



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 03:45 pm BST

PDB ID : 5JVH  
Title : The crystal structure large ribosomal subunit (50S) of *Deinococcus radiodurans* in complex with evernimicin  
Authors : Yonath, A.  
Deposited on : 2016-05-11  
Resolution : 3.58 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.

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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



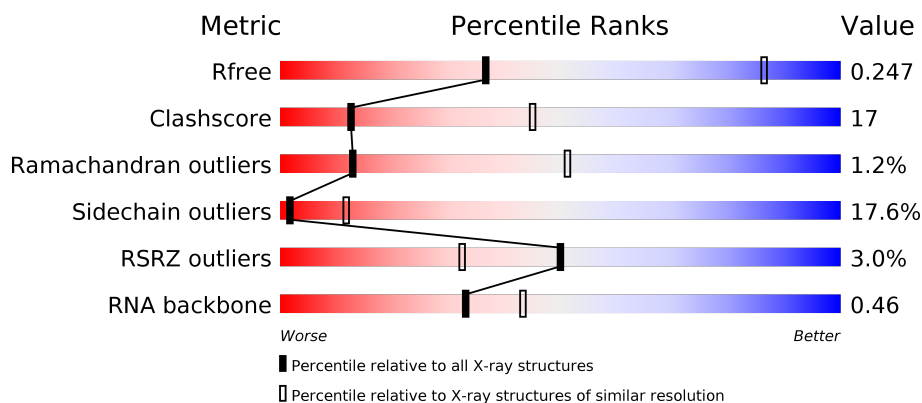
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.58 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)
RNA backbone	3102	1008 (4.10-3.00)

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 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	X	2880	
2	Y	123	
3	A	275	
4	B	211	

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	G	174	
9	H	134	
10	I	156	
11	J	141	
12	K	116	
13	L	114	
14	M	166	
15	N	118	
16	O	100	
17	P	134	
18	Q	95	
19	R	115	
20	S	237	
21	T	91	
22	U	81	
23	V	67	
24	W	55	
25	Z	60	
26	1	54	
27	2	47	
28	3	66	

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	2927	-	-	-	X
30	MG	X	2960	-	-	-	X
30	MG	X	3001	-	-	-	X
30	MG	X	3006	-	-	-	X
30	MG	X	3016	-	-	-	X
30	MG	X	3020	-	-	-	X



## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 83681 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2658	Total	C	N	O	P	0	0	0
			57052	25450	10532	18413	2657			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	259	Total	C	N	O	S	0	0	0
			1973	1226	395	349	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			



- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	134	Total	C	N	O	S	0	0	0
			1011	619	206	186				

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1078	690	196	185	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 13 is a protein called 50S ribosomal protein L18.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	108	Total	C	N	O	0	0	0
			859	537	166	156			

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 20 is a protein called 50S ribosomal protein L25.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	179	Total	C	N	O	S	0	0	0
			1374	867	240	261	6			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	S	0	0	0
			552	341	116	95				

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	53	Total	C	N	O	S	0	0	0
			427	271	79	76	1			

- Molecule 27 is a protein called 50S ribosomal protein L34.

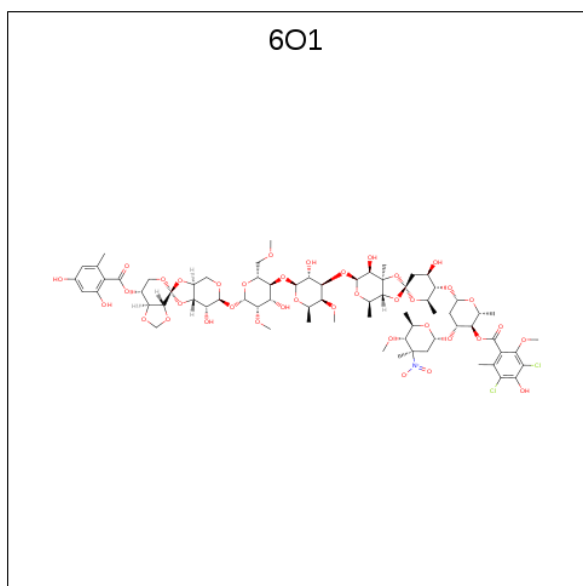


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 29 is Evernimicin (three-letter code: 6O1) (formula:  $C_{70}H_{97}Cl_2NO_{38}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	Cl	N	O	0	0
			111	70	2	1	38		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

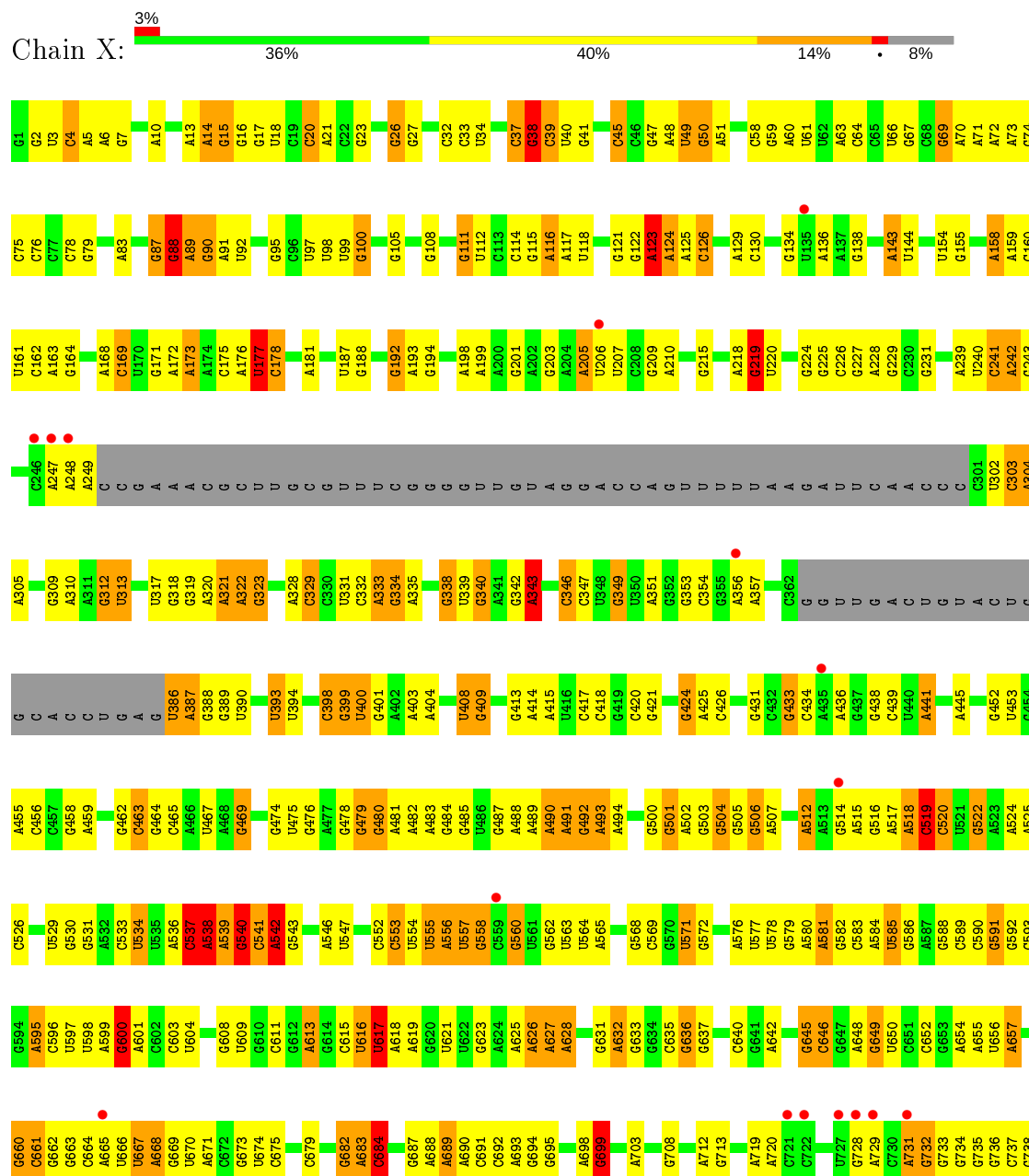
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	119	Total	Mg	0	0
			119	119		
30	Y	1	Total	Mg	0	0
			1	1		
30	K	2	Total	Mg	0	0
			2	2		
30	M	1	Total	Mg	0	0
			1	1		



