



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 08:40 PM BST

PDB ID : 4DV3  
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, C912A, bound with streptomycin  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2012-02-22  
Resolution : 3.55 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 : 2.13.1  
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) : 2.13.1

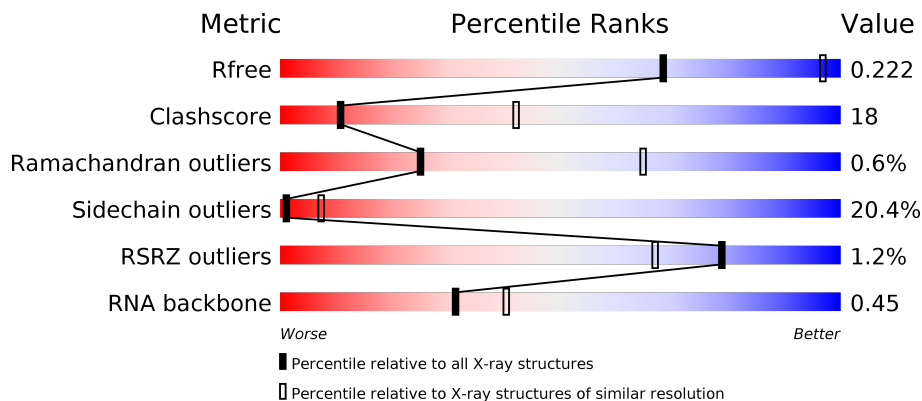
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.55 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.






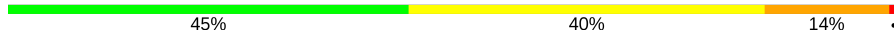
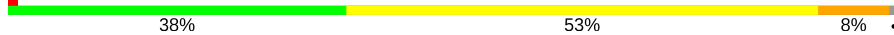
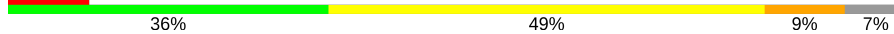
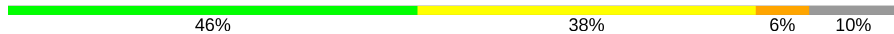
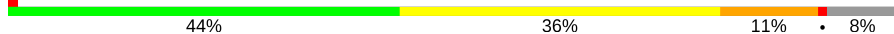
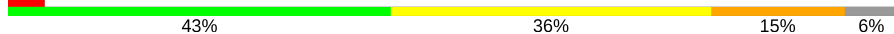
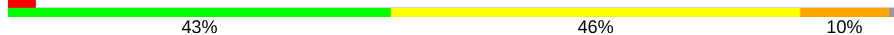

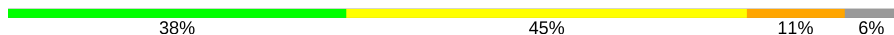
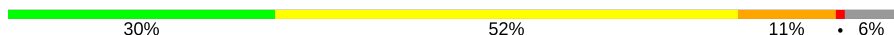




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)
RNA backbone	3102	1003 (4.02-3.00)

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	A	1522	 23% 41% 28% 8%
2	B	256	 41% 38% 11% 9%
3	C	239	 3% 38% 38% 10% 14%
4	D	209	 55% 35% 9%

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	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
1	PSU	A	1540	-	-	-	X
23	MG	A	1720	-	-	-	X
23	MG	A	1730	-	-	-	X
23	MG	A	1735	-	-	-	X
23	MG	A	1742	-	-	-	X
23	MG	A	1743	-	-	-	X
23	MG	A	1750	-	-	-	X
23	MG	A	1764	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
23	MG	A	1768	-	-	-	X
23	MG	A	1770	-	-	-	X
23	MG	A	1771	-	-	-	X
23	MG	A	1783	-	-	-	X
23	MG	A	1790	-	-	-	X
23	MG	A	1791	-	-	-	X
23	MG	A	1805	-	-	-	X
23	MG	A	1860	-	-	-	X
23	MG	H	204	-	-	-	X
23	MG	M	203	-	-	-	X
23	MG	P	102	-	-	-	X

## 2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 52302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32509	14478	6013	10506	1512	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	912	A	C	ENGINEERED MUTATION	GB M26923.1
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	116	864	537	164	160	3	0	0	0

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	124	972	612	195	163	2	0	0	0

- Molecule 13 is a protein called ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	118	937	579	193	163	2	0	0	0

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	87	729	457	146	124	2	0	0	0

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	99	823	528	152	141	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 18 is a protein called ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	70	574	367	112	95	0	0	0

- Molecule 19 is a protein called ribosomal protein S19.

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

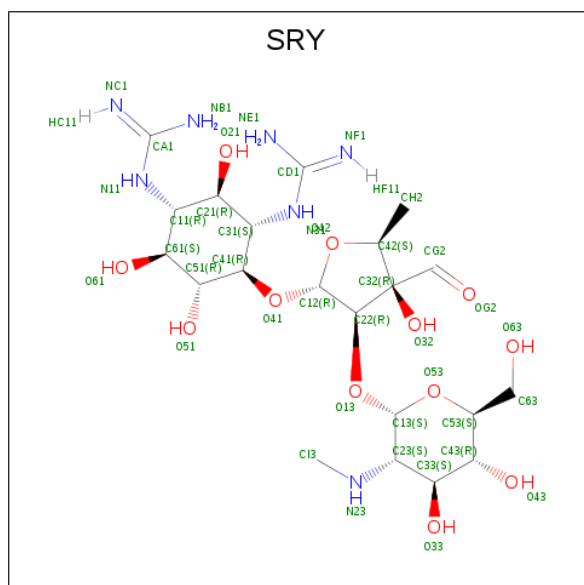
- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

- Molecule 22 is STREPTOMYCIN (three-letter code: SRY) (formula:  $C_{21}H_{39}N_7O_{12}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
22	A	1	40	21	7	12	0	0



- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	3	Total Mg 3 3	0	0
23	J	2	Total Mg 2 2	0	0
23	Q	2	Total Mg 2 2	0	0
23	D	1	Total Mg 1 1	0	0
23	K	1	Total Mg 1 1	0	0
23	E	1	Total Mg 1 1	0	0
23	H	4	Total Mg 4 4	0	0
23	B	2	Total Mg 2 2	0	0
23	A	259	Total Mg 259 259	0	0
23	T	1	Total Mg 1 1	0	0
23	N	1	Total Mg 1 1	0	0
23	S	1	Total Mg 1 1	0	0
23	M	3	Total Mg 3 3	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	369	Total O 369 369	0	0
25	D	1	Total O 1 1	0	0

