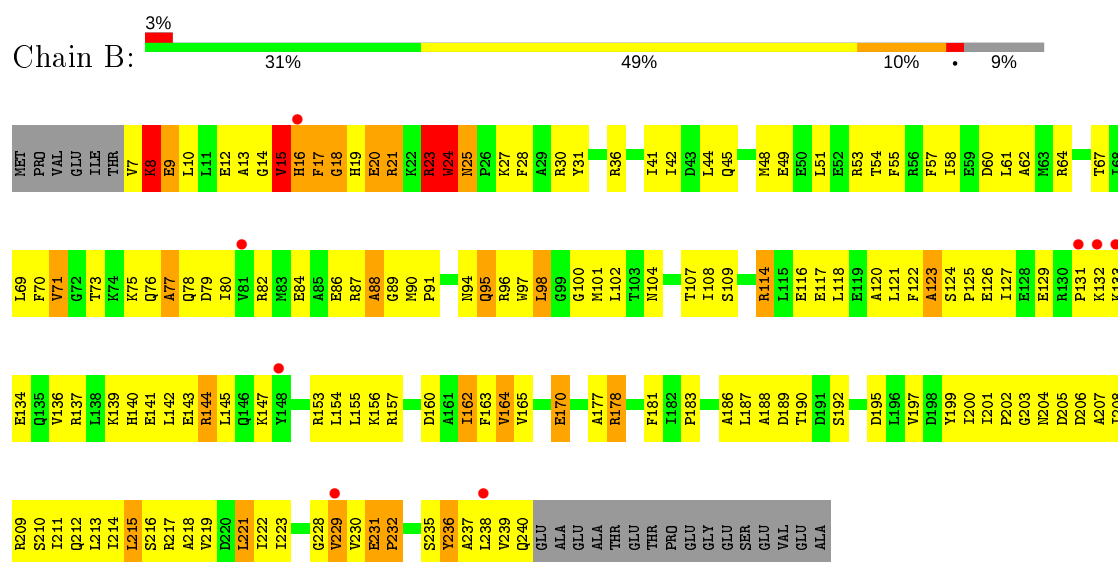
### • Molecule 2: A-Site Messenger RNA



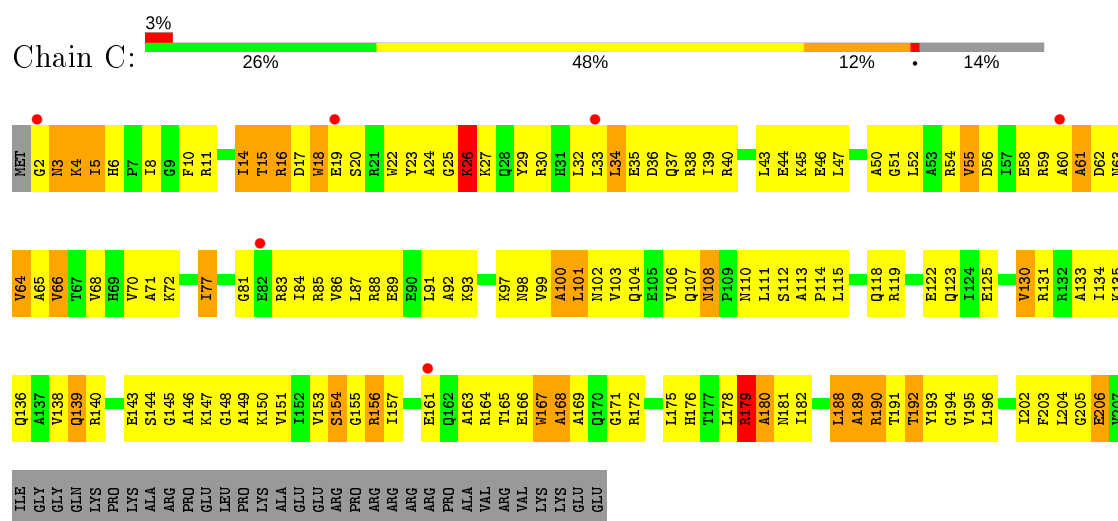
### • Molecule 3: Anticodon RNA



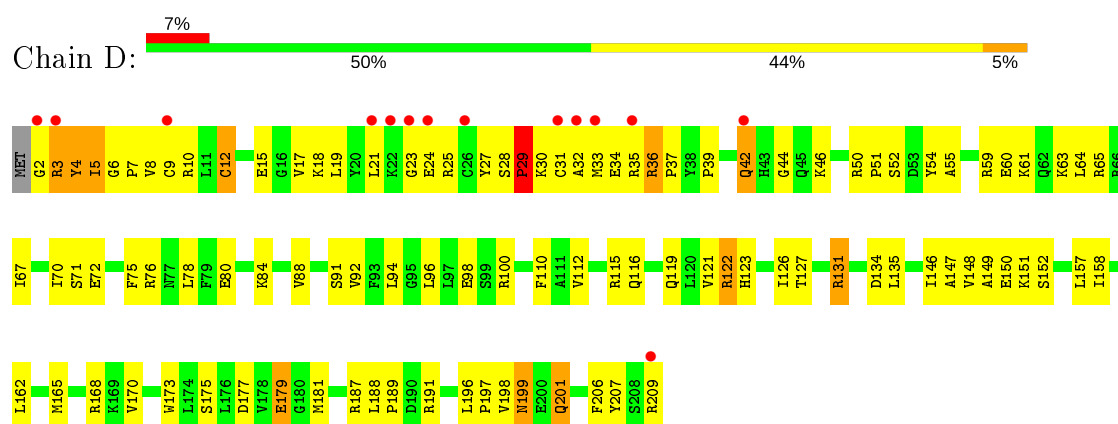
### • Molecule 4: 30S Ribosomal Protein S2



