



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 04:35 AM BST

PDB ID : 4JI3
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : Demirci, H.; Wang, L.; Murphy, F.V.; Murphy, E.L.; Carr, J.; Blanchard, S.;
Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on : 2013-03-05
Resolution : 3.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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

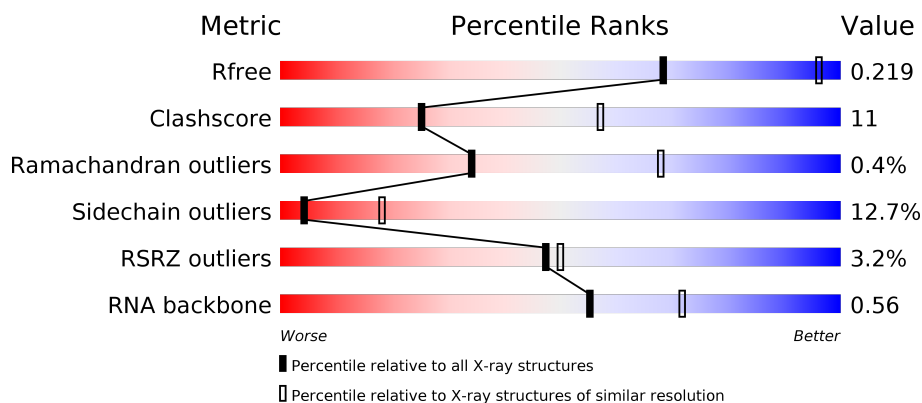
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>9%</div> <div>55% 34% 10% ..</div> </div>
2	B	256	<div> <div>54% 29% 8% 9%</div> </div>
3	C	239	<div> <div>9%</div> <div>44% 37% 5% 14%</div> </div>
4	D	209	<div> <div>67% 27% 6%</div> </div>

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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
1	PSU	A	1541	-	-	-	X
23	MG	A	1633	-	-	-	X
23	MG	A	1662	-	-	-	X
23	MG	A	1679	-	-	-	X
23	MG	A	1682	-	-	-	X
23	MG	A	1696	-	-	-	X
23	MG	A	1710	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1723	-	-	-	X
23	MG	A	1754	-	-	-	X
23	MG	A	1755	-	-	-	X
23	MG	A	1757	-	-	-	X
23	MG	A	1771	-	-	-	X
23	MG	A	1787	-	-	-	X
23	MG	A	1791	-	-	-	X
23	MG	A	1800	-	-	-	X
23	MG	A	1802	-	-	-	X
23	MG	A	1807	-	-	-	X
23	MG	A	1815	-	-	-	X
23	MG	A	1822	-	-	-	X
23	MG	A	1823	-	-	-	X
23	MG	K	201	-	-	-	X
23	MG	P	101	-	-	-	X
23	MG	P	102	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1511	Total	C	N	O	P	0	0	0
			32487	14468	6008	10500	1511			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			977	617	196	163	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	TRP	PRO	CONFLICT	UNP F6DEQ7

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

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

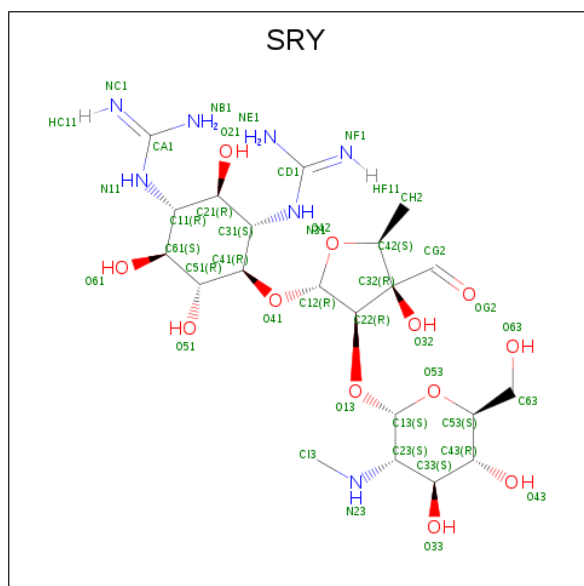
- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