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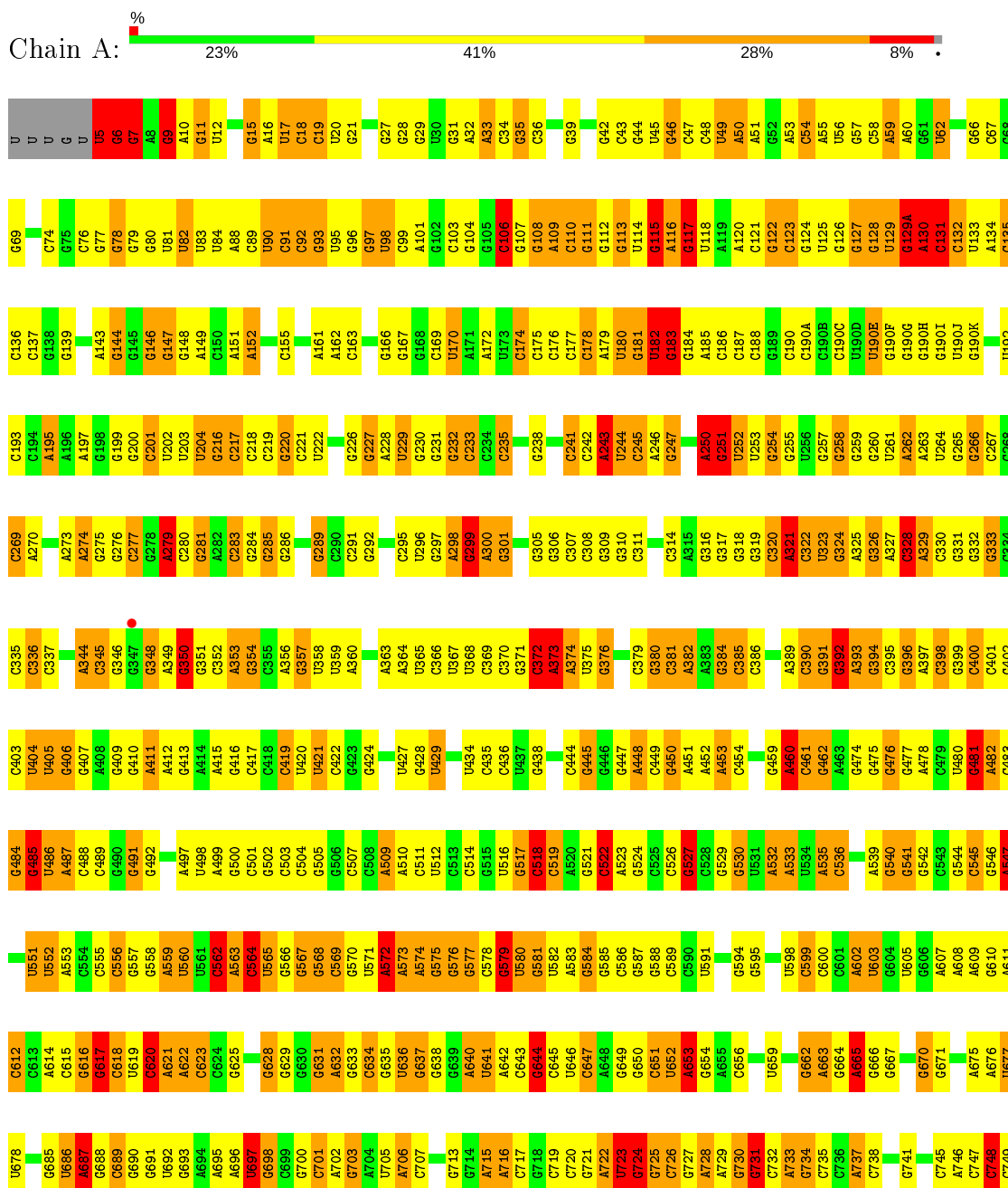
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
25	E	6	Total O 6 6	0	0
25	J	1	Total O 1 1	0	0
25	L	1	Total O 1 1	0	0
25	Q	1	Total O 1 1	0	0
25	T	2	Total O 2 2	0	0
25	U	1	Total O 1 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S rRNA