- Molecule 5: 30S Ribosomal Protein S3

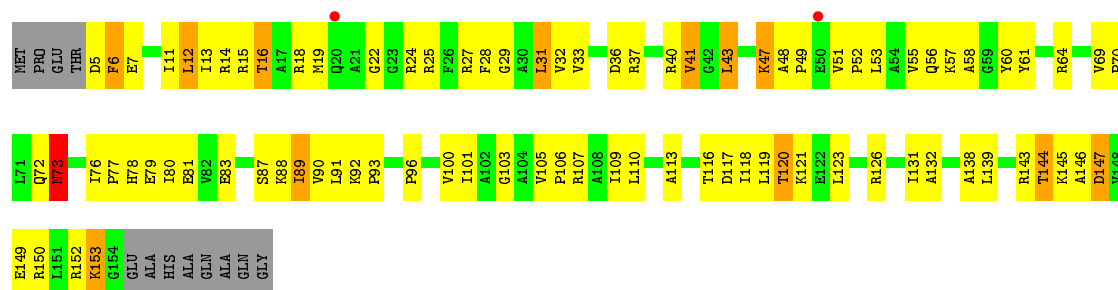


- Molecule 6: 30S Ribosomal Protein S4



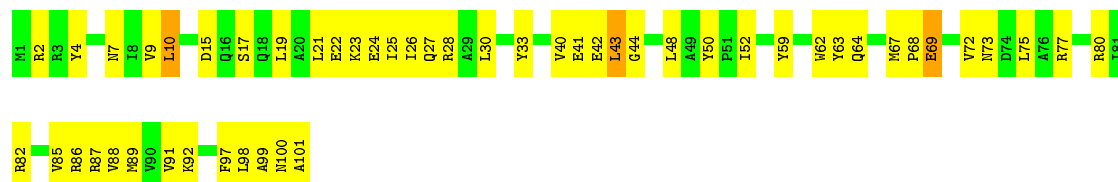
- Molecule 7: 30S Ribosomal Protein S5





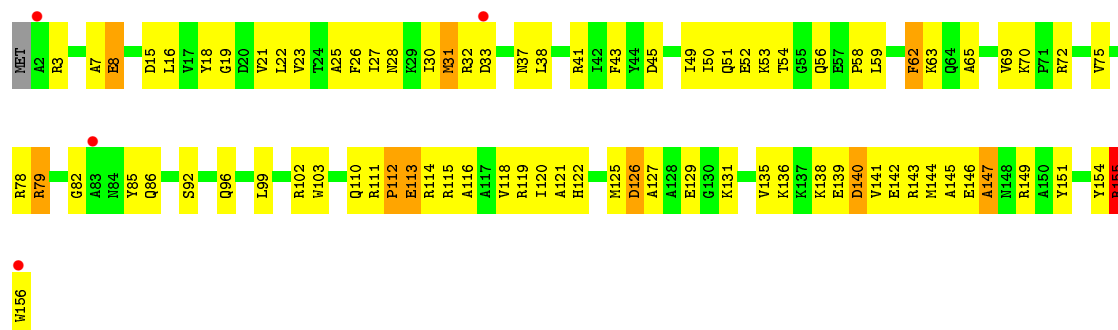
• Molecule 8: 30S Ribosomal Protein S6

Chain F: 50% 48%



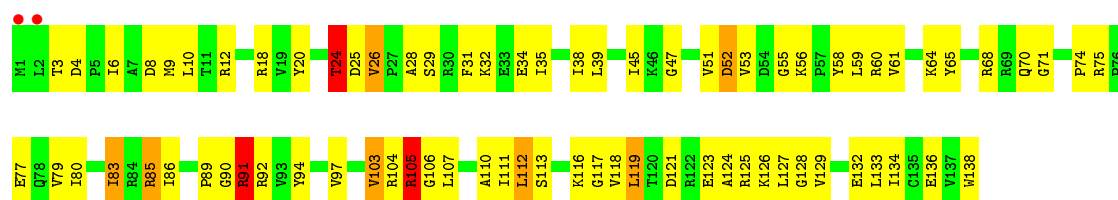
• Molecule 9: 30S Ribosomal Protein S7

Chain G: 3% 46% 47% 6%



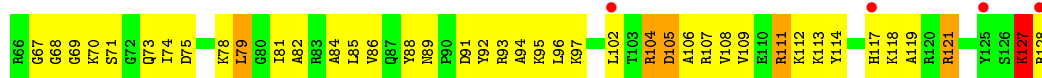
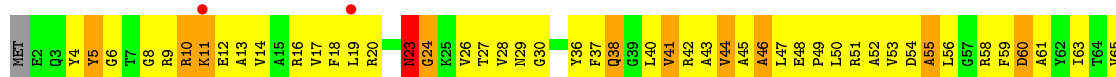
• Molecule 10: 30S Ribosomal Protein S8

Chain H: % 45% 48% 5%

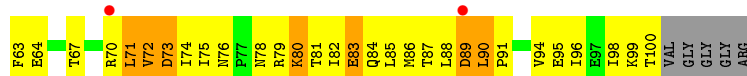
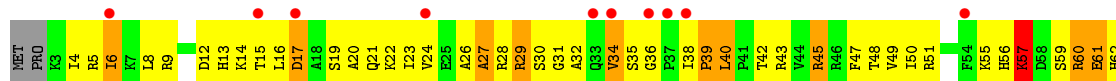


• Molecule 11: 30S Ribosomal Protein S9

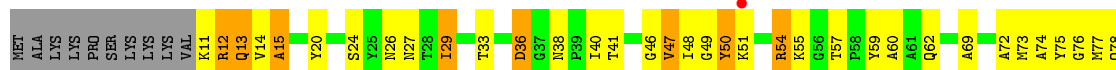
Chain I: 5% 30% 56% 12%



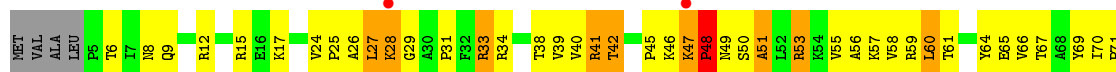
• Molecule 12: 30S Ribosomal Protein S10