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

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	P	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	Q	2	Total 2	Mg 2	0	0
23	D	2	Total 2	Mg 2	0	0
23	K	1	Total 1	Mg 1	0	0
23	E	1	Total 1	Mg 1	0	0
23	H	1	Total 1	Mg 1	0	0
23	B	2	Total 2	Mg 2	0	0
23	C	1	Total 1	Mg 1	0	0
23	A	231	Total 231	Mg 231	0	0
23	N	1	Total 1	Mg 1	0	0
23	L	1	Total 1	Mg 1	0	0
23	F	1	Total 1	Mg 1	0	0

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

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

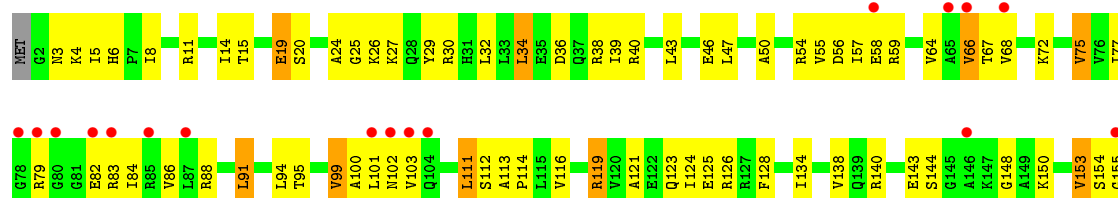
- Molecule 25 is water.

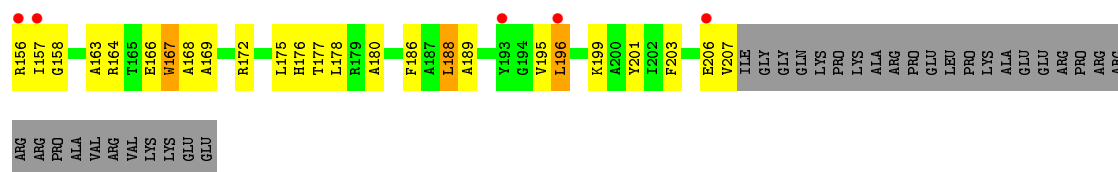
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	223	Total 223	O 223	0	0
25	D	1	Total 1	O 1	0	0
25	E	4	Total 4	O 4	0	0
25	L	1	Total 1	O 1	0	0

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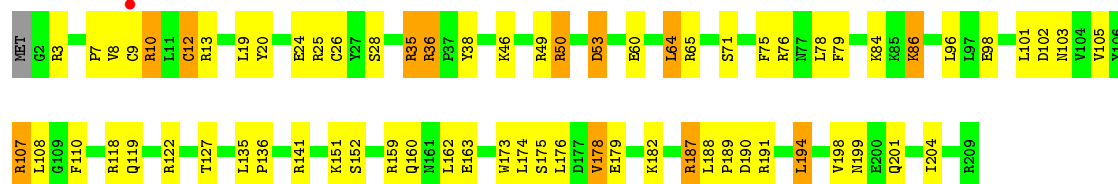
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	N	1	Total 1	O 1	0	0
25	Q	1	Total 1	O 1	0	0
25	T	1	Total 1	O 1	0	0
25	U	1	Total 1	O 1	0	0