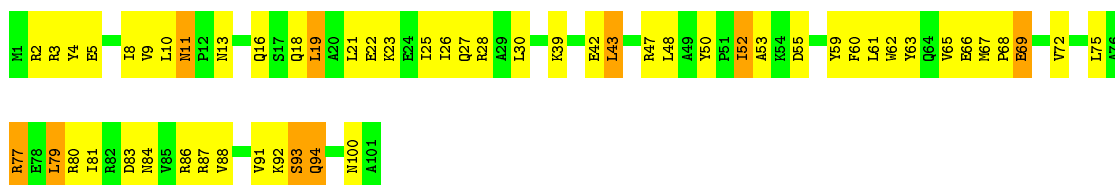




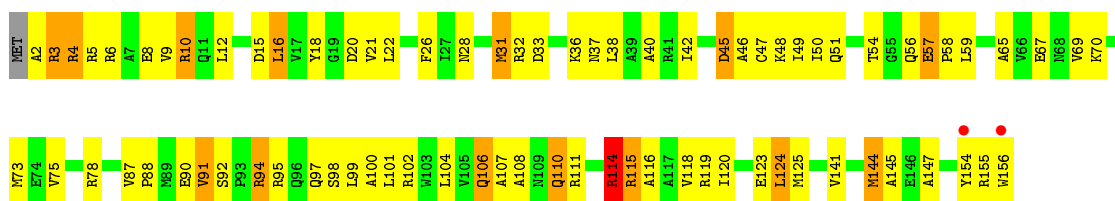




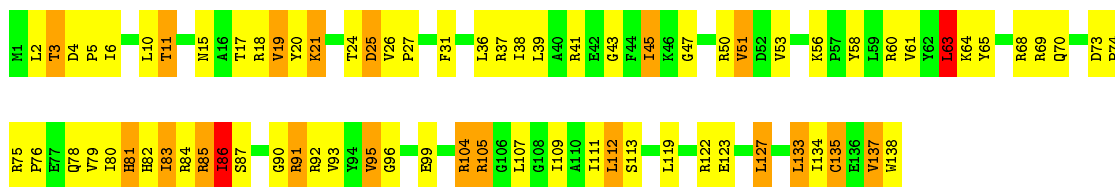
• Molecule 6: ribosomal protein S6



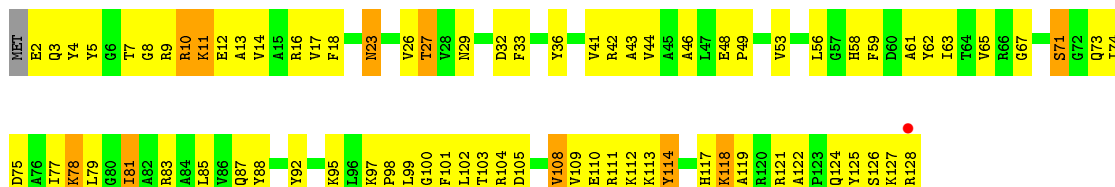
• Molecule 7: ribosomal protein S7



• Molecule 8: ribosomal protein S8

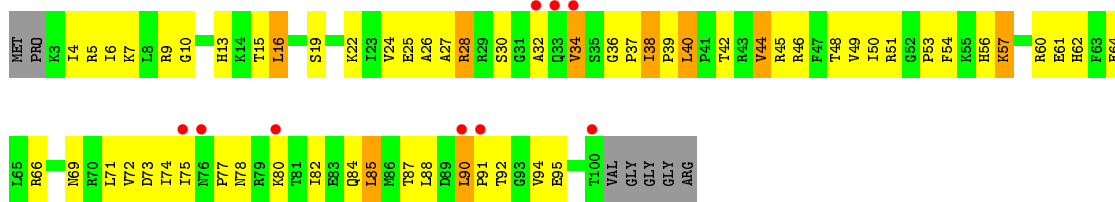


• Molecule 9: ribosomal protein S9

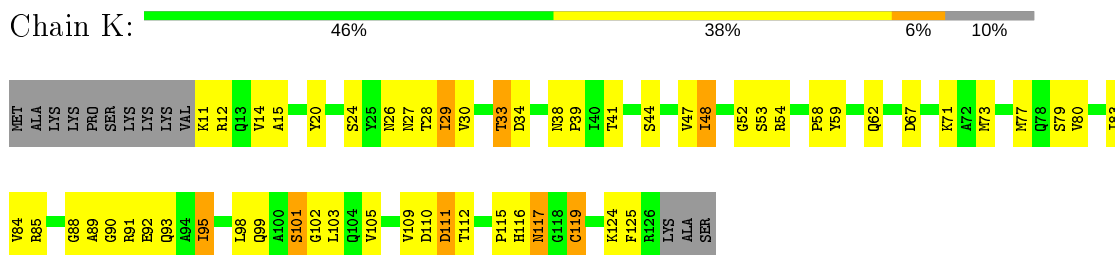


• Molecule 10: ribosomal protein S10

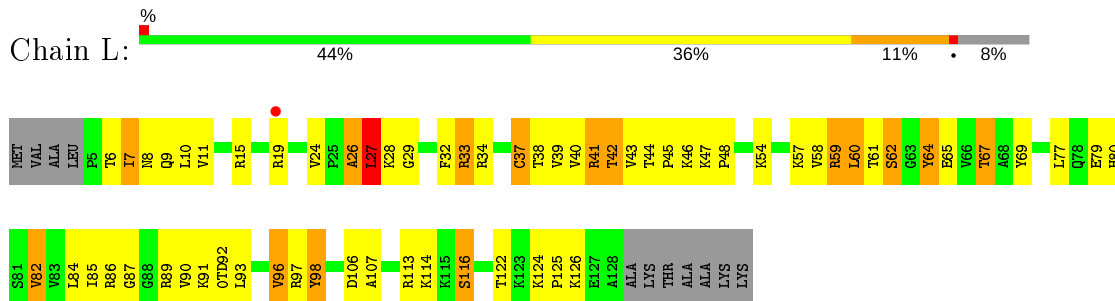




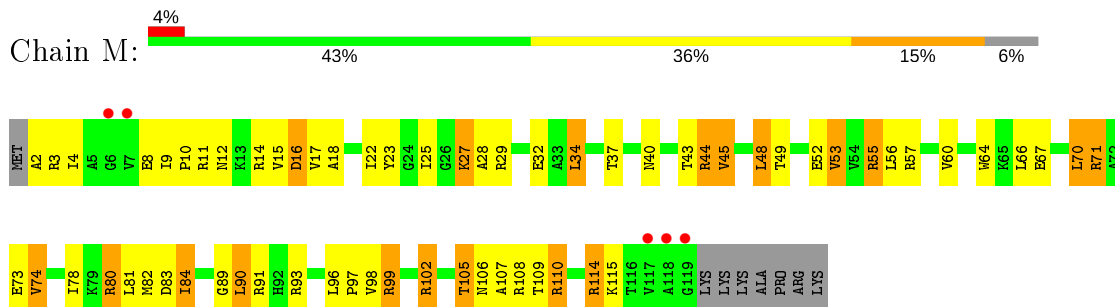
- Molecule 11: ribosomal protein S11



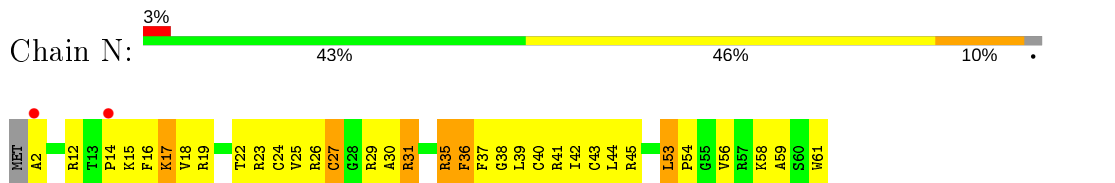
- Molecule 12: ribosomal protein S12



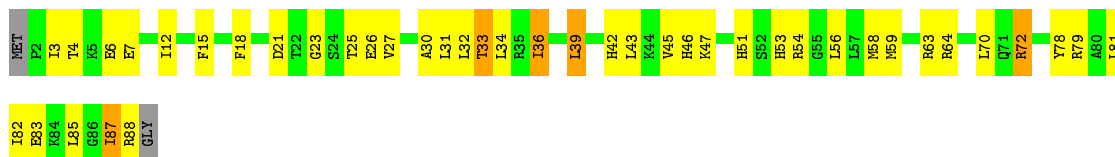
- Molecule 13: ribosomal protein S13



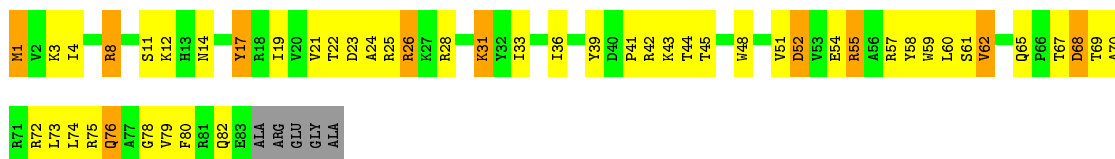
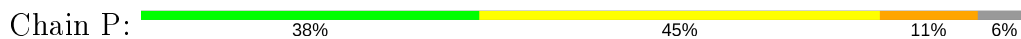
- Molecule 14: ribosomal protein S14



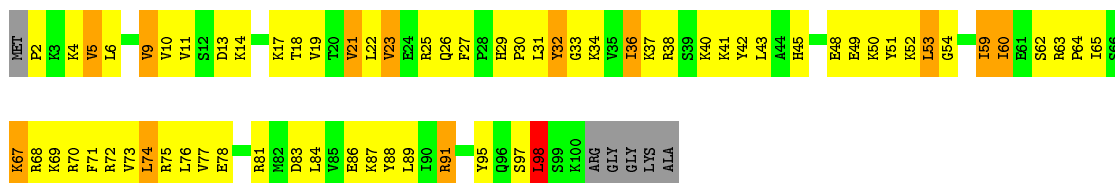
- Molecule 15: ribosomal protein S15



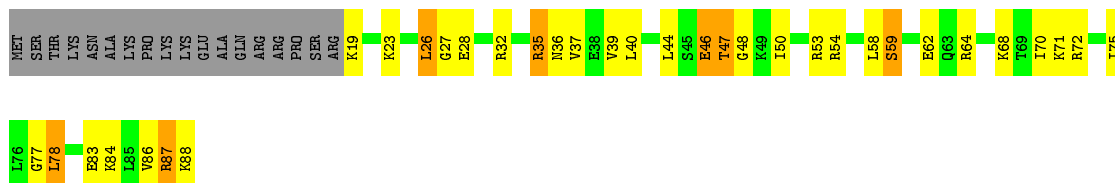
• Molecule 16: ribosomal protein S16



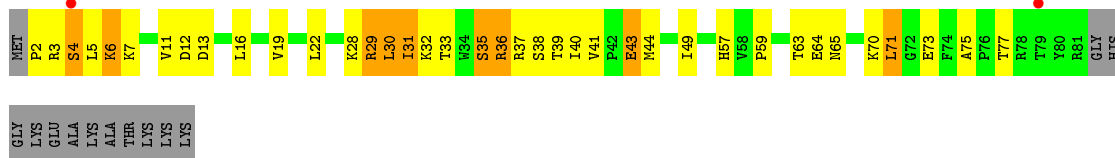
• Molecule 17: ribosomal protein S17



• Molecule 18: ribosomal protein S18



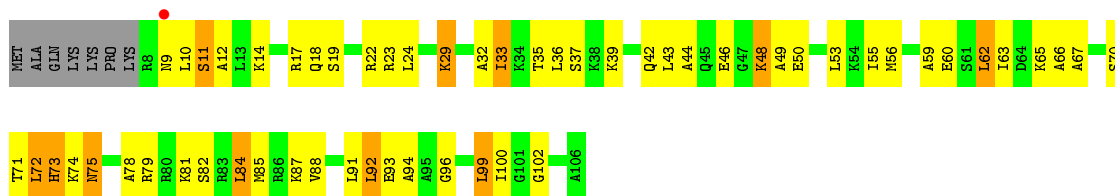
• Molecule 19: ribosomal protein S19



• Molecule 20: ribosomal protein S20







• Molecule 21: ribosomal protein THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.98Å 402.98Å 172.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.55 29.75 – 3.55	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.75-3.55) 96.3 (29.75-3.55)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 3.55Å)	Xtrriage
Refinement program	PHENIX dev_978	Depositor
R, $R_{free}$	0.166 , 0.220 0.167 , 0.222	Depositor DCC
$R_{free}$ test set	8254 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	118.0	Xtrriage
Anisotropy	0.504	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 97.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	52302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	152.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, PSU

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	1.20	169/36043 (0.5%)	1.90	1783/56248 (3.2%)
2	B	0.80	1/1935 (0.1%)	0.95	1/2609 (0.0%)
3	C	0.62	0/1636	0.82	2/2205 (0.1%)
4	D	0.73	1/1733 (0.1%)	0.93	6/2318 (0.3%)
5	E	0.93	0/1162	1.13	5/1564 (0.3%)
6	F	0.63	0/856	0.81	0/1154
7	G	0.62	0/1276	0.83	2/1709 (0.1%)
8	H	1.04	2/1136 (0.2%)	1.13	4/1527 (0.3%)
9	I	0.69	0/1029	0.88	0/1379
10	J	0.64	0/805	0.88	1/1082 (0.1%)
11	K	0.74	1/879 (0.1%)	0.92	0/1187
12	L	0.89	0/977	1.05	1/1306 (0.1%)
13	M	0.65	0/947	0.86	0/1270
14	N	0.65	1/501 (0.2%)	0.76	0/664
15	O	0.78	0/740	0.89	0/987
16	P	0.82	0/716	0.95	0/963
17	Q	1.07	2/836 (0.2%)	1.24	6/1117 (0.5%)
18	R	0.68	0/579	0.89	1/768 (0.1%)
19	S	0.54	0/661	0.75	0/890
20	T	0.77	0/765	1.10	1/1007 (0.1%)
21	U	0.62	0/212	0.80	0/277
All	All	1.07	177/55424 (0.3%)	1.66	1813/82231 (2.2%)

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
2	B	0	1
3	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	1
10	J	0	1
12	L	0	1
13	M	0	1
17	Q	0	1
20	T	0	1
All	All	0	11

The worst 5 of 177 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N3-C4	-11.12	1.28	1.34
1	A	1509	C	N1-C6	-10.10	1.31	1.37
1	A	1502	A	N9-C4	-10.09	1.31	1.37
1	A	266	G	N9-C4	-9.73	1.30	1.38
1	A	1377	A	N3-C4	-9.22	1.29	1.34