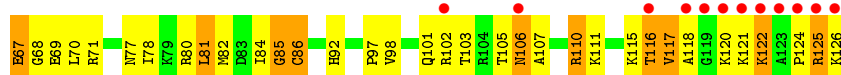
• Molecule 13: 30S Ribosomal Protein S11



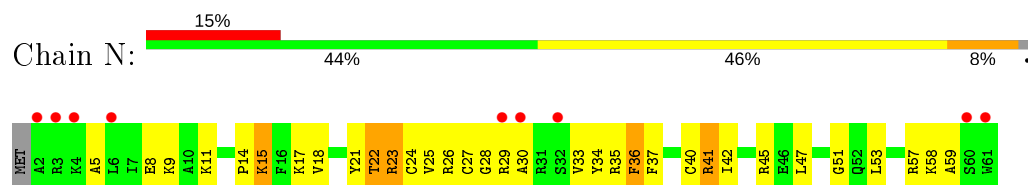
• Molecule 14: 30S Ribosomal Protein S12



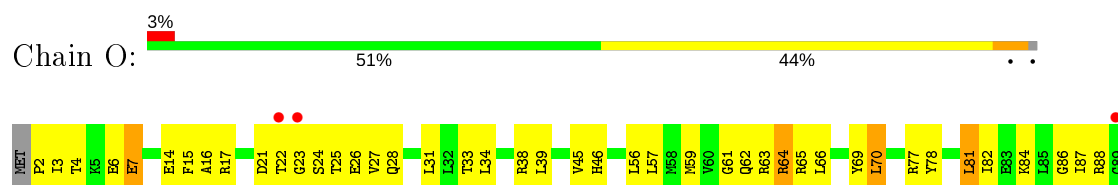
• Molecule 15: 30S Ribosomal Protein S13



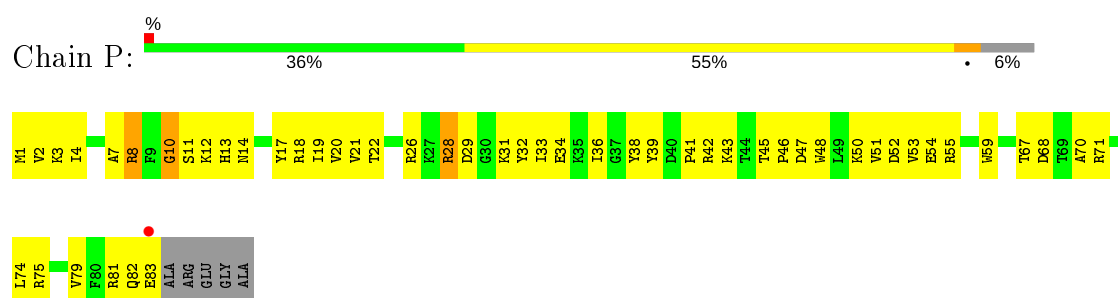
- Molecule 16: 30S Ribosomal Protein S14



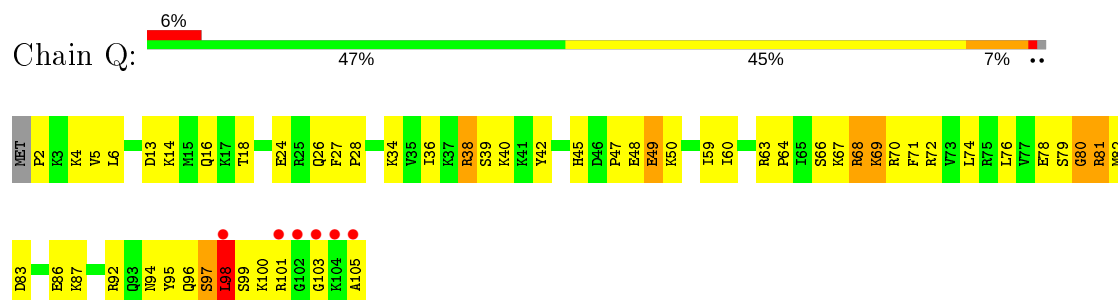
- Molecule 17: 30S Ribosomal Protein S15



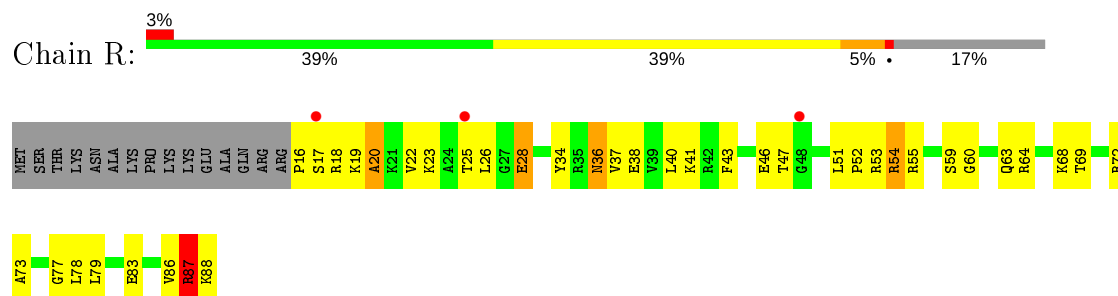
- Molecule 18: 30S Ribosomal Protein S16