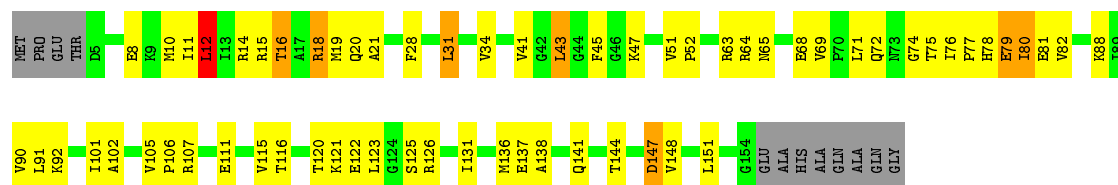




• Molecule 4: RIBOSOMAL PROTEIN S4



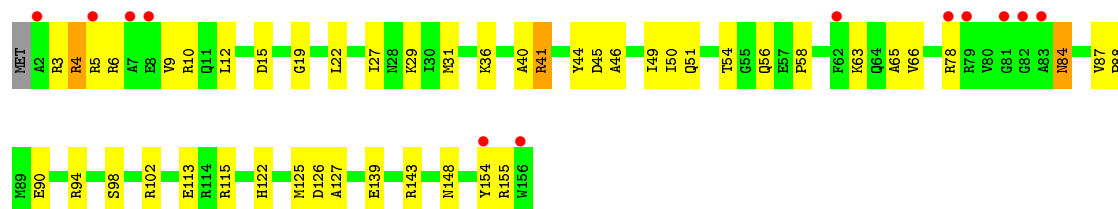
• Molecule 5: RIBOSOMAL PROTEIN S5



• Molecule 6: RIBOSOMAL PROTEIN S6

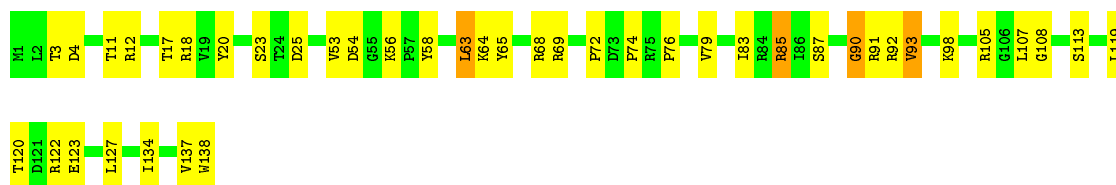


• Molecule 7: RIBOSOMAL PROTEIN S7

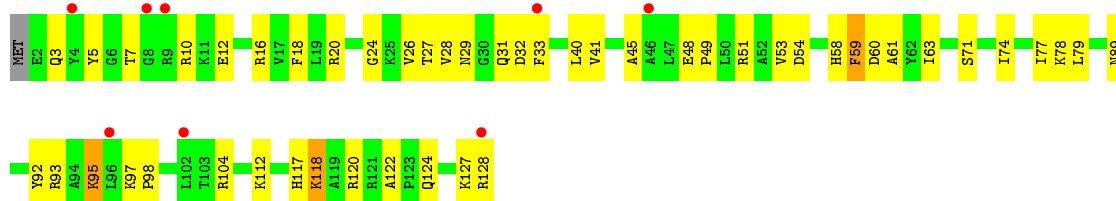


• Molecule 8: RIBOSOMAL PROTEIN S8

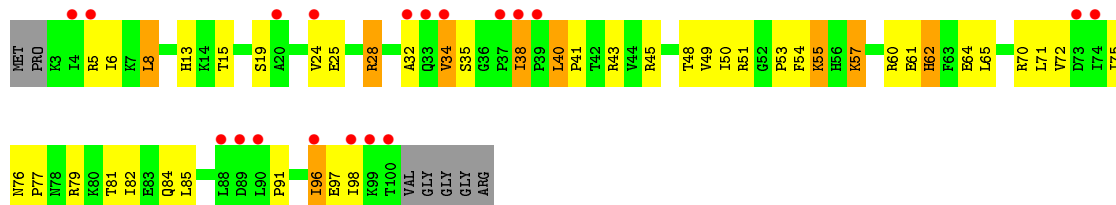




• Molecule 9: RIBOSOMAL PROTEIN S9



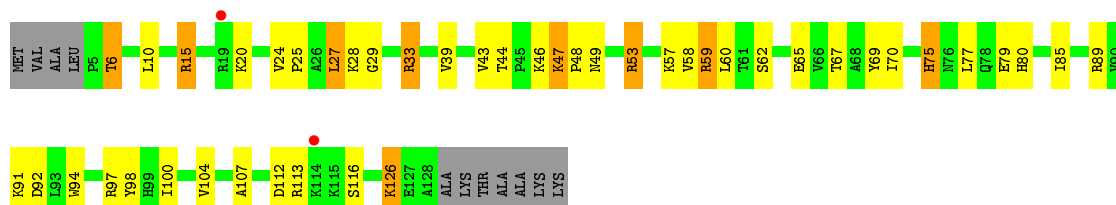
• Molecule 10: RIBOSOMAL PROTEIN S10



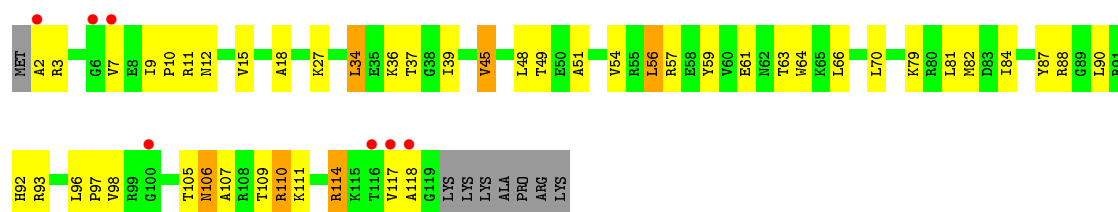
• Molecule 11: RIBOSOMAL PROTEIN S11



• Molecule 12: RIBOSOMAL PROTEIN S12



• Molecule 13: RIBOSOMAL PROTEIN S13



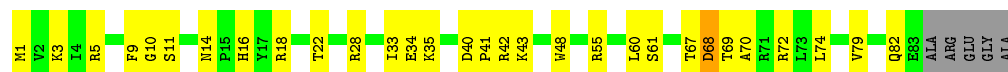
- Molecule 14: RIBOSOMAL PROTEIN S14



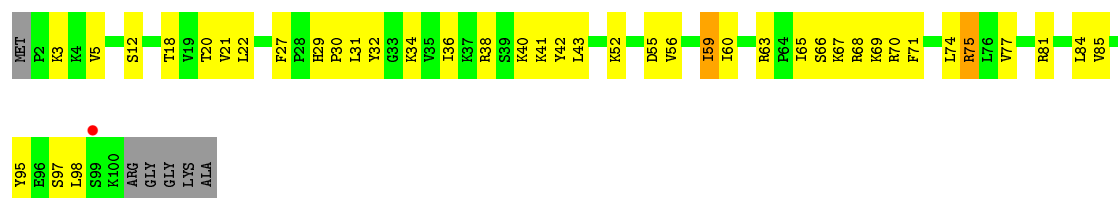
- Molecule 15: RIBOSOMAL PROTEIN S15



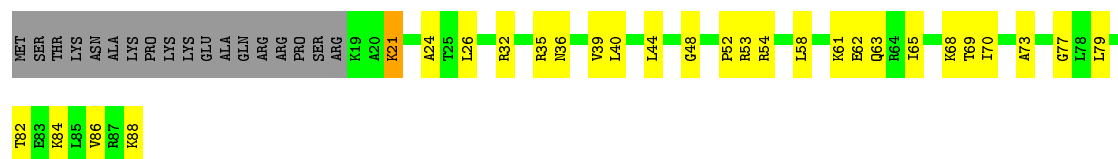
- Molecule 16: RIBOSOMAL PROTEIN S16