### 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: 23S ribosomal RNA



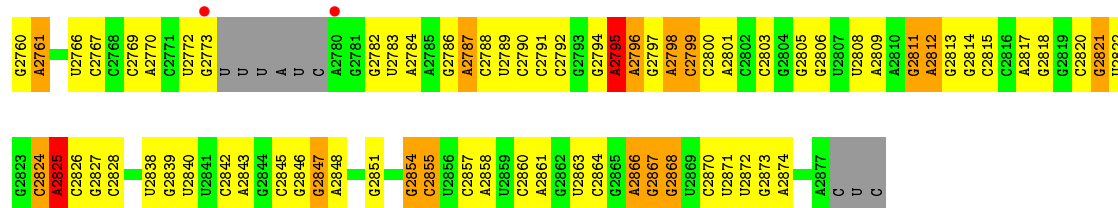




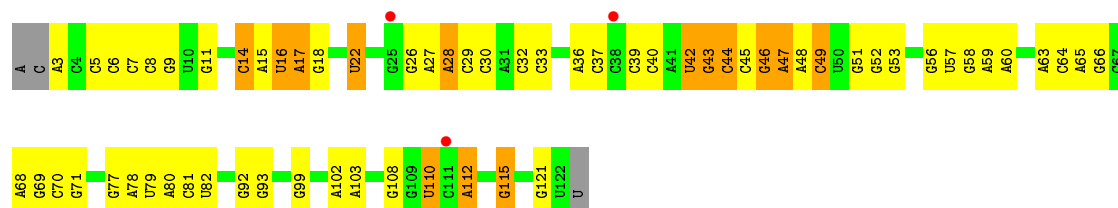




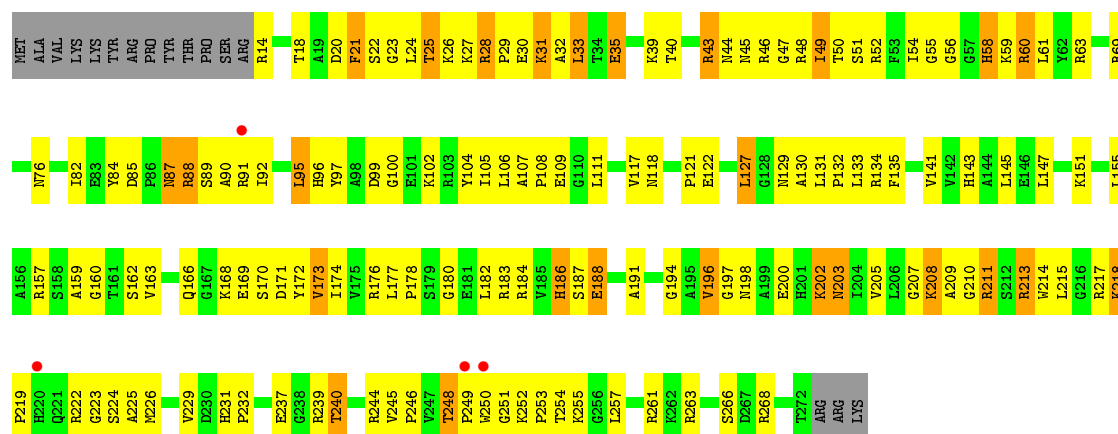
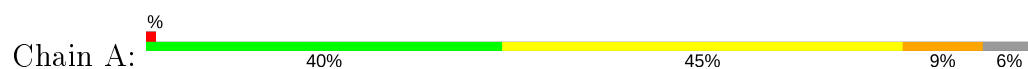




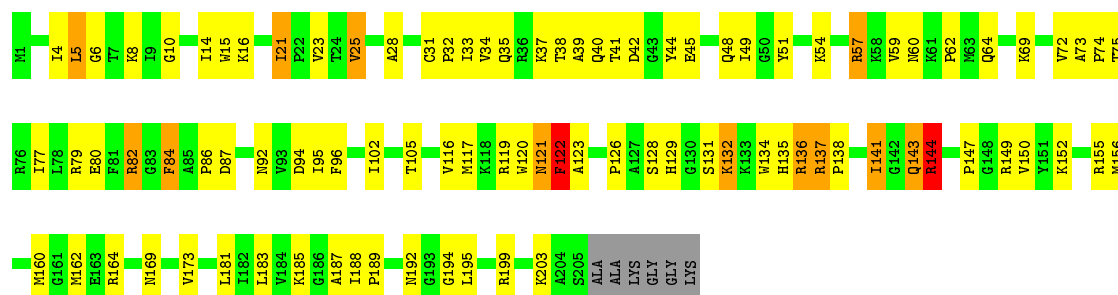
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2



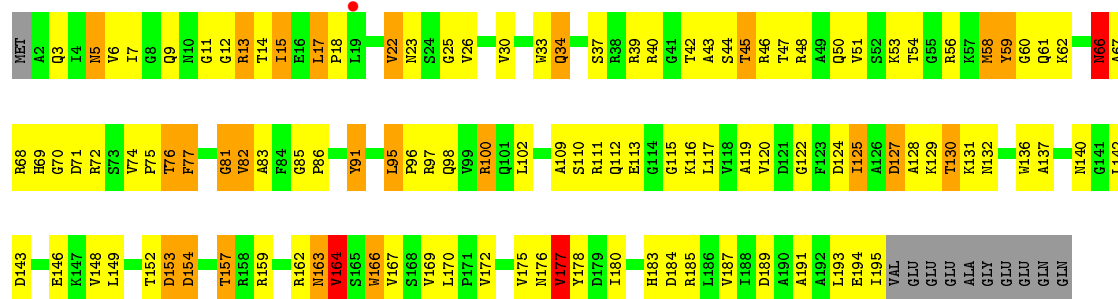
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