- Molecule 19: 30S Ribosomal Protein S17

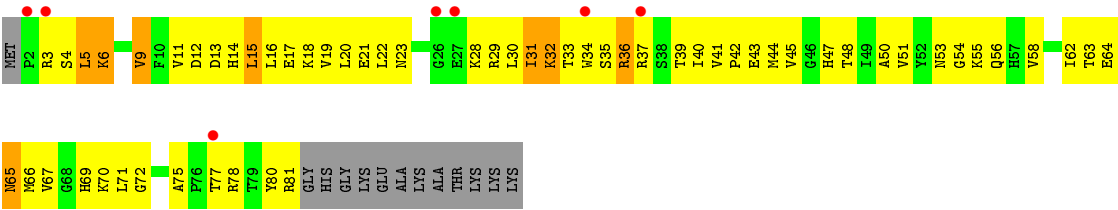


- Molecule 20: 30S Ribosomal Protein S18

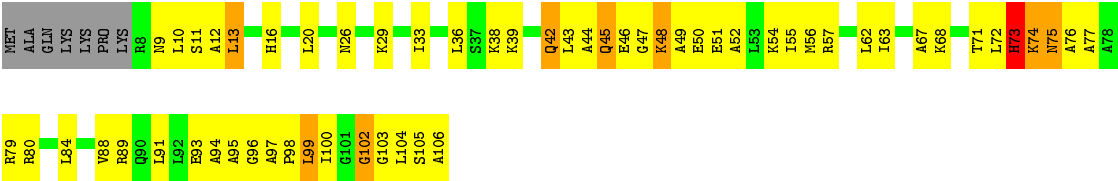
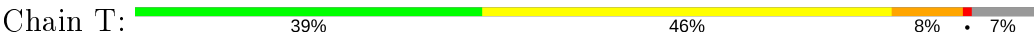


- Molecule 21: 30S Ribosomal Protein S19

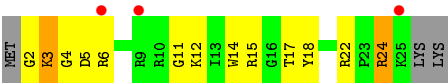




● Molecule 22: 30S Ribosomal Protein S20



● Molecule 23: 30S Ribosomal Protein Thx



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	400.72Å 400.72Å 175.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 3.00 283.35 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (99.00-3.00) 93.1 (283.35-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.222 , 0.236 0.215 , 0.253	Depositor DCC
$R_{free}$ test set	13422 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.2	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 71.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	52081	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, MG, T6A, 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	0.49	1/36244 (0.0%)	0.74	41/56567 (0.1%)
2	W	0.44	0/96	0.86	1/148 (0.7%)
3	X	0.44	0/226	0.78	0/349
4	B	0.32	0/1935	0.60	0/2609
5	C	0.35	0/1636	0.63	0/2205
6	D	0.36	0/1733	0.61	1/2318 (0.0%)
7	E	0.42	0/1162	0.67	0/1564
8	F	0.30	0/856	0.59	0/1154
9	G	0.32	0/1276	0.59	0/1709
10	H	0.40	0/1136	0.73	0/1527
11	I	0.33	0/1029	0.61	0/1378
12	J	0.35	0/805	0.63	0/1082
13	K	0.37	0/900	0.63	0/1213
14	L	0.42	0/986	0.75	0/1320
15	M	0.32	0/1008	0.62	0/1347
16	N	0.36	0/501	0.64	0/664
17	O	0.33	0/745	0.60	0/992
18	P	0.45	0/716	0.72	0/963
19	Q	0.43	0/870	0.75	0/1159
20	R	0.32	0/603	0.60	0/799
21	S	0.30	0/661	0.64	0/890
22	T	0.38	0/764	0.75	1/1006 (0.1%)
23	V	0.43	0/212	0.64	0/277
All	All	0.45	1/56100 (0.0%)	0.71	44/83240 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	40
3	X	1	0
All	All	5	40

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1361	G	C3'-O3'	5.66	1.50	1.42

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	G	C2'-C3'-O3'	10.04	131.59	109.50
1	A	1498	U	C2'-C3'-O3'	9.79	131.04	109.50
1	A	243	A	C2'-C3'-O3'	9.48	130.35	109.50
1	A	1302	U	C2'-C3'-O3'	9.13	129.59	109.50
1	A	366	C	C2'-C3'-O3'	9.11	129.55	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	243	A	C3'
1	A	281	G	C3'
1	A	366	C	C3'
1	A	1528	U	C3'
3	X	37	T6A	C14

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	C	Sidechain
1	A	190(K)	G	Sidechain
1	A	195	A	Sidechain
1	A	51	A	Sidechain
1	A	58	C	Sidechain

## 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	32380	0	16346	879	0
2	W	85	0	46	4	0
3	X	236	0	122	13	0
4	B	1900	0	1951	183	0
5	C	1612	0	1677	194	0
6	D	1703	0	1764	111	0
7	E	1146	0	1207	99	0
8	F	843	0	857	56	0
9	G	1257	0	1296	88	0
10	H	1116	0	1177	86	0
11	I	1011	0	1043	115	0
12	J	792	0	835	119	0
13	K	885	0	904	66	0
14	L	970	0	1057	107	0
15	M	997	0	1072	95	0
16	N	492	0	529	43	0
17	O	734	0	771	38	0
18	P	700	0	720	55	0
19	Q	857	0	930	57	0
20	R	597	0	668	58	0
21	S	647	0	673	91	0
22	T	762	0	856	58	0
23	V	208	0	221	18	0
24	A	42	0	45	2	0
25	A	104	0	0	0	0
25	N	1	0	0	0	0
25	X	2	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52081	0	36767	2401	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 27.

The worst 5 of 2401 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:A:972:C:H4'	12:J:57:LYS:HG2	1.31	1.08
4:B:84:GLU:HB3	4:B:219:VAL:HG21	1.35	1.06
19:Q:98:LEU:HD12	19:Q:98:LEU:H	1.20	1.05
21:S:33:THR:HG22	21:S:35:SER:H	1.16	1.04
1:A:1490:C:H5'	1:A:1490:C:H6	1.18	1.04