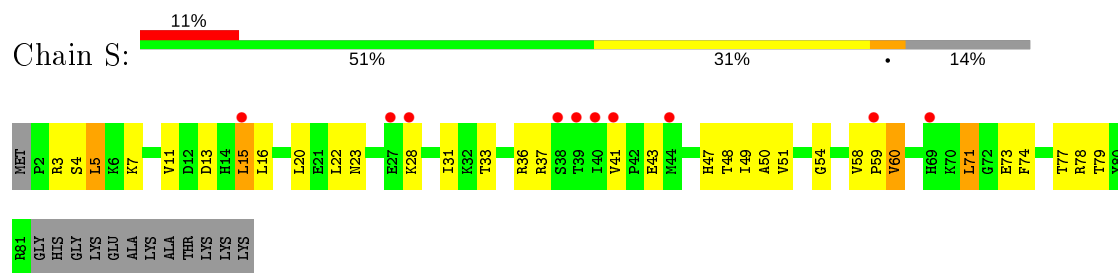
- Molecule 17: RIBOSOMAL PROTEIN S17



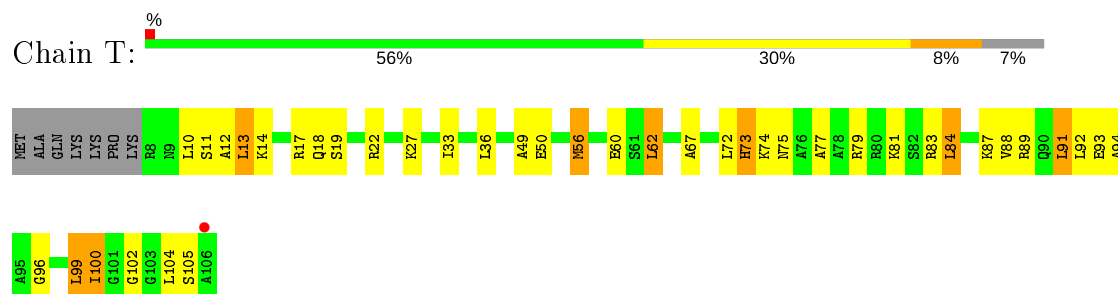
- Molecule 18: RIBOSOMAL PROTEIN S18



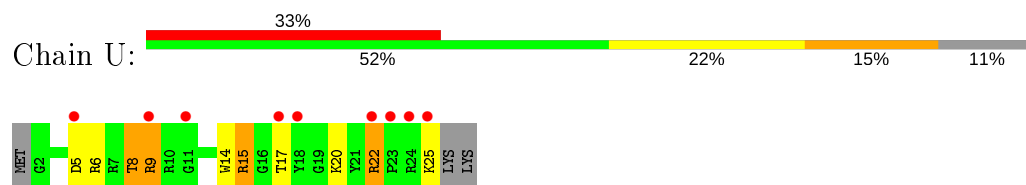
- Molecule 19: RIBOSOMAL PROTEIN S19



- 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, α , β , γ	402.98Å 402.98Å 173.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.00 – 3.35 34.00 – 3.35	Depositor EDS
% Data completeness (in resolution range)	87.8 (34.00-3.35) 87.6 (34.00-3.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.32Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.168 , 0.215 0.172 , 0.219	Depositor DCC
R_{free} test set	8993 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	116.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 105.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52101	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M2G, MA6, 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	0.51	1/36018 (0.0%)	1.01	72/56209 (0.1%)