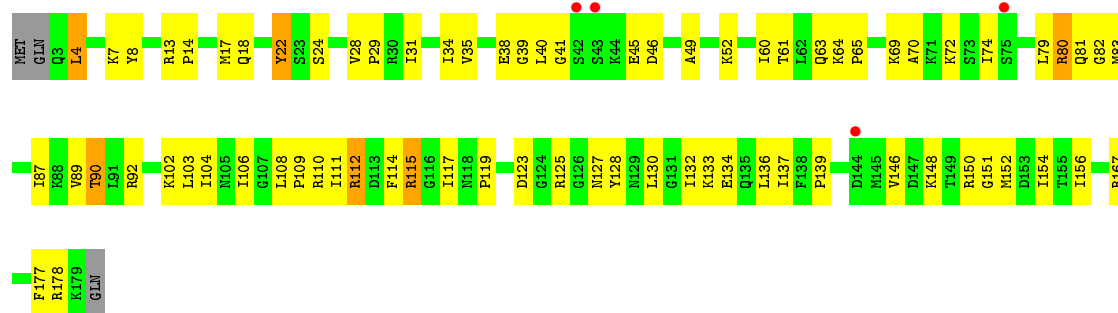


Chain C: 



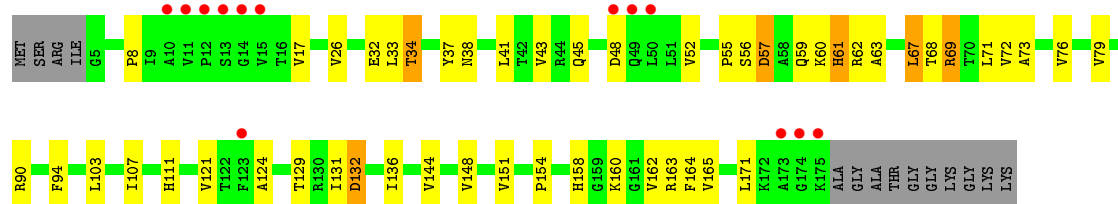
• Molecule 6: 50S ribosomal protein L5

Chain D: 



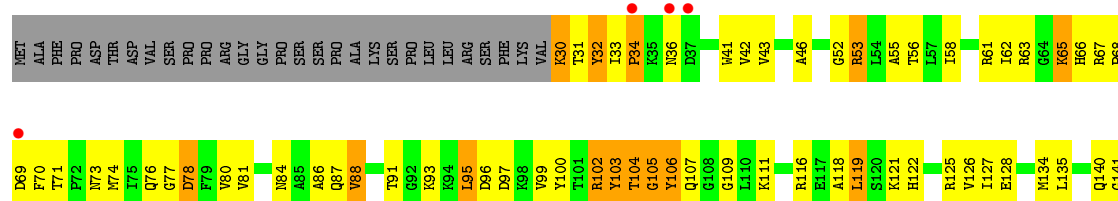
• Molecule 7: 50S ribosomal protein L6

Chain E: 



• Molecule 8: 50S ribosomal protein L13

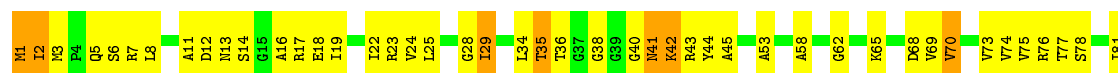
Chain G: 



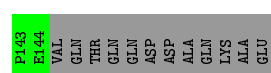
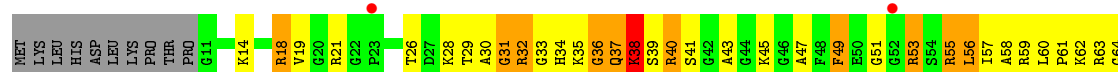




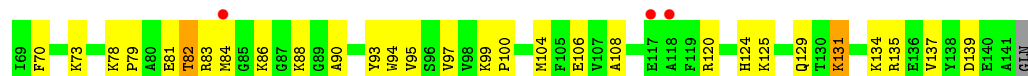
- Molecule 9: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L16

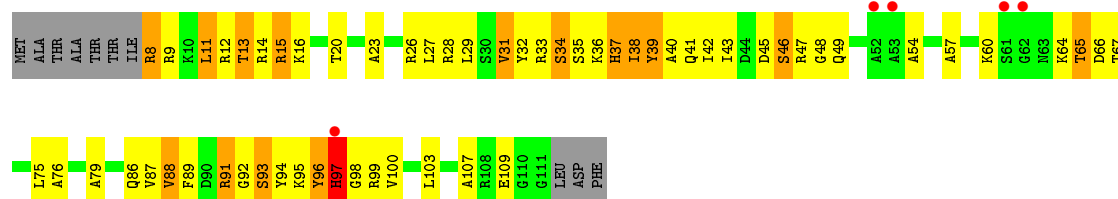
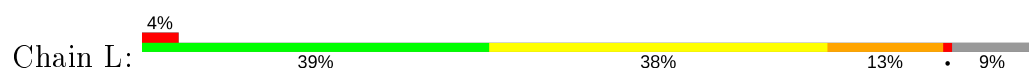


- Molecule 12: 50S ribosomal protein L17

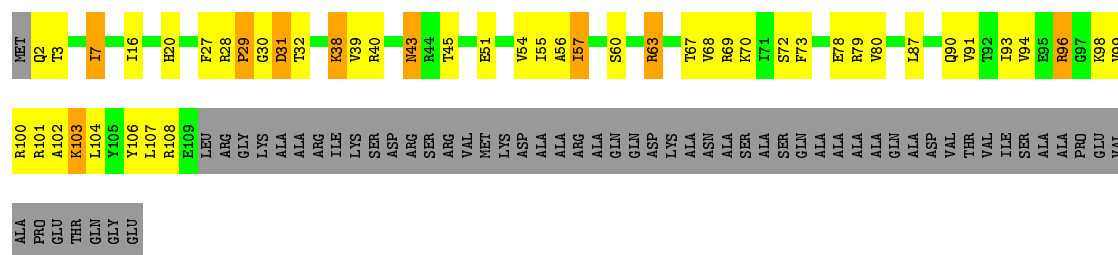


- Molecule 13: 50S ribosomal protein L18

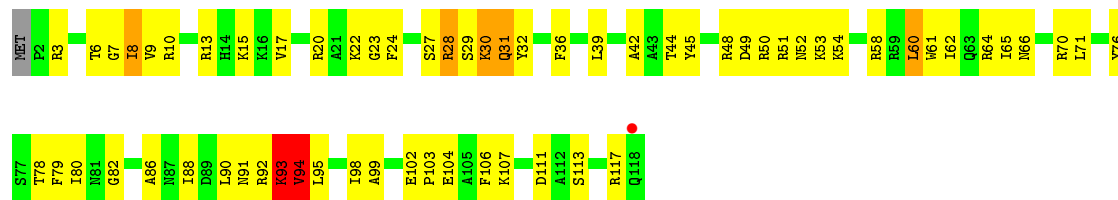




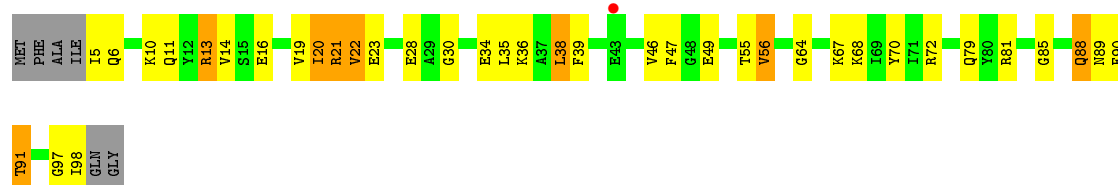
- Molecule 14: 50S ribosomal protein L19