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	
4	B	232/256 (91%)	176 (76%)	40 (17%)	16 (7%)	1	6
5	C	204/239 (85%)	131 (64%)	46 (22%)	27 (13%)	0	1
6	D	206/209 (99%)	168 (82%)	28 (14%)	10 (5%)	2	13
7	E	148/162 (91%)	140 (95%)	5 (3%)	3 (2%)	7	34
8	F	99/101 (98%)	80 (81%)	18 (18%)	1 (1%)	15	53
9	G	153/156 (98%)	122 (80%)	24 (16%)	7 (5%)	2	14
10	H	136/138 (99%)	116 (85%)	15 (11%)	5 (4%)	3	19
11	I	125/128 (98%)	94 (75%)	19 (15%)	12 (10%)	0	3
12	J	96/105 (91%)	60 (62%)	25 (26%)	11 (12%)	0	2
13	K	117/129 (91%)	88 (75%)	23 (20%)	6 (5%)	2	12
14	L	122/135 (90%)	97 (80%)	16 (13%)	9 (7%)	1	5
15	M	123/126 (98%)	88 (72%)	22 (18%)	13 (11%)	0	2
16	N	58/61 (95%)	44 (76%)	10 (17%)	4 (7%)	1	6
17	O	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	13	48
18	P	81/88 (92%)	69 (85%)	11 (14%)	1 (1%)	13	48
19	Q	102/105 (97%)	85 (83%)	9 (9%)	8 (8%)	1	4
20	R	71/88 (81%)	53 (75%)	16 (22%)	2 (3%)	5	25
21	S	78/93 (84%)	60 (77%)	12 (15%)	6 (8%)	1	5
22	T	97/106 (92%)	68 (70%)	20 (21%)	9 (9%)	0	3
23	V	22/27 (82%)	16 (73%)	5 (23%)	1 (4%)	2	14
All	All	2356/2541 (93%)	1832 (78%)	372 (16%)	152 (6%)	1	7

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	8	LYS
4	B	15	VAL
4	B	16	HIS
4	B	24	TRP
4	B	123	ALA

### 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	
4	B	202/220 (92%)	181 (90%)	21 (10%)	7	27
5	C	160/188 (85%)	145 (91%)	15 (9%)	8	32
6	D	180/181 (99%)	173 (96%)	7 (4%)	32	69
7	E	115/123 (94%)	101 (88%)	14 (12%)	5	21
8	F	90/90 (100%)	87 (97%)	3 (3%)	38	73
9	G	126/127 (99%)	120 (95%)	6 (5%)	25	62
10	H	119/119 (100%)	108 (91%)	11 (9%)	9	34
11	I	98/99 (99%)	89 (91%)	9 (9%)	9	34
12	J	87/92 (95%)	79 (91%)	8 (9%)	9	34
13	K	90/99 (91%)	83 (92%)	7 (8%)	12	42
14	L	104/111 (94%)	94 (90%)	10 (10%)	8	32
15	M	100/101 (99%)	91 (91%)	9 (9%)	9	35
16	N	49/50 (98%)	47 (96%)	2 (4%)	30	67
17	O	79/80 (99%)	71 (90%)	8 (10%)	7	29
18	P	72/74 (97%)	69 (96%)	3 (4%)	30	66
19	Q	96/97 (99%)	89 (93%)	7 (7%)	14	44
20	R	64/77 (83%)	60 (94%)	4 (6%)	18	51
21	S	71/80 (89%)	68 (96%)	3 (4%)	30	66
22	T	75/82 (92%)	71 (95%)	4 (5%)	22	58
23	V	19/22 (86%)	18 (95%)	1 (5%)	22	58

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1996/2112 (94%)	1844 (92%)	152 (8%)	13	43

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	25	ASP
11	I	127	LYS
20	R	28	GLU
10	H	52	ASP
11	I	5	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
8	F	64	GLN
10	H	82	HIS
21	S	14	HIS
8	F	100	ASN
9	G	68	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	241 (16%)	69 (4%)
2	W	3/4 (75%)	0	0
3	X	10/11 (90%)	1 (10%)	1 (10%)
All	All	1519/1537 (98%)	242 (15%)	70 (4%)

5 of 242 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 70 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	687	A
1	A	960	U
1	A	1498	U
1	A	701	C
1	A	819	A

## 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$
3	T6A	X	37	3	24,34,35	1.24	3 (12%)	24,49,52	4.20	8 (33%)

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
3	T6A	X	37	3	1/1/9/11	5/15/41/42	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	37	T6A	C15-C14	-3.14	1.42	1.51
3	X	37	T6A	O14-C14	-2.86	1.35	1.43
3	X	37	T6A	C12-N11	-2.47	1.41	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	37	T6A	O14-C14-C15	12.08	145.52	109.74
3	X	37	T6A	C12-N11-C10	11.64	135.18	122.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	37	T6A	O14-C14-C12	-7.17	94.80	109.14
3	X	37	T6A	N6-C10-N11	6.18	122.40	113.76
3	X	37	T6A	O10-C10-N6	-4.41	116.16	123.62

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	X	37	T6A	C14

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	37	T6A	C13-C12-N11-C10
3	X	37	T6A	N11-C12-C14-O14
3	X	37	T6A	C13-C12-C14-O14
3	X	37	T6A	O4'-C4'-C5'-O5'
3	X	37	T6A	C14-C12-N11-C10

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	37	T6A	8	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 109 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	1545	1	45,45,45	1.53	7 (15%)	64,67,67	1.27	6 (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
24	PAR	A	1545	1	-	4/18/94/94	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	C24-N24	4.14	1.53	1.47
24	A	1545	PAR	O54-C14	3.80	1.51	1.41
24	A	1545	PAR	C64-C54	3.43	1.56	1.52
24	A	1545	PAR	C11-C21	3.12	1.58	1.52
24	A	1545	PAR	C44-C34	2.23	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1545	PAR	C14-O54-C54	3.72	120.99	113.69
24	A	1545	PAR	O33-C14-C24	3.16	113.65	108.22
24	A	1545	PAR	O54-C54-C64	2.86	111.33	106.01
24	A	1545	PAR	O11-C11-C21	2.80	113.04	108.22
24	A	1545	PAR	O52-C13-C23	2.31	112.74	107.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