2	B	0.37	0/1935	0.59	1/2609 (0.0%)
3	C	0.32	0/1636	0.54	0/2205
4	D	0.39	1/1733 (0.1%)	0.59	1/2318 (0.0%)
5	E	0.47	0/1162	0.68	1/1564 (0.1%)
6	F	0.33	0/856	0.52	0/1154
7	G	0.30	0/1276	0.49	0/1709
8	H	0.47	0/1136	0.64	0/1527
9	I	0.33	0/1029	0.53	0/1379
10	J	0.28	0/805	0.59	0/1082
11	K	0.37	0/879	0.61	0/1187
12	L	0.41	0/994	0.67	0/1331
13	M	0.32	0/947	0.56	0/1270
14	N	0.35	0/501	0.52	0/664
15	O	0.38	0/740	0.55	0/987
16	P	0.42	0/716	0.61	0/963
17	Q	0.45	0/836	0.69	0/1117
18	R	0.34	0/579	0.55	0/768
19	S	0.27	0/661	0.56	0/890
20	T	0.39	0/765	0.65	1/1007 (0.1%)
21	U	0.30	0/212	0.45	0/277
All	All	0.47	2/55416 (0.0%)	0.90	76/82217 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
20	T	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	869	G	N7-C5	-5.53	1.35	1.39
4	D	12	CYS	CB-SG	5.07	1.90	1.82