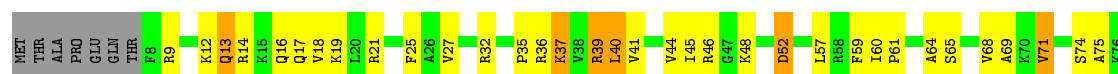
- Molecule 15: 50S ribosomal protein L20



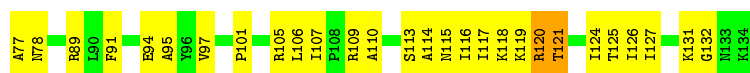
- Molecule 16: 50S ribosomal protein L21



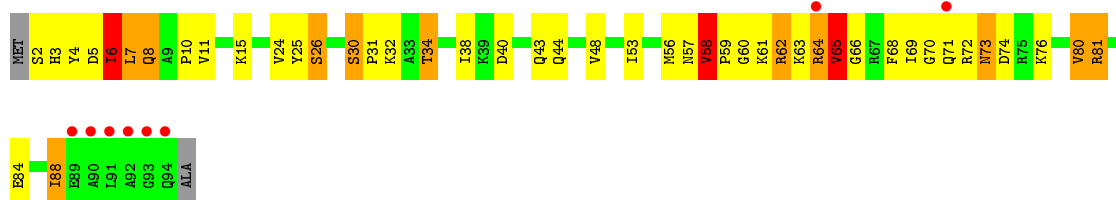
- Molecule 17: 50S ribosomal protein L22



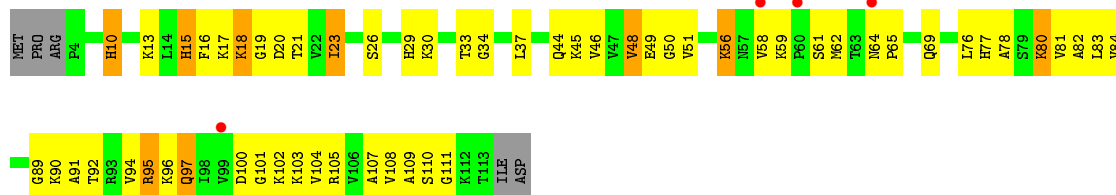




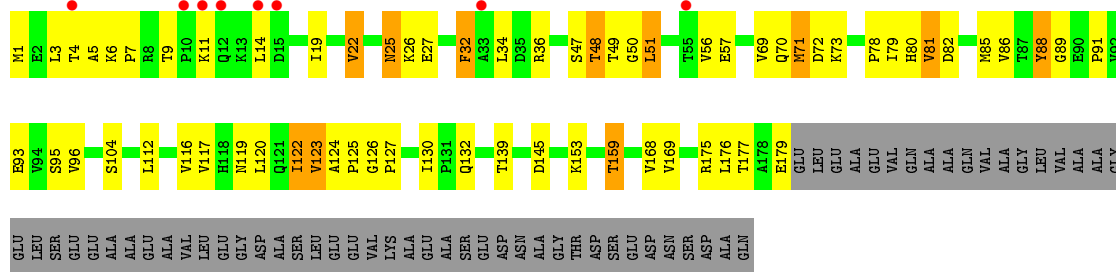
- Molecule 18: 50S ribosomal protein L23



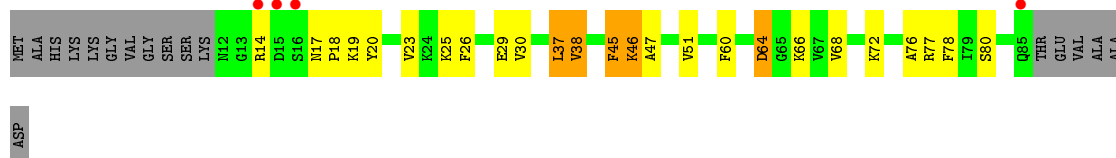
- Molecule 19: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L28











## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.47Å 407.38Å 692.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.58 29.84 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.84-3.58) 94.2 (29.84-3.57)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.204 , 0.247 0.204 , 0.247	Depositor DCC
$R_{free}$ test set	13397 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.0	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	83681	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6O1

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	X	0.69	20/63887 (0.0%)	1.25	500/99650 (0.5%)
2	Y	0.41	0/2863	0.93	0/4461
3	A	0.49	0/2011	0.79	4/2708 (0.1%)
4	B	0.58	0/1567	0.85	0/2105
5	C	0.49	0/1504	0.77	1/2036 (0.0%)
6	D	0.30	0/1419	0.51	0/1903
7	E	0.30	0/1308	0.54	0/1771
8	G	0.51	0/1138	0.81	1/1539 (0.1%)
9	H	0.56	0/1007	0.74	0/1352
10	I	0.61	0/1022	0.93	3/1366 (0.2%)
11	J	0.48	0/1101	0.71	0/1472
12	K	0.67	0/886	0.89	2/1188 (0.2%)
13	L	0.39	0/785	0.69	0/1048
14	M	0.67	1/872 (0.1%)	0.91	2/1172 (0.2%)
15	N	0.52	0/994	0.77	0/1323
16	O	0.46	0/750	0.81	2/1000 (0.2%)
17	P	0.58	0/1027	0.71	0/1373
18	Q	0.49	0/737	0.82	2/988 (0.2%)
19	R	0.45	0/835	0.75	0/1121
20	S	0.31	0/1399	0.57	0/1902
21	T	0.45	0/563	0.75	0/747
22	U	0.46	0/556	0.73	0/741
23	V	0.34	0/529	0.52	0/704
24	W	0.43	0/426	0.67	0/568
25	Z	0.56	0/464	0.77	0/622
26	1	0.55	0/434	0.83	0/579
27	2	0.58	0/387	1.04	2/509 (0.4%)
28	3	0.59	0/468	0.98	2/614 (0.3%)
All	All	0.63	21/90939 (0.0%)	1.14	521/136562 (0.4%)

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	A	0	1
4	B	0	1
5	C	0	2
8	G	0	4
10	I	0	5
11	J	0	1
13	L	0	1
15	N	0	2
19	R	0	1
25	Z	0	1
27	2	0	3
28	3	0	2
All	All	0	24

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	774	A	C5-C4	7.18	1.43	1.38
1	X	542	A	N9-C4	-7.12	1.33	1.37
14	M	29	PRO	CA-C	6.60	1.66	1.52
1	X	540	G	C2-N3	6.49	1.38	1.32
1	X	2548	G	C6-O6	6.47	1.29	1.24