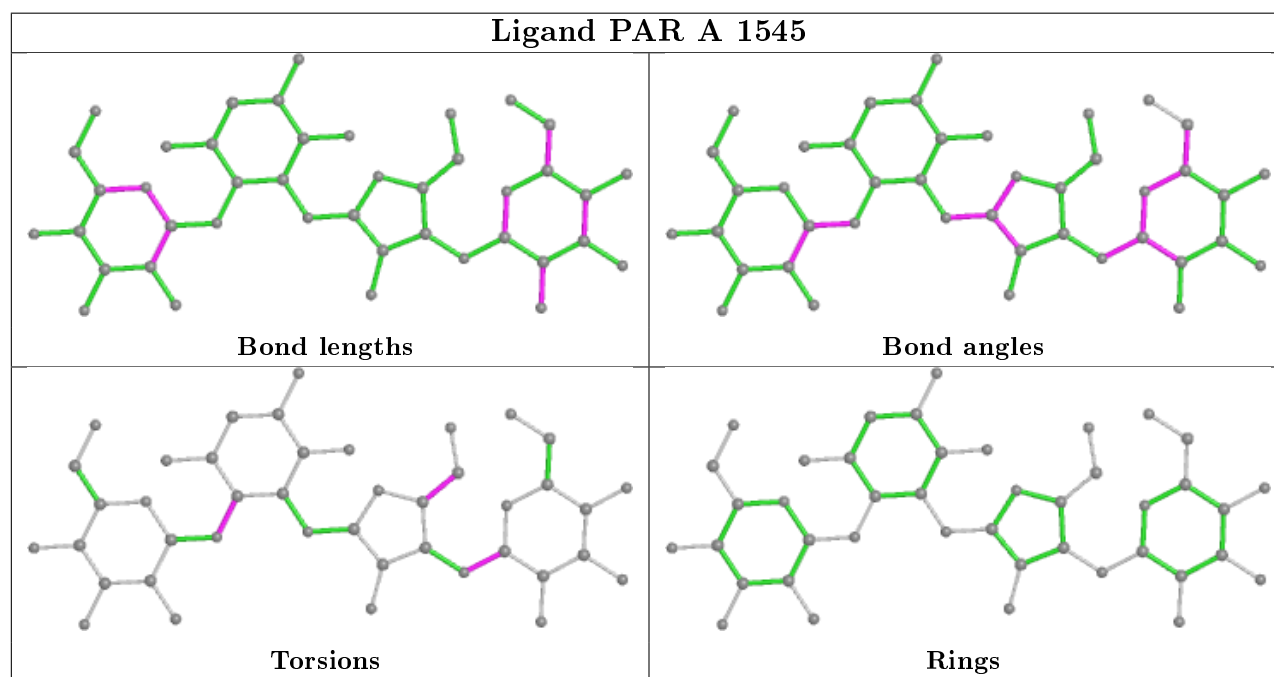
Mol	Chain	Res	Type	Atoms
24	A	1545	PAR	C33-C43-C53-O53
24	A	1545	PAR	O43-C43-C53-O53
24	A	1545	PAR	C24-C14-O33-C33
24	A	1545	PAR	C52-C42-O11-C11

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1545	PAR	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.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1506/1522 (98%)	0.96	65 (4%) 35 13	29, 61, 149, 201	0
2	W	4/4 (100%)	1.16	1 (25%) 0 0	49, 53, 55, 127	0
3	X	10/11 (90%)	0.49	0 100 100	63, 79, 146, 163	0
4	B	234/256 (91%)	0.27	8 (3%) 45 19	38, 106, 176, 201	0
5	C	206/239 (86%)	0.31	6 (2%) 51 23	41, 91, 159, 197	0
6	D	208/209 (99%)	0.46	14 (6%) 17 5	41, 72, 143, 200	0
7	E	150/162 (92%)	0.34	2 (1%) 77 51	33, 56, 107, 187	0
8	F	101/101 (100%)	0.05	0 100 100	51, 99, 138, 167	0
9	G	155/156 (99%)	0.24	4 (2%) 56 27	34, 82, 151, 191	0
10	H	138/138 (100%)	0.29	2 (1%) 75 49	32, 53, 99, 163	0
11	I	127/128 (99%)	0.45	6 (4%) 31 11	43, 96, 148, 200	0
12	J	98/105 (93%)	0.86	12 (12%) 4 1	47, 127, 197, 201	0
13	K	119/129 (92%)	0.35	2 (1%) 70 41	37, 67, 120, 182	0
14	L	124/135 (91%)	0.45	5 (4%) 38 15	31, 56, 135, 175	0
15	M	125/126 (99%)	1.03	13 (10%) 6 2	47, 83, 165, 201	0
16	N	60/61 (98%)	0.86	9 (15%) 2 1	50, 81, 133, 200	0
17	O	88/89 (98%)	0.31	3 (3%) 45 19	39, 74, 135, 195	0
18	P	83/88 (94%)	0.38	1 (1%) 79 54	36, 52, 94, 174	0
19	Q	104/105 (99%)	0.64	6 (5%) 23 7	29, 57, 139, 201	0
20	R	73/88 (82%)	0.28	3 (4%) 37 14	50, 74, 161, 193	0
21	S	80/93 (86%)	0.67	7 (8%) 10 3	55, 105, 165, 201	0
22	T	99/106 (93%)	0.28	0 100 100	28, 59, 118, 175	0
23	V	24/27 (88%)	0.95	3 (12%) 3 1	39, 67, 122, 166	0
All	All	3916/4078 (96%)	0.63	172 (4%) 34 13	28, 70, 158, 201	0

The worst 5 of 172 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	M	123	ALA	17.9
1	A	1539	C	13.4
15	M	126	LYS	12.6
15	M	124	PRO	12.6
1	A	424	G	11.9