The worst 5 of 1813 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	G	N1-C6-O6	17.30	130.28	119.90
1	A	117	G	C5-C6-N1	-16.49	103.26	111.50
1	A	1502	A	N1-C6-N6	16.22	128.33	118.60
1	A	284	G	N1-C6-O6	15.41	129.15	119.90
1	A	912	A	C2-N3-C4	-15.22	102.99	110.60

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
3	C	24	ALA	Peptide
7	G	154	TYR	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32509	0	16433	726	0
2	B	1900	0	1951	97	0
3	C	1612	0	1677	88	0
4	D	1703	0	1763	72	0
5	E	1146	0	1207	73	0
6	F	843	0	857	54	0
7	G	1257	0	1296	56	0
8	H	1116	0	1177	68	0
9	I	1010	0	1037	75	0
10	J	792	0	835	47	0
11	K	864	0	881	35	0
12	L	972	0	1058	51	0
13	M	937	0	995	47	0
14	N	492	0	529	36	0
15	O	729	0	768	25	0
16	P	700	0	720	44	0
17	Q	823	0	893	52	0
18	R	574	0	644	33	0
19	S	647	0	673	31	0
20	T	763	0	861	42	0
21	U	208	0	221	15	0
22	A	40	0	37	7	0
23	A	259	0	0	0	0
23	B	2	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	4	0	0	0	0
23	J	2	0	0	0	0
23	K	1	0	0	0	0
23	M	3	0	0	0	0
23	N	1	0	0	0	0
23	P	3	0	0	0	0
23	Q	2	0	0	0	0
23	S	1	0	0	0	0
23	T	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	369	0	0	11	0
25	D	1	0	0	0	0
25	E	6	0	0	0	0
25	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	L	1	0	0	0	0
25	Q	1	0	0	0	0
25	T	2	0	0	1	0
25	U	1	0	0	1	0
All	All	52302	0	36513	1594	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 18.

The worst 5 of 1594 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:1249:C:O2'	9:I:73:GLN:NE2	2.00	0.93
1:A:1125:U:OP2	1:A:1145:C:N4	2.03	0.91
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.53	0.91
1:A:1182:G:H4'	1:A:1183:A:H5'	1.53	0.90
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.38	0.89

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	
2	B	232/256 (91%)	199 (86%)	30 (13%)	3 (1%)	12	50
3	C	204/239 (85%)	171 (84%)	32 (16%)	1 (0%)	29	68
4	D	206/209 (99%)	187 (91%)	19 (9%)	0	100	100
5	E	148/162 (91%)	131 (88%)	16 (11%)	1 (1%)	22	62
6	F	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
7	G	153/156 (98%)	138 (90%)	14 (9%)	1 (1%)	22	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	19	60
10	J	96/105 (91%)	78 (81%)	16 (17%)	2 (2%)	7	40
11	K	114/129 (88%)	100 (88%)	13 (11%)	1 (1%)	17	58
12	L	121/135 (90%)	113 (93%)	7 (6%)	1 (1%)	19	60
13	M	116/126 (92%)	102 (88%)	14 (12%)	0	100	100
14	N	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
15	O	85/89 (96%)	76 (89%)	9 (11%)	0	100	100
16	P	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	Q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
18	R	68/88 (77%)	61 (90%)	7 (10%)	0	100	100
19	S	78/93 (84%)	70 (90%)	7 (9%)	1 (1%)	12	50
20	T	97/106 (92%)	80 (82%)	15 (16%)	2 (2%)	7	40
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	2336/2541 (92%)	2074 (89%)	248 (11%)	14 (1%)	25	65

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
19	S	31	ILE
12	L	28	LYS
3	C	15	THR
20	T	73	HIS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	157 (78%)	45 (22%)	1	5
3	C	160/188 (85%)	124 (78%)	36 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	180/181 (99%)	150 (83%)	30 (17%)	2	13
5	E	115/123 (94%)	89 (77%)	26 (23%)	1	5
6	F	90/90 (100%)	75 (83%)	15 (17%)	2	13
7	G	126/127 (99%)	101 (80%)	25 (20%)	1	8
8	H	119/119 (100%)	90 (76%)	29 (24%)	0	4
9	I	98/99 (99%)	78 (80%)	20 (20%)	1	7
10	J	87/92 (95%)	73 (84%)	14 (16%)	2	15
11	K	88/99 (89%)	73 (83%)	15 (17%)	2	13
12	L	103/110 (94%)	77 (75%)	26 (25%)	0	4
13	M	94/101 (93%)	67 (71%)	27 (29%)	0	3
14	N	49/50 (98%)	41 (84%)	8 (16%)	2	14
15	O	79/80 (99%)	64 (81%)	15 (19%)	1	9
16	P	72/74 (97%)	58 (81%)	14 (19%)	1	8
17	Q	94/97 (97%)	81 (86%)	13 (14%)	3	21
18	R	61/77 (79%)	50 (82%)	11 (18%)	1	10
19	S	71/80 (89%)	56 (79%)	15 (21%)	1	7
20	T	76/82 (93%)	59 (78%)	17 (22%)	1	5
21	U	19/22 (86%)	15 (79%)	4 (21%)	1	7
All	All	1983/2111 (94%)	1578 (80%)	405 (20%)	1	7

5 of 405 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	24	THR
10	J	4	ILE
19	S	30	LEU
8	H	45	ILE
8	H	133	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	11	ASN
20	T	18	GLN
10	J	62	HIS

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Mol	Chain	Res	Type
4	D	119	GLN
9	I	73	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	369 (24%)	48 (3%)

5 of 369 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	31	G
1	A	32	A

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	975	A
1	A	1347	G
1	A	748	C
1	A	870	U

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

15 non-standard protein/DNA/RNA residues are 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
1	MA6	A	1519	1	19,26,27	2.02	6 (31%)	18,38,41	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	1407	1	15,22,23	1.68	3 (20%)	19,32,35	0.98	1 (5%)
12	0TD	L	92	12	4,9,10	1.20	0	3,11,13	2.65	2 (66%)
1	PSU	A	516	1,23	17,21,22	1.32	3 (17%)	20,30,33	2.93	6 (30%)
1	MA6	A	1518	1	19,26,27	1.07	1 (5%)	18,38,41	1.59	2 (11%)
1	5MC	A	1400	1	15,22,23	1.27	2 (13%)	19,32,35	1.38	3 (15%)
1	4OC	A	1402	1	16,23,24	1.24	3 (18%)	17,32,35	1.62	1 (5%)
1	2MG	A	1207	1	19,26,27	2.41	4 (21%)	21,38,41	2.20	3 (14%)
1	5MC	A	967	1	15,22,23	0.81	0	19,32,35	1.21	2 (10%)
1	5MC	A	1404	1	15,22,23	1.35	2 (13%)	19,32,35	1.04	1 (5%)
1	M2G	A	966	1	20,27,28	2.50	5 (25%)	22,40,43	2.33	3 (13%)
1	PSU	A	1540	1,23	17,21,22	1.14	1 (5%)	20,30,33	3.62	5 (25%)
1	7MG	A	527	1	22,26,27	2.24	8 (36%)	28,39,42	1.46	7 (25%)
1	UR3	A	1498	1	14,22,23	1.21	1 (7%)	15,32,35	1.33	2 (13%)
1	PSU	A	1541	1	17,21,22	1.27	2 (11%)	20,30,33	3.60	8 (40%)

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
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
12	0TD	L	92	12	-	1/3/12/14	-
1	PSU	A	516	1,23	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	4OC	A	1402	1	-	6/9/29/30	0/2/2/2
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	M2G	A	966	1	-	6/7/29/30	0/3/3/3
1	PSU	A	1540	1,23	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	UR3	A	1498	1	-	4/5/25/26	0/2/2/2
1	PSU	A	1541	1	-	4/7/25/26	0/2/2/2

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	7.29	1.40	1.34
1	A	1207	2MG	C6-N1	6.36	1.44	1.33
1	A	966	M2G	C6-N1	6.35	1.44	1.33
1	A	966	M2G	C2-N2	5.86	1.44	1.34
1	A	527	7MG	C6-C5	5.06	1.48	1.41

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	N1-C2-N3	-12.22	118.72	128.43
1	A	1540	PSU	N1-C2-N3	-11.71	119.12	128.43
1	A	516	PSU	N1-C2-N3	-9.33	121.01	128.43
1	A	1207	2MG	C5-C6-N1	-8.23	112.18	123.43
1	A	966	M2G	C5-C6-N1	-8.02	112.46	123.43