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	G	N1-C6-O6	11.85	127.01	119.90
1	A	254	G	O5'-P-OP1	-9.37	97.27	105.70
1	A	117	G	C6-C5-N7	-9.03	124.98	130.40
1	A	328	C	N1-C2-O2	7.78	123.57	118.90
1	A	839	U	C2-N1-C1'	7.74	126.98	117.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
8	H	90	GLY	Peptide
12	L	27	LEU	Peptide
20	T	93	GLU	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	32487	0	16421	443	0
2	B	1900	0	1951	58	0
3	C	1612	0	1677	66	0
4	D	1703	0	1763	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1146	0	1207	36	0
6	F	843	0	857	14	0
7	G	1257	0	1296	30	0
8	H	1116	0	1177	25	0
9	I	1010	0	1037	29	0
10	J	792	0	835	39	0
11	K	864	0	881	25	0
12	L	977	0	1060	38	0
13	M	937	0	995	28	0
14	N	492	0	529	16	0
15	O	729	0	768	20	0
16	P	700	0	720	20	0
17	Q	823	0	891	36	0
18	R	574	0	644	18	0
19	S	647	0	673	21	0
20	T	763	0	861	33	0
21	U	208	0	221	7	0
22	A	40	0	37	4	0
23	A	231	0	0	0	0
23	B	2	0	0	0	0
23	C	1	0	0	0	0
23	D	2	0	0	0	0
23	E	1	0	0	0	0
23	F	1	0	0	0	0
23	H	1	0	0	0	0
23	K	1	0	0	0	0
23	L	1	0	0	0	0
23	N	1	0	0	0	0
23	P	2	0	0	0	0
23	Q	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	223	0	0	3	0
25	D	1	0	0	0	0
25	E	4	0	0	0	0
25	L	1	0	0	0	0
25	N	1	0	0	0	0
25	Q	1	0	0	0	0
25	T	1	0	0	0	0
25	U	1	0	0	0	0
All	All	52101	0	36501	927	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 11.

The worst 5 of 927 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:1443:G:H5''	1:A:1446:A:H5'	1.43	0.99
17:Q:29:HIS:HD2	17:Q:32:TYR:H	1.11	0.89
1:A:279:A:OP2	17:Q:95:TYR:OH	1.88	0.89
1:A:411:A:H62	1:A:413:G:H21	1.23	0.87
1:A:298:A:N6	25:A:2054:HOH:O	2.06	0.85

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%)	210 (90%)	19 (8%)	3 (1%)	12	42
3	C	204/239 (85%)	182 (89%)	21 (10%)	1 (0%)	29	63
4	D	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
5	E	148/162 (91%)	141 (95%)	6 (4%)	1 (1%)	22	56
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
8	H	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
9	I	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	15	49
11	K	114/129 (88%)	105 (92%)	9 (8%)	0	100	100
12	L	122/135 (90%)	109 (89%)	13 (11%)	0	100	100
13	M	116/126 (92%)	104 (90%)	12 (10%)	0	100	100
14	N	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	85/89 (96%)	82 (96%)	2 (2%)	1 (1%)	13	44
16	P	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	Q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	R	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
19	S	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	12	42
20	T	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2337/2541 (92%)	2169 (93%)	159 (7%)	9 (0%)	34	68

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
2	B	21	ARG
2	B	24	TRP
5	E	16	THR
14	N	23	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	173 (86%)	29 (14%)	3	14
3	C	160/188 (85%)	140 (88%)	20 (12%)	4	18
4	D	180/181 (99%)	153 (85%)	27 (15%)	3	12
5	E	115/123 (94%)	97 (84%)	18 (16%)	2	11
6	F	90/90 (100%)	81 (90%)	9 (10%)	7	29
7	G	126/127 (99%)	116 (92%)	10 (8%)	12	40
8	H	119/119 (100%)	110 (92%)	9 (8%)	13	41
9	I	98/99 (99%)	84 (86%)	14 (14%)	3	14
10	J	87/92 (95%)	74 (85%)	13 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	88/99 (89%)	78 (89%)	10 (11%)	5	22
12	L	104/111 (94%)	86 (83%)	18 (17%)	2	8
13	M	94/101 (93%)	80 (85%)	14 (15%)	3	13
14	N	49/50 (98%)	39 (80%)	10 (20%)	1	4
15	O	79/80 (99%)	66 (84%)	13 (16%)	2	10
16	P	72/74 (97%)	68 (94%)	4 (6%)	21	53
17	Q	94/97 (97%)	90 (96%)	4 (4%)	29	60
18	R	61/77 (79%)	56 (92%)	5 (8%)	11	38
19	S	71/80 (89%)	62 (87%)	9 (13%)	4	18
20	T	76/82 (93%)	65 (86%)	11 (14%)	3	14
21	U	19/22 (86%)	15 (79%)	4 (21%)	1	4
All	All	1984/2112 (94%)	1733 (87%)	251 (13%)	4	18