The worst 5 of 521 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	774	A	N7-C8-N9	14.67	121.13	113.80
1	X	774	A	C8-N9-C4	-14.58	99.97	105.80
1	X	542	A	C2-N3-C4	-13.70	103.75	110.60
1	X	1333	G	N3-C4-N9	-12.51	118.49	126.00
1	X	2018	G	C4-C5-N7	11.72	115.49	110.80

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	58	HIS	Peptide
4	B	122	PHE	Peptide
5	C	176	ASN	Peptide

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Mol	Chain	Res	Type	Group
5	C	66	ASN	Peptide
8	G	34	PRO	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	X	57052	0	28750	1265	0
2	Y	2561	0	1306	59	0
3	A	1973	0	2034	131	0
4	B	1539	0	1600	81	0
5	C	1481	0	1504	97	0
6	D	1400	0	1481	60	0
7	E	1286	0	1336	31	0
8	G	1114	0	1144	83	0
9	H	997	0	1046	55	0
10	I	1011	0	1047	76	0
11	J	1078	0	1103	47	0
12	K	878	0	930	34	0
13	L	779	0	820	49	0
14	M	859	0	872	35	0
15	N	978	0	1020	66	0
16	O	741	0	756	34	0
17	P	1014	0	1096	49	0
18	Q	726	0	753	29	0
19	R	825	0	881	57	0
20	S	1374	0	1401	44	0
21	T	556	0	579	24	0
22	U	552	0	604	42	0
23	V	525	0	546	14	0
24	W	424	0	470	16	0
25	Z	452	0	457	34	0
26	1	427	0	445	35	0
27	2	383	0	414	37	0
28	3	462	0	506	36	0
29	X	111	0	0	2	0
30	K	2	0	0	0	0
30	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	119	0	0	0	0
30	Y	1	0	0	0	0
All	All	83681	0	54901	2278	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 17.

The worst 5 of 2278 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:X:356:A:HO2'	1:X:357:A:H8	1.10	0.99
8:G:100:TYR:HB2	8:G:116:ARG:HE	1.25	0.96
10:I:56:LEU:H	10:I:59:ARG:HD3	1.30	0.94
1:X:1277:G:OP1	25:Z:19:ARG:NH2	2.01	0.93
1:X:1264:C:H5''	15:N:13:ARG:HH12	1.34	0.93

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
3	A	257/275 (94%)	219 (85%)	37 (14%)	1 (0%)	34	71
4	B	203/211 (96%)	183 (90%)	15 (7%)	5 (2%)	5	36
5	C	192/205 (94%)	161 (84%)	25 (13%)	6 (3%)	4	32
6	D	175/180 (97%)	151 (86%)	24 (14%)	0	100	100
7	E	169/185 (91%)	155 (92%)	13 (8%)	1 (1%)	25	64
8	G	140/174 (80%)	124 (89%)	15 (11%)	1 (1%)	22	62
9	H	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	19	59
10	I	132/156 (85%)	98 (74%)	30 (23%)	4 (3%)	4	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	134/141 (95%)	117 (87%)	16 (12%)	1 (1%)	22	62
12	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	17	57
13	L	102/114 (90%)	80 (78%)	22 (22%)	0	100	100
14	M	106/166 (64%)	100 (94%)	6 (6%)	0	100	100
15	N	115/118 (98%)	100 (87%)	13 (11%)	2 (2%)	9	44
16	O	92/100 (92%)	83 (90%)	9 (10%)	0	100	100
17	P	125/134 (93%)	121 (97%)	4 (3%)	0	100	100
18	Q	91/95 (96%)	69 (76%)	19 (21%)	3 (3%)	4	31
19	R	108/115 (94%)	80 (74%)	28 (26%)	0	100	100
20	S	177/237 (75%)	150 (85%)	25 (14%)	2 (1%)	14	53
21	T	72/91 (79%)	63 (88%)	9 (12%)	0	100	100
22	U	70/81 (86%)	51 (73%)	17 (24%)	2 (3%)	4	33
23	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
24	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
25	Z	55/60 (92%)	45 (82%)	10 (18%)	0	100	100
26	1	51/54 (94%)	36 (71%)	12 (24%)	3 (6%)	1	18
27	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	2	23
28	3	57/66 (86%)	44 (77%)	11 (19%)	2 (4%)	3	30
All	All	3026/3377 (90%)	2598 (86%)	391 (13%)	37 (1%)	13	51

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	94	VAL
18	Q	6	ILE
5	C	177	VAL
20	S	122	ILE
26	1	9	ILE

### 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	
3	A	200/216 (93%)	160 (80%)	40 (20%)	1	8
4	B	155/157 (99%)	132 (85%)	23 (15%)	3	20
5	C	154/163 (94%)	117 (76%)	37 (24%)	0	5
6	D	153/156 (98%)	144 (94%)	9 (6%)	19	54
7	E	136/144 (94%)	124 (91%)	12 (9%)	10	40
8	G	118/146 (81%)	100 (85%)	18 (15%)	2	19
9	H	103/103 (100%)	83 (81%)	20 (19%)	1	9
10	I	101/121 (84%)	77 (76%)	24 (24%)	0	5
11	J	108/115 (94%)	89 (82%)	19 (18%)	2	12
12	K	90/93 (97%)	74 (82%)	16 (18%)	2	11
13	L	74/82 (90%)	50 (68%)	24 (32%)	0	2
14	M	92/134 (69%)	76 (83%)	16 (17%)	2	12
15	N	96/97 (99%)	87 (91%)	9 (9%)	8	38
16	O	75/79 (95%)	64 (85%)	11 (15%)	3	20
17	P	109/115 (95%)	90 (83%)	19 (17%)	2	12
18	Q	75/76 (99%)	53 (71%)	22 (29%)	0	3
19	R	91/96 (95%)	77 (85%)	14 (15%)	2	18
20	S	152/192 (79%)	130 (86%)	22 (14%)	3	20
21	T	55/67 (82%)	47 (86%)	8 (14%)	3	20
22	U	57/66 (86%)	43 (75%)	14 (25%)	0	5
23	V	53/55 (96%)	49 (92%)	4 (8%)	13	45
24	W	48/48 (100%)	42 (88%)	6 (12%)	4	25
25	Z	51/53 (96%)	36 (71%)	15 (29%)	0	3
26	1	45/47 (96%)	33 (73%)	12 (27%)	0	3
27	2	39/40 (98%)	29 (74%)	10 (26%)	0	4
28	3	46/52 (88%)	34 (74%)	12 (26%)	0	4
All	All	2476/2713 (91%)	2040 (82%)	436 (18%)	2	12

5 of 436 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	106	GLU

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Mol	Chain	Res	Type
14	M	31	ASP
26	1	8	ILE
12	K	11	ASN
13	L	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
10	I	103	ASN
12	K	35	GLN
25	Z	44	HIS
11	J	58	HIS
13	L	41	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2650/2880 (92%)	580 (21%)	49 (1%)
2	Y	119/123 (96%)	23 (19%)	1 (0%)
All	All	2769/3003 (92%)	603 (21%)	50 (1%)

5 of 603 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	4	C
1	X	7	G
1	X	10	A
1	X	14	A

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1182	U
1	X	1475	U
1	X	2736	U
1	X	1223	G
1	X	1391	A