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	N1-C6-N6-C9
12	L	92	0TD	CG-CB-SB-CSB
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519	MA6	3	0
1	A	1407	5MC	3	0
1	A	1518	MA6	3	0
1	A	1400	5MC	2	0
1	A	967	5MC	2	0
1	A	1404	5MC	2	0
1	A	966	M2G	1	0
1	A	527	7MG	3	0
1	A	1498	UR3	4	0
1	A	1541	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 284 ligands modelled in this entry, 283 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
22	SRY	A	1601	-	40,42,42	2.33	11 (27%)	49,63,63	2.37	17 (34%)

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
22	SRY	A	1601	-	-	3/20/87/87	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.51	1.49	1.33
22	A	1601	SRY	CA1-N11	6.17	1.44	1.33
22	A	1601	SRY	O53-C53	-3.75	1.35	1.44
22	A	1601	SRY	C23-N23	-2.57	1.43	1.47
22	A	1601	SRY	O51-C51	-2.53	1.37	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	C13-O13-C22	-5.93	105.96	116.25
22	A	1601	SRY	CI3-N23-C23	-5.08	106.98	114.38
22	A	1601	SRY	O13-C13-C23	5.00	116.87	108.24
22	A	1601	SRY	C61-C11-N11	-4.35	102.40	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	O41-C12-O42	-4.27	106.81	111.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

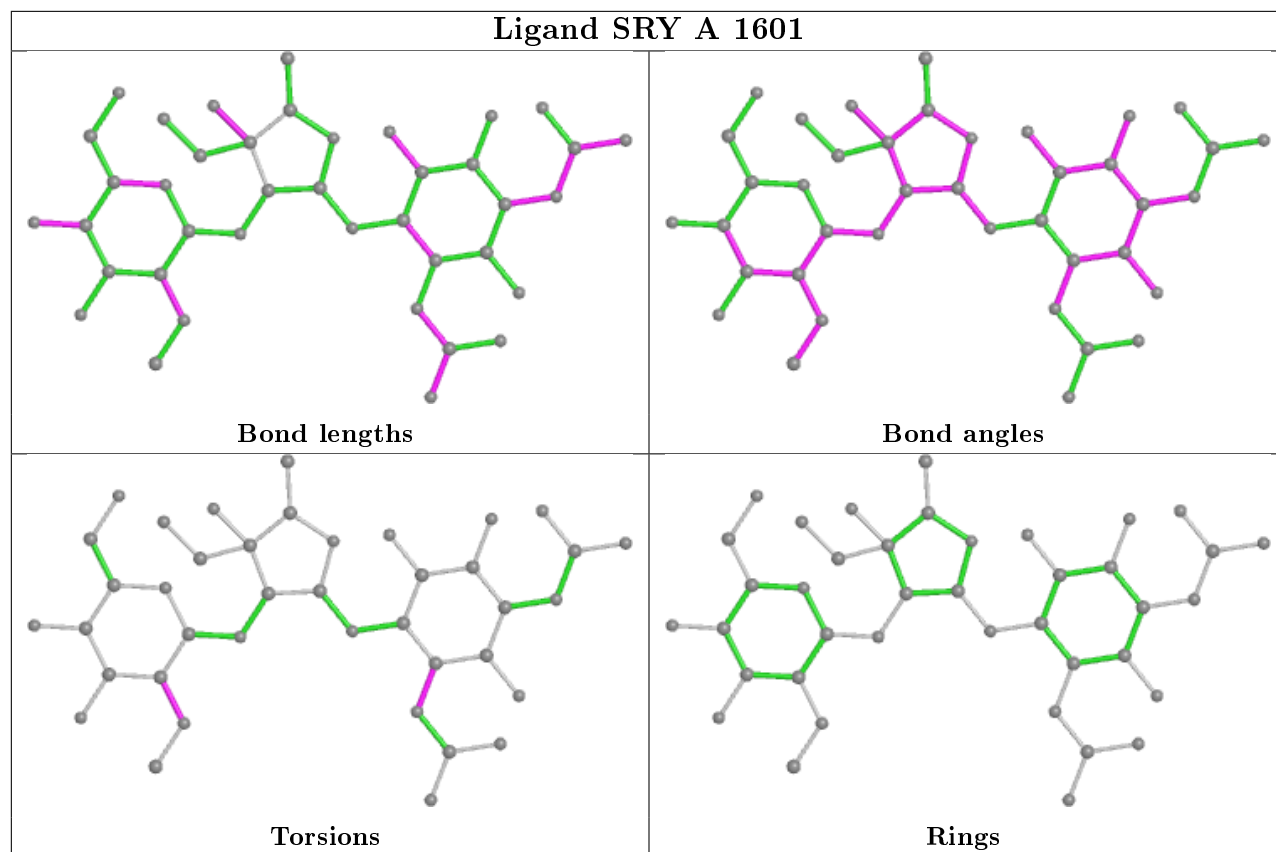
Mol	Chain	Res	Type	Atoms
22	A	1601	SRY	C13-C23-N23-CI3
22	A	1601	SRY	C41-C31-N31-CD1
22	A	1601	SRY	C21-C31-N31-CD1

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1498/1522 (98%)	-0.38	14 (0%) 84 73	77, 136, 263, 391	0
2	B	234/256 (91%)	-0.62	0 100 100	102, 148, 207, 245	0
3	C	206/239 (86%)	-0.19	8 (3%) 39 28	129, 192, 249, 279	0
4	D	208/209 (99%)	-0.54	0 100 100	85, 139, 187, 218	0
5	E	150/162 (92%)	-0.68	0 100 100	74, 111, 149, 166	0
6	F	101/101 (100%)	-0.67	0 100 100	115, 160, 188, 229	0
7	G	155/156 (99%)	-0.46	2 (1%) 77 65	138, 187, 250, 276	0
8	H	138/138 (100%)	-0.75	0 100 100	63, 98, 143, 166	0
9	I	127/128 (99%)	-0.31	1 (0%) 86 75	141, 207, 248, 258	0
10	J	98/105 (93%)	0.12	9 (9%) 9 7	171, 230, 284, 340	0
11	K	116/129 (89%)	-0.71	0 100 100	104, 131, 179, 211	0
12	L	123/135 (91%)	-0.60	1 (0%) 86 75	75, 131, 171, 211	0
13	M	118/126 (93%)	-0.40	5 (4%) 36 26	123, 166, 204, 229	0
14	N	60/61 (98%)	-0.05	2 (3%) 46 34	136, 206, 243, 259	0
15	O	87/89 (97%)	-0.64	0 100 100	79, 120, 171, 185	0
16	P	83/88 (94%)	-0.67	0 100 100	93, 128, 165, 189	0
17	Q	99/105 (94%)	-0.76	0 100 100	81, 109, 146, 174	0
18	R	70/88 (79%)	-0.68	0 100 100	93, 136, 177, 203	0
19	S	80/93 (86%)	-0.22	2 (2%) 57 43	164, 214, 256, 290	0
20	T	99/106 (93%)	-0.65	1 (1%) 82 71	94, 132, 176, 217	0
21	U	24/27 (88%)	0.53	3 (12%) 3 4	139, 191, 208, 221	0
All	All	3874/4063 (95%)	-0.45	48 (1%) 79 67	63, 145, 243, 391	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	65	ALA	8.6
3	C	102	ASN	5.5
10	J	90	LEU	5.4
1	A	1129	C	5.3
3	C	103	VAL	5.0