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	T6A	X	37	32/33	0.92	0.28	67,76,76,76	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1608	1/1	0.34	0.58	29,29,29,29	1
25	MG	A	1548	1/1	0.53	0.32	29,29,29,29	1
25	MG	A	1607	1/1	0.58	0.32	29,29,29,29	1
25	MG	A	1602	1/1	0.64	0.18	29,29,29,29	1
25	MG	A	1614	1/1	0.68	0.23	29,29,29,29	0
25	MG	A	1613	1/1	0.68	0.48	29,29,29,29	1
25	MG	A	1630	1/1	0.69	0.33	29,29,29,29	1
25	MG	N	423	1/1	0.69	0.24	29,29,29,29	1
25	MG	A	1595	1/1	0.69	0.34	29,29,29,29	1
25	MG	A	1620	1/1	0.70	0.34	29,29,29,29	1
25	MG	A	493	1/1	0.70	0.69	29,29,29,29	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	441	1/1	0.72	0.24	29,29,29,29	1
25	MG	A	1575	1/1	0.73	0.29	29,29,29,29	1
25	MG	A	1562	1/1	0.73	0.39	29,29,29,29	1
25	MG	A	1585	1/1	0.74	0.39	29,29,29,29	1
25	MG	A	470	1/1	0.75	0.21	29,29,29,29	1
25	MG	A	1627	1/1	0.77	0.42	29,29,29,29	1
25	MG	A	1628	1/1	0.78	0.33	29,29,29,29	1
25	MG	A	467	1/1	0.78	0.27	29,29,29,29	1
25	MG	A	1633	1/1	0.79	0.33	29,29,29,29	1
25	MG	A	1554	1/1	0.79	0.23	29,29,29,29	1
25	MG	A	87	1/1	0.80	0.38	29,29,29,29	1
25	MG	A	1601	1/1	0.81	0.09	29,29,29,29	0
25	MG	A	1634	1/1	0.81	0.41	29,29,29,29	1
25	MG	A	1597	1/1	0.81	0.13	29,29,29,29	0
25	MG	A	1610	1/1	0.82	0.41	29,29,29,29	1
25	MG	A	1632	1/1	0.82	0.43	29,29,29,29	1
25	MG	A	1564	1/1	0.83	0.23	29,29,29,29	0
25	MG	A	214	1/1	0.83	0.24	29,29,29,29	1
25	MG	A	471	1/1	0.84	0.31	29,29,29,29	1
25	MG	A	1603	1/1	0.84	0.43	29,29,29,29	1
25	MG	A	1596	1/1	0.84	0.23	29,29,29,29	0
25	MG	A	1594	1/1	0.85	0.29	29,29,29,29	1
25	MG	X	500	1/1	0.85	0.44	29,29,29,29	1
25	MG	A	1565	1/1	0.85	0.40	29,29,29,29	1
25	MG	A	1600	1/1	0.86	0.21	29,29,29,29	1
25	MG	A	210	1/1	0.87	0.16	29,29,29,29	1
25	MG	A	71	1/1	0.87	0.34	29,29,29,29	1
25	MG	A	1635	1/1	0.87	0.22	29,29,29,29	0
25	MG	X	502	1/1	0.87	0.39	29,29,29,29	1
25	MG	A	1591	1/1	0.87	0.26	29,29,29,29	0
25	MG	A	1615	1/1	0.87	0.17	29,29,29,29	1
25	MG	A	1584	1/1	0.88	0.27	29,29,29,29	0
25	MG	A	1571	1/1	0.88	0.21	29,29,29,29	0
25	MG	A	1558	1/1	0.89	0.14	29,29,29,29	1
25	MG	A	1611	1/1	0.89	0.19	29,29,29,29	1
25	MG	A	1559	1/1	0.89	0.27	29,29,29,29	1
25	MG	A	1578	1/1	0.89	0.16	29,29,29,29	0
25	MG	A	1624	1/1	0.89	0.35	29,29,29,29	1
25	MG	A	1612	1/1	0.90	0.24	29,29,29,29	1
25	MG	A	1547	1/1	0.90	0.35	29,29,29,29	0
25	MG	A	1616	1/1	0.90	0.15	29,29,29,29	1
25	MG	A	1563	1/1	0.90	0.34	29,29,29,29	1