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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 124 ligands modelled in this entry, 123 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	$\# Z  > 2$
29	6O1	X	2901	-	117,123,123	1.60	14 (11%)	155,191,191	1.86	27 (17%)

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
29	6O1	X	2901	-	-	10/50/234/234	0/13/13/13

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	6O1	O71-N65	6.73	1.36	1.22
29	X	2901	6O1	C08-C05	-5.84	1.39	1.51
29	X	2901	6O1	O53-C49	5.39	1.45	1.40
29	X	2901	6O1	C62-C61	-5.28	1.40	1.51
29	X	2901	6O1	C04-C09	-4.34	1.40	1.50

The worst 5 of 27 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	6O1	O50-C50-C51	-10.43	97.90	106.63
29	X	2901	6O1	O51-C51-C50	-6.40	98.11	106.41
29	X	2901	6O1	C44-O44-C36	-5.12	105.27	114.42
29	X	2901	6O1	C36-C37-C38	-4.77	102.16	110.38
29	X	2901	6O1	C01-C06-C05	-4.45	119.97	122.79

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	2901	6O1	O67-C63-O12-C12
29	X	2901	6O1	O33-C29-O39-C39
29	X	2901	6O1	O40-C36-O44-C44
29	X	2901	6O1	C37-C36-O44-C44
29	X	2901	6O1	O55-C55-C56-C61

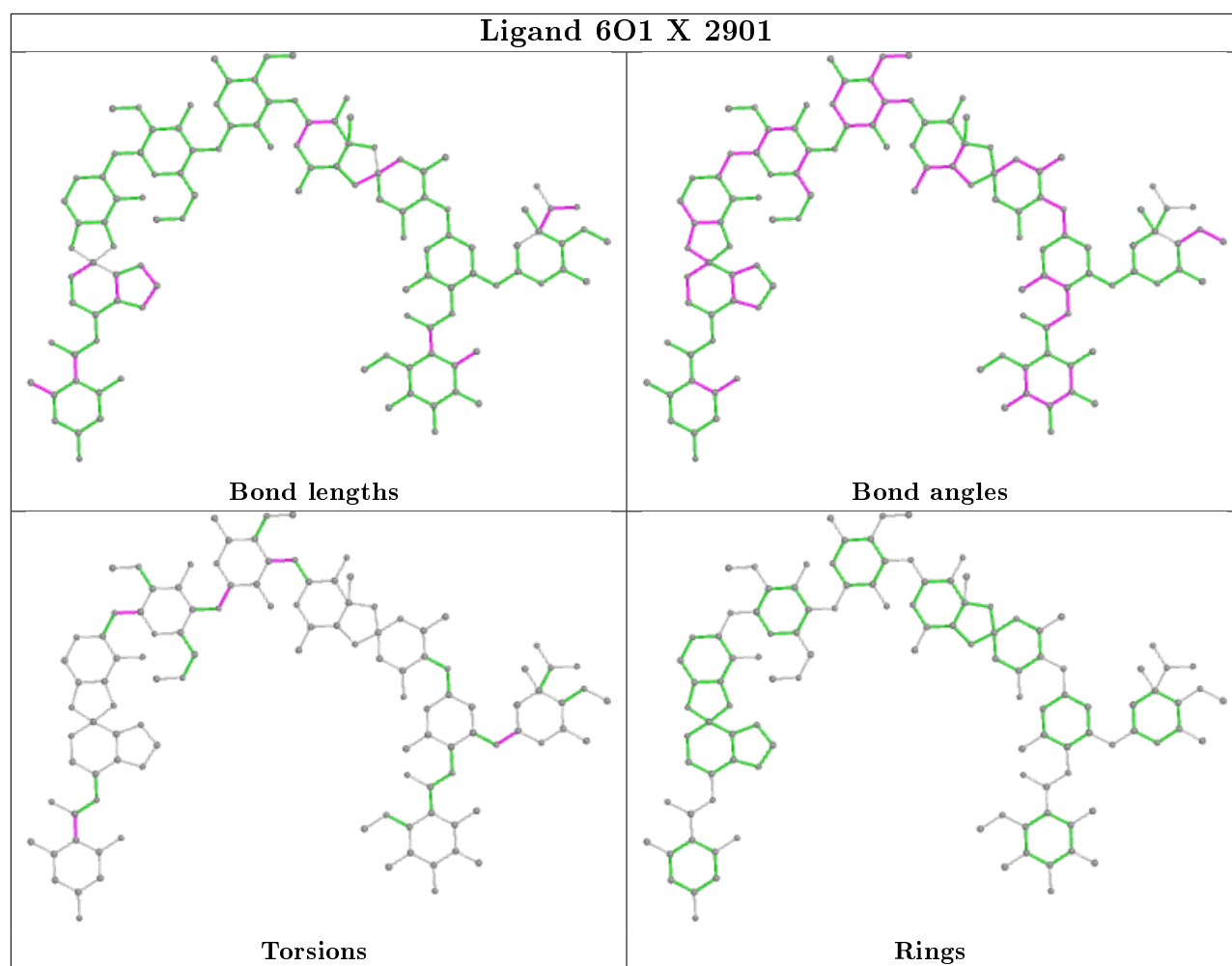
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	2901	6O1	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	X	2658/2880 (92%)	-0.12	95 (3%) 42 27	30, 77, 204, 337	0
2	Y	120/123 (97%)	-0.07	3 (2%) 57 39	80, 150, 187, 207	0
3	A	259/275 (94%)	-0.19	4 (1%) 73 58	50, 105, 160, 212	0
4	B	205/211 (97%)	-0.49	0 100 100	30, 51, 113, 199	0
5	C	194/205 (94%)	-0.38	1 (0%) 91 82	35, 103, 180, 254	0
6	D	177/180 (98%)	-0.14	4 (2%) 60 42	128, 183, 249, 280	0
7	E	171/185 (92%)	-0.08	13 (7%) 13 7	70, 142, 203, 254	0
8	G	142/174 (81%)	-0.12	6 (4%) 36 22	38, 78, 188, 245	0
9	H	134/134 (100%)	-0.43	0 100 100	40, 55, 108, 175	0
10	I	134/156 (85%)	-0.10	2 (1%) 73 58	50, 120, 191, 236	0
11	J	136/141 (96%)	-0.04	3 (2%) 62 43	65, 106, 170, 225	0
12	K	113/116 (97%)	-0.54	0 100 100	30, 37, 91, 200	0
13	L	104/114 (91%)	0.01	5 (4%) 30 18	120, 154, 189, 241	0
14	M	108/166 (65%)	-0.66	0 100 100	37, 50, 117, 169	0
15	N	117/118 (99%)	-0.47	1 (0%) 84 71	42, 82, 136, 279	0
16	O	94/100 (94%)	-0.37	1 (1%) 80 66	48, 101, 170, 216	0
17	P	127/134 (94%)	-0.53	0 100 100	34, 53, 105, 192	0
18	Q	93/95 (97%)	-0.28	8 (8%) 10 6	49, 88, 174, 215	0
19	R	110/115 (95%)	-0.28	4 (3%) 42 27	62, 117, 213, 259	0
20	S	179/237 (75%)	-0.10	8 (4%) 33 19	97, 158, 213, 289	0
21	T	74/91 (81%)	-0.09	4 (5%) 25 14	67, 104, 157, 206	0
22	U	72/81 (88%)	0.10	5 (6%) 16 9	70, 125, 187, 215	0
23	V	65/67 (97%)	-0.23	3 (4%) 32 19	83, 125, 197, 216	0
24	W	55/55 (100%)	-0.61	0 100 100	68, 90, 135, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Z	57/60 (95%)	-0.28	1 (1%) 68 51	32, 43, 104, 182	0
26	1	53/54 (98%)	0.36	6 (11%) 5 3	101, 129, 224, 259	0
27	2	46/47 (97%)	-0.29	1 (2%) 62 43	44, 59, 103, 162	0
28	3	59/66 (89%)	0.04	0 100 100	72, 100, 161, 239	0
All	All	5856/6380 (91%)	-0.19	178 (3%) 50 32	30, 91, 201, 337	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	1523	A	15.5
6	D	43	SER	8.1
22	U	29	GLY	6.4
1	X	1522	C	6.2
1	X	1073	G	5.9