## 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(Å <sup>2</sup> )	Q<0.9
1	PSU	A	1540	20/21	0.77	0.57	284,295,304,304	0
1	PSU	A	1541	20/21	0.82	0.36	194,232,275,275	0
1	2MG	A	1207	24/25	0.93	0.20	171,214,228,232	0
1	5MC	A	1407	21/22	0.95	0.17	137,157,169,173	0
1	5MC	A	967	21/22	0.95	0.14	122,133,140,142	0
1	PSU	A	516	20/21	0.95	0.14	143,147,160,163	0
1	5MC	A	1400	21/22	0.95	0.17	97,136,144,154	0
1	MA6	A	1518	24/25	0.96	0.13	109,126,150,152	0
1	UR3	A	1498	21/22	0.96	0.17	119,127,136,154	0
1	M2G	A	966	25/26	0.96	0.15	111,131,155,159	0
1	4OC	A	1402	22/23	0.97	0.16	111,116,133,174	0
12	0TD	L	92	10/11	0.97	0.24	99,116,135,216	0
1	MA6	A	1519	24/25	0.97	0.14	106,122,139,141	0
1	5MC	A	1404	21/22	0.97	0.18	105,128,135,142	0
1	7MG	A	527	24/25	0.98	0.14	95,109,116,120	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
23	MG	A	1742	1/1	-0.22	1.39	151,151,151,151	0
23	MG	S	101	1/1	0.42	0.18	107,107,107,107	0
23	MG	A	1735	1/1	0.43	0.94	98,98,98,98	0
23	MG	A	1771	1/1	0.44	0.42	113,113,113,113	0
23	MG	A	1860	1/1	0.55	0.64	113,113,113,113	0
23	MG	A	1768	1/1	0.56	0.44	152,152,152,152	0
23	MG	A	1770	1/1	0.58	0.62	107,107,107,107	0
23	MG	P	102	1/1	0.58	0.47	123,123,123,123	0
23	MG	A	1764	1/1	0.60	0.49	108,108,108,108	0
23	MG	A	1743	1/1	0.61	0.56	108,108,108,108	0
23	MG	A	1790	1/1	0.61	0.59	98,98,98,98	0
23	MG	A	1720	1/1	0.65	0.43	110,110,110,110	0
23	MG	A	1655	1/1	0.68	0.20	129,129,129,129	0
23	MG	A	1805	1/1	0.68	0.72	117,117,117,117	0
23	MG	N	102	1/1	0.69	0.19	118,118,118,118	0
23	MG	A	1773	1/1	0.70	0.22	116,116,116,116	0
23	MG	A	1648	1/1	0.70	0.21	122,122,122,122	0
23	MG	A	1750	1/1	0.70	0.67	106,106,106,106	0
23	MG	M	203	1/1	0.71	0.45	135,135,135,135	0
23	MG	A	1807	1/1	0.71	0.36	114,114,114,114	0
23	MG	A	1783	1/1	0.71	1.56	126,126,126,126	0
23	MG	A	1804	1/1	0.72	0.37	107,107,107,107	0
23	MG	A	1791	1/1	0.73	0.43	116,116,116,116	0
23	MG	A	1737	1/1	0.74	0.39	131,131,131,131	0
23	MG	A	1712	1/1	0.74	0.28	89,89,89,89	0
23	MG	A	1665	1/1	0.75	0.28	121,121,121,121	0
23	MG	D	302	1/1	0.75	0.08	121,121,121,121	0
23	MG	A	1803	1/1	0.76	0.33	109,109,109,109	0
23	MG	H	204	1/1	0.77	0.69	106,106,106,106	0
23	MG	P	103	1/1	0.77	0.25	98,98,98,98	0
23	MG	A	1843	1/1	0.77	0.34	101,101,101,101	0
23	MG	A	1706	1/1	0.78	0.38	129,129,129,129	0
23	MG	B	301	1/1	0.79	0.34	118,118,118,118	0
23	MG	A	1730	1/1	0.79	0.54	112,112,112,112	0
23	MG	A	1667	1/1	0.79	0.25	135,135,135,135	0
23	MG	A	1767	1/1	0.80	0.22	152,152,152,152	0
23	MG	A	1806	1/1	0.80	0.39	109,109,109,109	0
23	MG	A	1675	1/1	0.80	0.26	83,83,83,83	0
23	MG	A	1792	1/1	0.81	0.45	106,106,106,106	0
23	MG	A	1666	1/1	0.81	0.40	112,112,112,112	0
23	MG	A	1810	1/1	0.81	0.29	131,131,131,131	0
23	MG	A	1745	1/1	0.82	0.77	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1722	1/1	0.82	0.37	101,101,101,101	0
23	MG	A	1733	1/1	0.82	0.23	107,107,107,107	0
23	MG	A	1626	1/1	0.82	0.83	124,124,124,124	0
23	MG	A	1786	1/1	0.83	0.17	114,114,114,114	0
23	MG	A	1687	1/1	0.83	0.23	277,277,277,277	0
23	MG	A	1715	1/1	0.83	0.34	108,108,108,108	0
23	MG	A	1763	1/1	0.83	0.36	94,94,94,94	0
23	MG	A	1813	1/1	0.83	0.33	103,103,103,103	0
23	MG	A	1808	1/1	0.83	0.38	105,105,105,105	0
23	MG	A	1697	1/1	0.83	0.39	147,147,147,147	0
23	MG	A	1839	1/1	0.83	0.31	118,118,118,118	0
23	MG	A	1838	1/1	0.84	0.26	101,101,101,101	0
23	MG	A	1642	1/1	0.84	0.24	91,91,91,91	0
23	MG	A	1749	1/1	0.85	0.29	102,102,102,102	0
23	MG	H	202	1/1	0.85	0.13	73,73,73,73	0
23	MG	A	1621	1/1	0.85	0.27	128,128,128,128	0
23	MG	A	1855	1/1	0.85	0.28	295,295,295,295	0
23	MG	A	1751	1/1	0.85	0.31	100,100,100,100	0
23	MG	A	1756	1/1	0.86	0.20	154,154,154,154	0
23	MG	A	1673	1/1	0.86	1.25	126,126,126,126	0
23	MG	A	1859	1/1	0.86	0.26	102,102,102,102	0
23	MG	A	1676	1/1	0.86	0.28	96,96,96,96	0
23	MG	A	1845	1/1	0.86	0.29	154,154,154,154	0
23	MG	Q	201	1/1	0.86	0.37	101,101,101,101	0
23	MG	A	1609	1/1	0.86	0.31	99,99,99,99	0
23	MG	A	1704	1/1	0.86	0.31	108,108,108,108	0
23	MG	A	1840	1/1	0.86	0.27	127,127,127,127	0
23	MG	A	1634	1/1	0.86	0.26	125,125,125,125	0
23	MG	A	1748	1/1	0.87	0.40	103,103,103,103	0
23	MG	A	1755	1/1	0.87	0.18	114,114,114,114	0
23	MG	A	1654	1/1	0.87	0.29	115,115,115,115	0
23	MG	M	201	1/1	0.87	0.26	126,126,126,126	0
23	MG	A	1785	1/1	0.88	1.13	116,116,116,116	0
23	MG	A	1699	1/1	0.88	0.24	128,128,128,128	0
23	MG	A	1709	1/1	0.88	0.09	107,107,107,107	0
23	MG	A	1832	1/1	0.88	0.48	218,218,218,218	0
23	MG	A	1711	1/1	0.88	0.42	130,130,130,130	0
23	MG	A	1798	1/1	0.88	0.90	126,126,126,126	0
23	MG	A	1663	1/1	0.88	0.23	121,121,121,121	0
23	MG	Q	202	1/1	0.88	0.38	72,72,72,72	0
23	MG	A	1607	1/1	0.88	0.12	252,252,252,252	0
23	MG	A	1809	1/1	0.88	0.52	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1734	1/1	0.88	0.43	102,102,102,102	0
23	MG	A	1617	1/1	0.89	0.25	103,103,103,103	0
23	MG	A	1684	1/1	0.89	0.24	172,172,172,172	0
23	MG	A	1776	1/1	0.89	0.14	133,133,133,133	0
23	MG	A	1714	1/1	0.89	0.38	107,107,107,107	0
23	MG	A	1725	1/1	0.89	0.30	91,91,91,91	0
23	MG	A	1624	1/1	0.89	0.26	98,98,98,98	0
23	MG	A	1670	1/1	0.89	1.12	181,181,181,181	0
23	MG	A	1784	1/1	0.89	0.11	110,110,110,110	0
23	MG	A	1616	1/1	0.89	0.23	84,84,84,84	0
23	MG	A	1708	1/1	0.90	0.24	93,93,93,93	0
23	MG	A	1788	1/1	0.90	0.30	103,103,103,103	0