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	11	THR
10	J	38	ILE
19	S	43	GLU
8	H	68	ARG
9	I	40	LEU

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

Mol	Chain	Res	Type
9	I	124	GLN
17	Q	29	HIS
12	L	75	HIS
9	I	73	GLN
16	P	16	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	259 (17%)	38 (2%)

5 of 259 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	748	C
1	A	913	A
1	A	1347	G
1	A	812	C
1	A	960	U

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

14 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	1518	1	19,26,27	1.28	2 (10%)	18,38,41	1.21	2 (11%)
1	M2G	A	966	1	20,27,28	1.65	4 (20%)	22,40,43	2.24	2 (9%)
1	PSU	A	516	1,23	17,21,22	1.24	3 (17%)	20,30,33	3.08	6 (30%)
1	2MG	A	1207	1	19,26,27	2.31	4 (21%)	21,38,41	1.95	3 (14%)
1	MA6	A	1519	1	19,26,27	1.38	4 (21%)	18,38,41	0.59	0
1	UR3	A	1498	1	14,22,23	0.57	0	15,32,35	1.17	1 (6%)
1	5MC	A	1400	1	15,22,23	0.77	0	19,32,35	1.25	2 (10%)
1	PSU	A	1540	1	17,21,22	1.09	2 (11%)	20,30,33	3.14	6 (30%)
1	5MC	A	1404	1	15,22,23	0.82	0	19,32,35	1.12	2 (10%)
1	5MC	A	967	1	15,22,23	0.88	0	19,32,35	0.99	0
1	5MC	A	1407	1	15,22,23	1.17	1 (6%)	19,32,35	1.08	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	A	1402	1	16,23,24	0.76	1 (6%)	17,32,35	0.92	1 (5%)
1	PSU	A	1541	1	17,21,22	1.03	1 (5%)	20,30,33	3.15	5 (25%)
1	7MG	A	527	1	22,26,27	2.11	6 (27%)	28,39,42	1.67	6 (21%)

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

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	6.80	1.39	1.34
1	A	1207	2MG	C6-N1	6.22	1.43	1.33
1	A	966	M2G	C6-N1	5.33	1.42	1.33
1	A	527	7MG	C2-N2	5.23	1.44	1.33
1	A	527	7MG	C8-N9	-5.08	1.33	1.45

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	N1-C2-N3	-10.78	119.86	128.43
1	A	1540	PSU	N1-C2-N3	-10.65	119.96	128.43
1	A	516	PSU	N1-C2-N3	-10.37	120.19	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	966	M2G	C5-C6-N1	-7.85	112.69	123.43
1	A	1207	2MG	C5-C6-N1	-7.31	113.43	123.43

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM2
1	A	1519	MA6	C5-C6-N6-C9

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	1	0
1	A	1400	5MC	1	0
1	A	1407	5MC	1	0
1	A	527	7MG	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 249 ligands modelled in this entry, 248 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	2.31	9 (22%)	49,63,63	1.71	9 (18%)

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	SRV	A	1601	-	-	4/20/87/87	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRV	CD1-N31	9.19	1.49	1.33
22	A	1601	SRV	CA1-N11	6.98	1.45	1.33
22	A	1601	SRV	O53-C53	-3.49	1.35	1.44
22	A	1601	SRV	O51-C51	-2.57	1.36	1.43
22	A	1601	SRV	CA1-NB1	2.50	1.45	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRV	C12-O42-C42	-5.33	99.99	108.38
22	A	1601	SRV	C61-C11-N11	-4.54	102.04	110.62
22	A	1601	SRV	C13-O13-C22	-3.54	110.10	116.25
22	A	1601	SRV	O41-C12-O42	-3.26	107.90	111.43
22	A	1601	SRV	C13-O53-C53	-3.24	107.34	113.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1601	SRV	C61-C11-N11-CA1
22	A	1601	SRV	C21-C11-N11-CA1
22	A	1601	SRV	C13-C23-N23-CI3
22	A	1601	SRV	C21-C31-N31-CD1