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

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

## 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(Å <sup>2</sup> )	Q<0.9
30	MG	X	3020	1/1	0.53	1.58	64,64,64,64	0
30	MG	X	3016	1/1	0.71	1.26	74,74,74,74	0
30	MG	X	3012	1/1	0.73	0.39	52,52,52,52	0
30	MG	X	3006	1/1	0.74	0.50	34,34,34,34	0
30	MG	X	2927	1/1	0.79	0.54	57,57,57,57	0
30	MG	X	2960	1/1	0.79	0.89	34,34,34,34	0
30	MG	X	2999	1/1	0.80	0.77	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MG	X	3001	1/1	0.80	1.62	86,86,86,86	0
30	MG	X	2916	1/1	0.81	1.06	51,51,51,51	0
30	MG	X	3019	1/1	0.83	1.06	46,46,46,46	0
30	MG	K	201	1/1	0.83	0.70	31,31,31,31	0
30	MG	X	2974	1/1	0.87	0.84	30,30,30,30	0
30	MG	X	2933	1/1	0.88	1.35	38,38,38,38	0
30	MG	X	3017	1/1	0.88	0.77	52,52,52,52	0
30	MG	X	2935	1/1	0.88	2.22	41,41,41,41	0
30	MG	X	2982	1/1	0.89	0.86	31,31,31,31	0
30	MG	X	2975	1/1	0.89	1.36	49,49,49,49	0
30	MG	X	3007	1/1	0.89	0.50	40,40,40,40	0
30	MG	X	2979	1/1	0.89	0.29	46,46,46,46	0
30	MG	X	3015	1/1	0.89	0.55	98,98,98,98	0
30	MG	X	2907	1/1	0.90	1.25	49,49,49,49	0
30	MG	X	2992	1/1	0.90	1.04	34,34,34,34	0
30	MG	X	2967	1/1	0.90	0.37	55,55,55,55	0
30	MG	X	2913	1/1	0.91	0.63	36,36,36,36	0
30	MG	X	2964	1/1	0.91	0.53	60,60,60,60	0
30	MG	X	2904	1/1	0.91	1.01	32,32,32,32	0
30	MG	X	2906	1/1	0.91	0.88	42,42,42,42	0
30	MG	X	2942	1/1	0.91	0.25	31,31,31,31	0
30	MG	X	2940	1/1	0.91	0.41	34,34,34,34	0
29	6O1	X	2901	111/111	0.91	0.39	106,116,136,139	0
30	MG	X	2928	1/1	0.91	0.17	41,41,41,41	0
30	MG	X	2978	1/1	0.92	0.42	49,49,49,49	0
30	MG	X	2925	1/1	0.92	0.53	43,43,43,43	0
30	MG	M	201	1/1	0.92	1.58	35,35,35,35	0
30	MG	X	2981	1/1	0.92	0.61	99,99,99,99	0
30	MG	X	2972	1/1	0.92	0.63	36,36,36,36	0
30	MG	X	2971	1/1	0.92	0.61	33,33,33,33	0
30	MG	X	2937	1/1	0.93	0.73	32,32,32,32	0
30	MG	X	2945	1/1	0.93	1.20	55,55,55,55	0
30	MG	X	2987	1/1	0.93	0.46	43,43,43,43	0
30	MG	X	2995	1/1	0.93	0.82	83,83,83,83	0
30	MG	X	2970	1/1	0.94	1.02	63,63,63,63	0
30	MG	X	2902	1/1	0.94	1.16	32,32,32,32	0
30	MG	X	2947	1/1	0.94	1.18	52,52,52,52	0
30	MG	X	2973	1/1	0.94	0.35	52,52,52,52	0
30	MG	X	2976	1/1	0.94	0.49	53,53,53,53	0
30	MG	X	2998	1/1	0.94	0.22	35,35,35,35	0
30	MG	X	2909	1/1	0.94	0.72	36,36,36,36	0
30	MG	X	2938	1/1	0.94	0.33	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MG	X	2944	1/1	0.94	0.88	37,37,37,37	0
30	MG	X	2968	1/1	0.94	0.26	35,35,35,35	0
30	MG	X	3011	1/1	0.94	0.34	58,58,58,58	0
30	MG	X	2994	1/1	0.94	0.37	77,77,77,77	0
30	MG	X	3008	1/1	0.94	0.62	39,39,39,39	0
30	MG	X	2917	1/1	0.94	0.21	33,33,33,33	0
30	MG	X	2920	1/1	0.95	0.74	34,34,34,34	0
30	MG	X	2922	1/1	0.95	0.44	35,35,35,35	0
30	MG	X	3003	1/1	0.95	0.88	63,63,63,63	0
30	MG	X	2910	1/1	0.95	0.62	34,34,34,34	0
30	MG	X	2956	1/1	0.95	0.57	32,32,32,32	0
30	MG	X	2903	1/1	0.95	0.61	37,37,37,37	0
30	MG	X	2943	1/1	0.95	0.29	33,33,33,33	0
30	MG	K	202	1/1	0.95	0.19	31,31,31,31	0
30	MG	X	2912	1/1	0.95	0.46	34,34,34,34	0
30	MG	X	2988	1/1	0.95	0.65	55,55,55,55	0
30	MG	X	3002	1/1	0.95	0.31	44,44,44,44	0
30	MG	X	2908	1/1	0.95	0.67	34,34,34,34	0
30	MG	X	2932	1/1	0.95	0.32	53,53,53,53	0
30	MG	X	2986	1/1	0.96	0.47	46,46,46,46	0
30	MG	X	3004	1/1	0.96	0.30	54,54,54,54	0
30	MG	X	2991	1/1	0.96	0.69	72,72,72,72	0
30	MG	X	2939	1/1	0.96	0.61	30,30,30,30	0
30	MG	X	2951	1/1	0.96	0.22	35,35,35,35	0
30	MG	X	2931	1/1	0.96	0.58	32,32,32,32	0
30	MG	X	3005	1/1	0.96	0.92	66,66,66,66	0
30	MG	X	2959	1/1	0.96	0.69	54,54,54,54	0
30	MG	X	2955	1/1	0.96	0.39	31,31,31,31	0
30	MG	X	2977	1/1	0.96	1.03	78,78,78,78	0
30	MG	X	2990	1/1	0.96	0.64	39,39,39,39	0
30	MG	X	2989	1/1	0.96	0.67	56,56,56,56	0
30	MG	Y	201	1/1	0.96	0.90	77,77,77,77	0
30	MG	X	2957	1/1	0.96	0.33	42,42,42,42	0
30	MG	X	2914	1/1	0.96	0.46	43,43,43,43	0
30	MG	X	2950	1/1	0.96	0.52	36,36,36,36	0
30	MG	X	2961	1/1	0.96	0.68	68,68,68,68	0
30	MG	X	2949	1/1	0.96	0.36	32,32,32,32	0
30	MG	X	2958	1/1	0.96	0.86	38,38,38,38	0
30	MG	X	2921	1/1	0.96	0.98	37,37,37,37	0
30	MG	X	3018	1/1	0.96	0.28	32,32,32,32	0
30	MG	X	2930	1/1	0.97	0.64	46,46,46,46	0
30	MG	X	3010	1/1	0.97	0.27	41,41,41,41	0