23	MG	A	1702	1/1	0.90	0.23	84,84,84,84	0
23	MG	A	1740	1/1	0.90	0.21	141,141,141,141	0
23	MG	A	1829	1/1	0.90	0.20	244,244,244,244	0
23	MG	A	1698	1/1	0.90	0.09	128,128,128,128	0
23	MG	P	101	1/1	0.90	0.53	82,82,82,82	0
23	MG	A	1678	1/1	0.90	0.16	96,96,96,96	0
23	MG	A	1643	1/1	0.90	0.27	110,110,110,110	0
23	MG	A	1695	1/1	0.90	0.12	118,118,118,118	0
23	MG	A	1736	1/1	0.91	0.19	108,108,108,108	0
23	MG	A	1732	1/1	0.91	0.30	89,89,89,89	0
23	MG	A	1778	1/1	0.91	0.16	314,314,314,314	0
23	MG	A	1682	1/1	0.91	0.28	134,134,134,134	0
23	MG	K	201	1/1	0.91	0.11	154,154,154,154	0
23	MG	A	1727	1/1	0.91	0.31	97,97,97,97	0
23	MG	J	201	1/1	0.91	0.25	113,113,113,113	0
23	MG	A	1821	1/1	0.91	0.14	278,278,278,278	0
23	MG	A	1718	1/1	0.91	0.12	147,147,147,147	0
23	MG	H	203	1/1	0.91	0.27	103,103,103,103	0
23	MG	A	1775	1/1	0.91	0.34	87,87,87,87	0
23	MG	A	1816	1/1	0.91	0.17	120,120,120,120	0
23	MG	A	1793	1/1	0.91	0.09	125,125,125,125	0
23	MG	A	1723	1/1	0.91	0.19	120,120,120,120	0
23	MG	A	1729	1/1	0.92	0.42	102,102,102,102	0
23	MG	A	1744	1/1	0.92	0.37	124,124,124,124	0
23	MG	A	1656	1/1	0.92	0.14	149,149,149,149	0
23	MG	A	1794	1/1	0.92	0.58	115,115,115,115	0
23	MG	A	1853	1/1	0.92	0.18	208,208,208,208	0
23	MG	A	1658	1/1	0.93	0.21	202,202,202,202	0
23	MG	A	1799	1/1	0.93	0.20	114,114,114,114	0
23	MG	A	1683	1/1	0.93	0.14	256,256,256,256	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1659	1/1	0.93	0.20	142,142,142,142	0
23	MG	A	1811	1/1	0.93	0.08	102,102,102,102	0
23	MG	A	1691	1/1	0.93	0.15	102,102,102,102	0
23	MG	T	201	1/1	0.93	0.19	135,135,135,135	0
23	MG	A	1801	1/1	0.93	0.48	130,130,130,130	0
23	MG	A	1789	1/1	0.93	0.19	80,80,80,80	0
23	MG	A	1752	1/1	0.93	0.84	142,142,142,142	0
23	MG	A	1826	1/1	0.93	0.15	196,196,196,196	0
23	MG	A	1844	1/1	0.93	0.20	116,116,116,116	0
23	MG	A	1661	1/1	0.93	0.13	98,98,98,98	0
23	MG	A	1668	1/1	0.93	0.12	167,167,167,167	0
23	MG	A	1834	1/1	0.93	0.27	335,335,335,335	0
23	MG	A	1828	1/1	0.93	0.18	400,400,400,400	0
23	MG	A	1669	1/1	0.93	0.22	138,138,138,138	0
23	MG	A	1707	1/1	0.94	0.08	99,99,99,99	0
23	MG	A	1703	1/1	0.94	0.30	93,93,93,93	0
23	MG	A	1664	1/1	0.94	0.14	120,120,120,120	0
23	MG	A	1650	1/1	0.94	0.23	107,107,107,107	0
23	MG	A	1680	1/1	0.94	0.17	121,121,121,121	0
23	MG	A	1692	1/1	0.94	0.18	331,331,331,331	0
23	MG	A	1856	1/1	0.94	0.15	231,231,231,231	0
23	MG	A	1651	1/1	0.94	0.10	239,239,239,239	0
23	MG	A	1620	1/1	0.94	0.18	143,143,143,143	0
23	MG	A	1627	1/1	0.94	0.18	168,168,168,168	0
23	MG	A	1772	1/1	0.94	0.23	118,118,118,118	0
23	MG	A	1823	1/1	0.94	0.39	365,365,365,365	0
23	MG	A	1787	1/1	0.94	0.16	140,140,140,140	0
23	MG	A	1696	1/1	0.94	0.11	125,125,125,125	0
23	MG	A	1635	1/1	0.94	0.16	75,75,75,75	0
23	MG	A	1713	1/1	0.94	0.26	72,72,72,72	0
23	MG	A	1625	1/1	0.94	0.36	178,178,178,178	0
23	MG	A	1689	1/1	0.94	0.14	230,230,230,230	0
23	MG	A	1846	1/1	0.94	0.22	396,396,396,396	0
23	MG	A	1604	1/1	0.94	0.22	114,114,114,114	0
23	MG	A	1841	1/1	0.94	0.13	96,96,96,96	0
23	MG	A	1747	1/1	0.94	0.22	116,116,116,116	0
23	MG	A	1819	1/1	0.94	0.33	175,175,175,175	0
23	MG	A	1662	1/1	0.94	0.09	161,161,161,161	0
23	MG	A	1701	1/1	0.95	0.21	205,205,205,205	0
23	MG	A	1761	1/1	0.95	0.18	100,100,100,100	0
23	MG	A	1817	1/1	0.95	0.10	97,97,97,97	0
23	MG	A	1717	1/1	0.95	0.29	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	MG	A	1660	1/1	0.95	0.19	118,118,118,118	0
23	MG	A	1850	1/1	0.95	0.29	350,350,350,350	0
23	MG	A	1631	1/1	0.95	0.37	95,95,95,95	0
23	MG	A	1825	1/1	0.95	0.22	199,199,199,199	0
23	MG	A	1739	1/1	0.95	0.21	107,107,107,107	0
23	MG	A	1847	1/1	0.95	0.27	328,328,328,328	0
23	MG	A	1719	1/1	0.95	0.19	118,118,118,118	0
23	MG	B	302	1/1	0.95	0.11	97,97,97,97	0
23	MG	A	1836	1/1	0.95	0.17	341,341,341,341	0
23	MG	A	1738	1/1	0.95	0.19	114,114,114,114	0
23	MG	A	1731	1/1	0.95	0.16	82,82,82,82	0
23	MG	E	201	1/1	0.95	0.05	232,232,232,232	0
23	MG	A	1857	1/1	0.95	0.07	287,287,287,287	0
23	MG	A	1636	1/1	0.95	0.43	85,85,85,85	0
23	MG	A	1710	1/1	0.95	0.15	104,104,104,104	0
23	MG	A	1854	1/1	0.95	0.29	359,359,359,359	0
23	MG	A	1827	1/1	0.95	0.11	162,162,162,162	0
23	MG	A	1694	1/1	0.95	0.22	142,142,142,142	0
23	MG	H	201	1/1	0.95	0.30	77,77,77,77	0
23	MG	A	1741	1/1	0.95	0.31	87,87,87,87	0
23	MG	A	1815	1/1	0.95	0.48	98,98,98,98	0
23	MG	A	1679	1/1	0.95	0.27	94,94,94,94	0
23	MG	A	1820	1/1	0.96	0.16	376,376,376,376	0
23	MG	A	1830	1/1	0.96	0.19	312,312,312,312	0
23	MG	A	1632	1/1	0.96	0.07	100,100,100,100	0
23	MG	A	1638	1/1	0.96	0.18	192,192,192,192	0
23	MG	A	1690	1/1	0.96	0.17	75,75,75,75	0
23	MG	A	1766	1/1	0.96	0.18	124,124,124,124	0
23	MG	A	1779	1/1	0.96	0.12	213,213,213,213	0
23	MG	A	1637	1/1	0.96	0.04	62,62,62,62	0
23	MG	A	1608	1/1	0.96	0.27	93,93,93,93	0
23	MG	A	1782	1/1	0.96	0.12	94,94,94,94	0
23	MG	A	1611	1/1	0.96	0.21	105,105,105,105	0
23	MG	A	1795	1/1	0.96	0.17	115,115,115,115	0
23	MG	A	1753	1/1	0.96	0.14	89,89,89,89	0
23	MG	A	1762	1/1	0.96	0.16	97,97,97,97	0
23	MG	A	1724	1/1	0.96	0.19	133,133,133,133	0
23	MG	A	1640	1/1	0.96	0.16	118,118,118,118	0
22	SRY	A	1601	40/40	0.96	0.18	88,116,133,137	0
23	MG	A	1700	1/1	0.96	0.09	174,174,174,174	0
23	MG	A	1757	1/1	0.97	0.15	190,190,190,190	0
23	MG	A	1769	1/1	0.97	0.48	131,131,131,131	0