*Continued on next page...*

*Continued from previous page...*

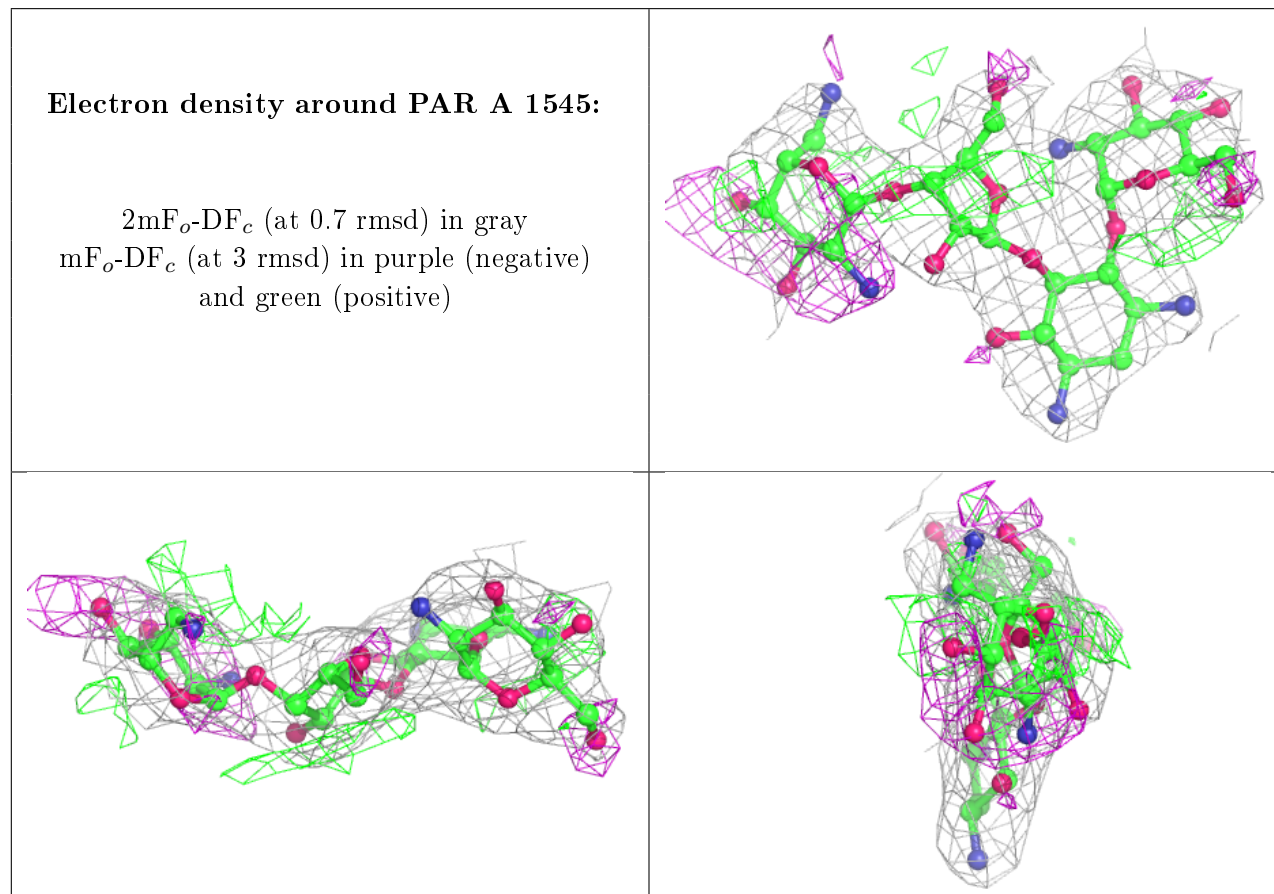
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1569	1/1	0.90	0.33	29,29,29,29	1
25	MG	A	1568	1/1	0.91	0.21	29,29,29,29	0
25	MG	A	469	1/1	0.91	0.27	29,29,29,29	1
25	MG	A	1592	1/1	0.91	0.23	29,29,29,29	0
25	MG	A	1631	1/1	0.91	0.15	29,29,29,29	1
25	MG	A	473	1/1	0.91	0.29	29,29,29,29	1
25	MG	A	211	1/1	0.91	0.33	29,29,29,29	1
25	MG	A	1619	1/1	0.91	0.16	29,29,29,29	0
25	MG	A	1572	1/1	0.91	0.14	29,29,29,29	1
25	MG	A	1583	1/1	0.92	0.25	29,29,29,29	0
25	MG	A	1546	1/1	0.92	0.26	29,29,29,29	0
25	MG	A	1622	1/1	0.92	0.23	29,29,29,29	1
24	PAR	A	1545	42/42	0.92	0.30	28,28,28,28	0
25	MG	A	1580	1/1	0.92	0.34	29,29,29,29	1
25	MG	A	1621	1/1	0.93	0.37	29,29,29,29	1
25	MG	A	1623	1/1	0.93	0.24	29,29,29,29	1
25	MG	A	1581	1/1	0.93	0.34	29,29,29,29	1
25	MG	A	1617	1/1	0.93	0.16	29,29,29,29	1
25	MG	A	1599	1/1	0.93	0.24	29,29,29,29	1
25	MG	A	1593	1/1	0.93	0.27	29,29,29,29	0
25	MG	A	1551	1/1	0.93	0.28	29,29,29,29	0
25	MG	A	1574	1/1	0.93	0.30	29,29,29,29	0
25	MG	A	1577	1/1	0.93	0.14	29,29,29,29	0
25	MG	A	1586	1/1	0.94	0.29	29,29,29,29	0
25	MG	A	1550	1/1	0.94	0.26	29,29,29,29	1
25	MG	A	1556	1/1	0.94	0.34	29,29,29,29	0
25	MG	A	466	1/1	0.94	0.29	29,29,29,29	1
25	MG	A	1557	1/1	0.94	0.32	29,29,29,29	0
25	MG	A	1549	1/1	0.94	0.28	29,29,29,29	1
25	MG	A	1604	1/1	0.95	0.25	29,29,29,29	1
25	MG	A	1561	1/1	0.95	0.10	29,29,29,29	1
25	MG	A	1629	1/1	0.95	0.24	29,29,29,29	1
25	MG	A	86	1/1	0.95	0.22	29,29,29,29	1
25	MG	A	1553	1/1	0.95	0.36	29,29,29,29	0
25	MG	A	1582	1/1	0.95	0.20	29,29,29,29	0
25	MG	A	1609	1/1	0.95	0.29	29,29,29,29	1
25	MG	A	1566	1/1	0.96	0.37	29,29,29,29	1
25	MG	A	1576	1/1	0.96	0.31	29,29,29,29	0
25	MG	A	1560	1/1	0.96	0.25	29,29,29,29	0
25	MG	A	1552	1/1	0.96	0.29	29,29,29,29	0
25	MG	A	1573	1/1	0.96	0.32	29,29,29,29	0
25	MG	A	1618	1/1	0.96	0.18	29,29,29,29	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1579	1/1	0.96	0.23	29,29,29,29	1
25	MG	A	1598	1/1	0.96	0.26	29,29,29,29	0
25	MG	A	1606	1/1	0.97	0.18	29,29,29,29	0
25	MG	A	1570	1/1	0.97	0.19	29,29,29,29	0
25	MG	A	1555	1/1	0.97	0.28	29,29,29,29	0
25	MG	A	1587	1/1	0.97	0.32	29,29,29,29	0
26	ZN	D	306	1/1	0.97	0.39	29,29,29,29	1
25	MG	A	1590	1/1	0.98	0.23	29,29,29,29	0
25	MG	A	1625	1/1	0.98	0.22	29,29,29,29	0
25	MG	A	1589	1/1	0.98	0.34	29,29,29,29	0
25	MG	A	1626	1/1	0.98	0.17	29,29,29,29	1
25	MG	A	1605	1/1	0.98	0.25	29,29,29,29	1
25	MG	A	1567	1/1	0.98	0.37	29,29,29,29	1
26	ZN	N	307	1/1	0.98	0.24	29,29,29,29	1
25	MG	A	1588	1/1	0.98	0.30	29,29,29,29	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.