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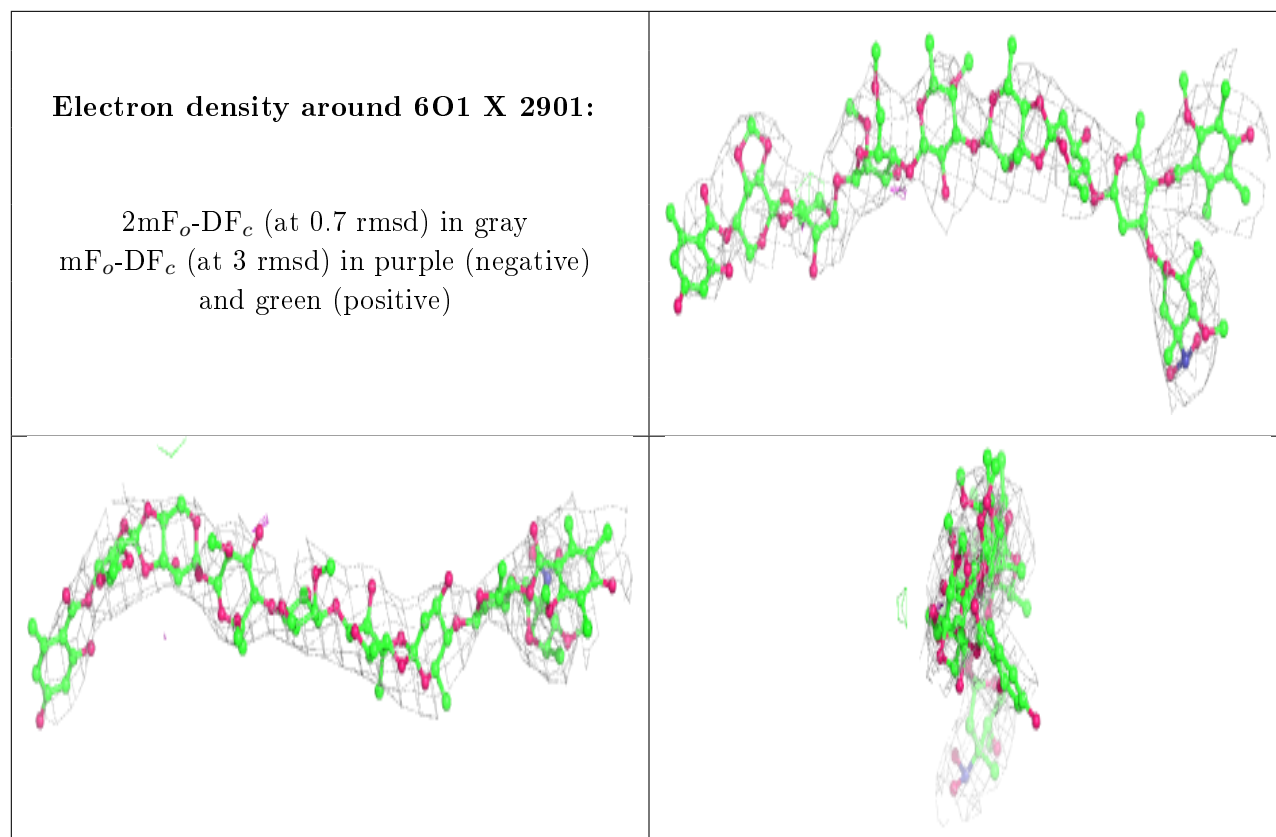


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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MG	X	2905	1/1	0.97	0.82	30,30,30,30	0
30	MG	X	2911	1/1	0.97	0.66	46,46,46,46	0
30	MG	X	2984	1/1	0.97	0.57	49,49,49,49	0
30	MG	X	2926	1/1	0.97	0.32	32,32,32,32	0
30	MG	X	2952	1/1	0.97	1.27	54,54,54,54	0
30	MG	X	2941	1/1	0.97	0.43	55,55,55,55	0
30	MG	X	2965	1/1	0.97	0.48	40,40,40,40	0
30	MG	X	2980	1/1	0.97	0.44	49,49,49,49	0
30	MG	X	3014	1/1	0.97	0.28	43,43,43,43	0
30	MG	X	2948	1/1	0.97	0.26	30,30,30,30	0
30	MG	X	2953	1/1	0.97	0.29	38,38,38,38	0
30	MG	X	3013	1/1	0.98	0.49	47,47,47,47	0
30	MG	X	2985	1/1	0.98	0.28	55,55,55,55	0
30	MG	X	2963	1/1	0.98	0.67	71,71,71,71	0
30	MG	X	2983	1/1	0.98	0.30	63,63,63,63	0
30	MG	X	2946	1/1	0.98	0.43	34,34,34,34	0
30	MG	X	2923	1/1	0.98	0.39	30,30,30,30	0
30	MG	X	2966	1/1	0.98	0.34	37,37,37,37	0
30	MG	X	2996	1/1	0.98	0.19	43,43,43,43	0
30	MG	X	2993	1/1	0.98	0.42	44,44,44,44	0
30	MG	X	2915	1/1	0.98	0.36	36,36,36,36	0
30	MG	X	2934	1/1	0.98	0.81	39,39,39,39	0
30	MG	X	2936	1/1	0.98	0.47	53,53,53,53	0
30	MG	X	3000	1/1	0.98	0.28	39,39,39,39	0
30	MG	X	2962	1/1	0.98	0.20	41,41,41,41	0
30	MG	X	2929	1/1	0.98	0.73	39,39,39,39	0
30	MG	X	2918	1/1	0.98	0.47	45,45,45,45	0
30	MG	X	2919	1/1	0.98	0.31	33,33,33,33	0
30	MG	X	3009	1/1	0.99	0.33	41,41,41,41	0
30	MG	X	2924	1/1	0.99	0.39	30,30,30,30	0
30	MG	X	2954	1/1	0.99	0.56	41,41,41,41	0
30	MG	X	2997	1/1	0.99	0.35	38,38,38,38	0
30	MG	X	2969	1/1	0.99	0.64	43,43,43,43	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.