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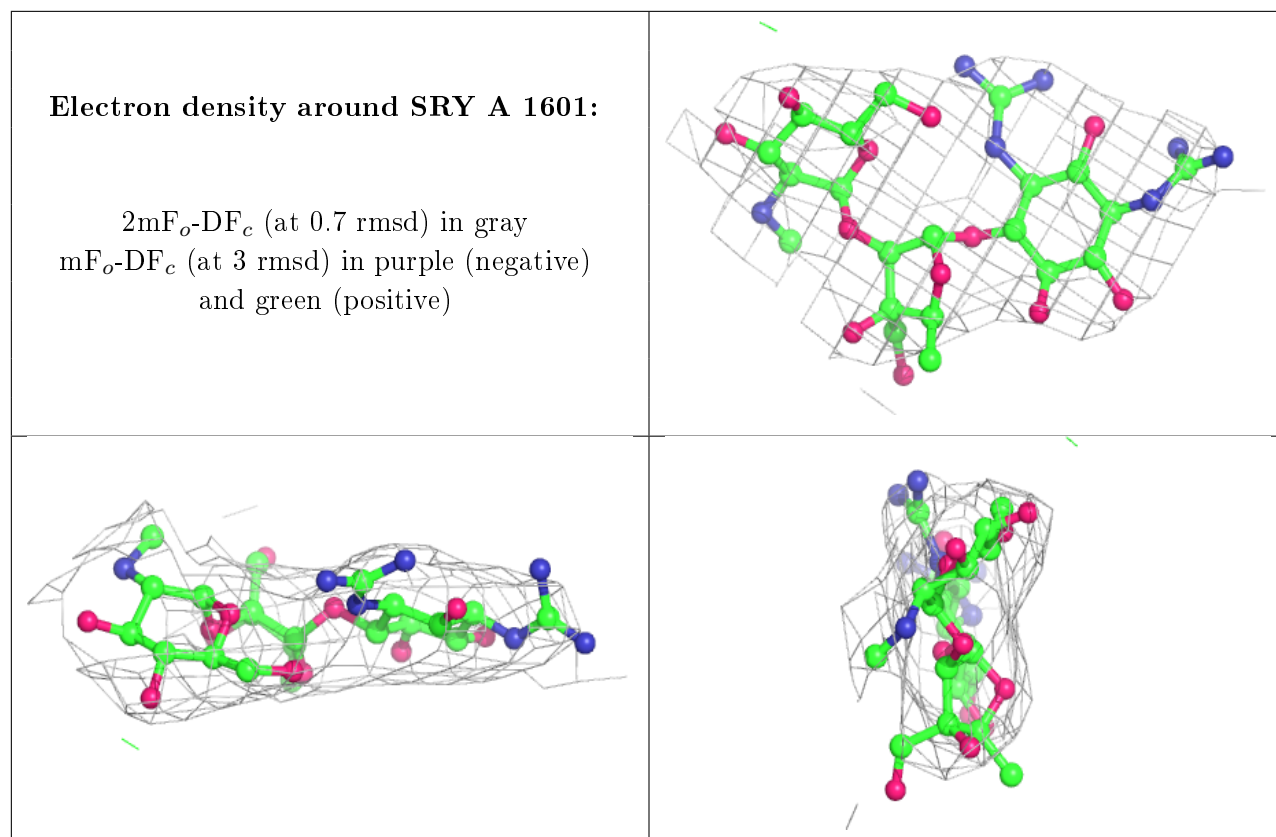
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1685	1/1	0.97	0.19	129,129,129,129	0
23	MG	A	1728	1/1	0.97	0.20	84,84,84,84	0
23	MG	A	1780	1/1	0.97	0.25	211,211,211,211	0
23	MG	A	1822	1/1	0.97	0.08	300,300,300,300	0
23	MG	A	1705	1/1	0.97	0.09	135,135,135,135	0
23	MG	A	1672	1/1	0.97	0.46	140,140,140,140	0
23	MG	A	1796	1/1	0.97	0.12	100,100,100,100	0
23	MG	A	1774	1/1	0.97	0.44	126,126,126,126	0
23	MG	A	1606	1/1	0.97	0.15	100,100,100,100	0
23	MG	A	1688	1/1	0.97	0.16	112,112,112,112	0
23	MG	A	1858	1/1	0.97	0.14	279,279,279,279	0
23	MG	A	1777	1/1	0.97	0.12	219,219,219,219	0
23	MG	A	1824	1/1	0.97	0.07	200,200,200,200	0
23	MG	A	1781	1/1	0.97	0.06	490,490,490,490	0
23	MG	A	1797	1/1	0.97	0.23	110,110,110,110	0
23	MG	A	1629	1/1	0.97	0.35	87,87,87,87	0
23	MG	A	1818	1/1	0.97	0.15	209,209,209,209	0
23	MG	J	202	1/1	0.97	0.33	133,133,133,133	0
23	MG	A	1612	1/1	0.97	0.08	115,115,115,115	0
23	MG	A	1754	1/1	0.97	0.10	120,120,120,120	0
23	MG	A	1693	1/1	0.97	0.22	144,144,144,144	0
23	MG	A	1759	1/1	0.97	0.16	197,197,197,197	0
23	MG	A	1800	1/1	0.97	0.16	124,124,124,124	0
23	MG	A	1765	1/1	0.98	0.42	128,128,128,128	0
23	MG	A	1646	1/1	0.98	0.13	102,102,102,102	0
23	MG	A	1849	1/1	0.98	0.21	235,235,235,235	0
23	MG	A	1619	1/1	0.98	0.41	113,113,113,113	0
23	MG	A	1726	1/1	0.98	0.17	84,84,84,84	0
23	MG	A	1812	1/1	0.98	0.11	68,68,68,68	0
23	MG	A	1686	1/1	0.98	0.23	264,264,264,264	0
23	MG	A	1645	1/1	0.98	0.13	91,91,91,91	0
23	MG	M	202	1/1	0.98	0.58	130,130,130,130	0
23	MG	A	1644	1/1	0.98	0.12	83,83,83,83	0
23	MG	A	1833	1/1	0.98	0.13	180,180,180,180	0
23	MG	A	1603	1/1	0.98	0.25	106,106,106,106	0
23	MG	A	1746	1/1	0.98	0.24	91,91,91,91	0
23	MG	A	1602	1/1	0.98	0.14	155,155,155,155	0
23	MG	A	1758	1/1	0.98	0.12	305,305,305,305	0
23	MG	A	1639	1/1	0.98	0.31	120,120,120,120	0
23	MG	A	1671	1/1	0.98	0.48	124,124,124,124	0
23	MG	A	1622	1/1	0.98	0.20	106,106,106,106	0
23	MG	A	1831	1/1	0.98	0.78	231,231,231,231	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	ZN	D	301	1/1	0.98	0.34	106,106,106,106	0
24	ZN	N	101	1/1	0.98	0.14	173,173,173,173	0
23	MG	A	1630	1/1	0.98	0.16	139,139,139,139	0
23	MG	A	1677	1/1	0.98	0.14	128,128,128,128	0
23	MG	A	1681	1/1	0.98	0.07	93,93,93,93	0
23	MG	A	1613	1/1	0.98	0.11	84,84,84,84	0
23	MG	A	1623	1/1	0.98	0.11	159,159,159,159	0
23	MG	A	1647	1/1	0.98	0.16	133,133,133,133	0
23	MG	A	1852	1/1	0.98	0.18	353,353,353,353	0
23	MG	A	1674	1/1	0.98	0.12	186,186,186,186	0
23	MG	A	1716	1/1	0.98	0.11	112,112,112,112	0
23	MG	A	1605	1/1	0.99	0.05	114,114,114,114	0
23	MG	A	1760	1/1	0.99	0.17	194,194,194,194	0
23	MG	A	1851	1/1	0.99	0.18	246,246,246,246	0
23	MG	A	1721	1/1	0.99	0.04	101,101,101,101	0
23	MG	A	1614	1/1	0.99	0.12	80,80,80,80	0
23	MG	A	1628	1/1	0.99	0.18	84,84,84,84	0
23	MG	A	1618	1/1	0.99	0.07	69,69,69,69	0
23	MG	A	1615	1/1	0.99	0.11	75,75,75,75	0
23	MG	A	1652	1/1	0.99	0.19	137,137,137,137	0
23	MG	A	1835	1/1	0.99	0.17	103,103,103,103	0
23	MG	A	1842	1/1	0.99	0.20	187,187,187,187	0
23	MG	A	1848	1/1	0.99	0.10	235,235,235,235	0
23	MG	A	1802	1/1	0.99	0.14	150,150,150,150	0
23	MG	A	1653	1/1	0.99	0.24	154,154,154,154	0
23	MG	A	1610	1/1	0.99	0.15	83,83,83,83	0
23	MG	A	1641	1/1	0.99	0.08	119,119,119,119	0
23	MG	A	1814	1/1	0.99	0.19	103,103,103,103	0
23	MG	A	1649	1/1	0.99	0.10	117,117,117,117	0
23	MG	A	1633	1/1	0.99	0.16	67,67,67,67	0
23	MG	A	1837	1/1	1.00	0.07	134,134,134,134	0
23	MG	A	1657	1/1	1.00	0.15	97,97,97,97	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.