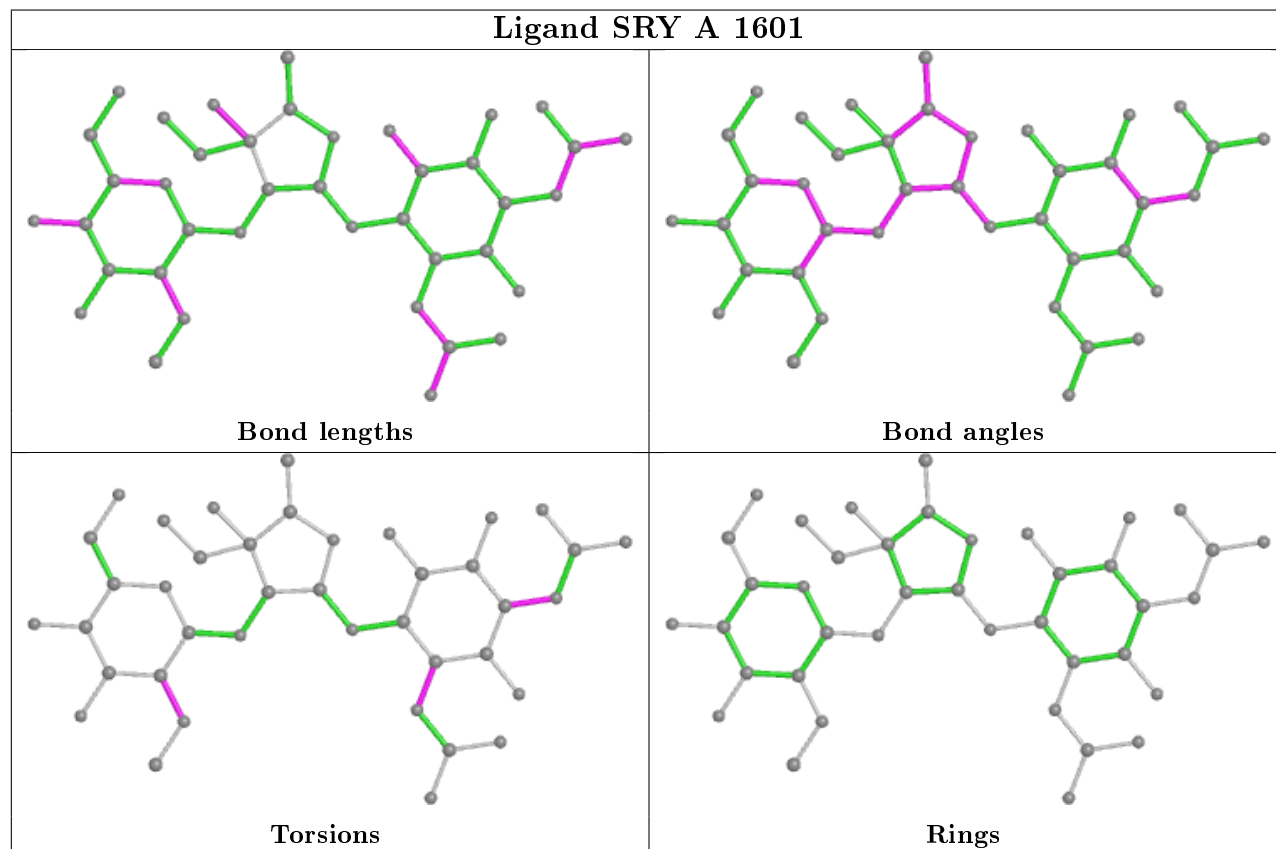
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRV	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1497/1522 (98%)	-0.32	17 (1%) 80 84	75, 126, 254, 372	0
2	B	234/256 (91%)	-0.35	2 (0%) 84 87	102, 148, 210, 229	0
3	C	206/239 (86%)	0.28	22 (10%) 6 7	130, 188, 244, 266	0
4	D	208/209 (99%)	-0.23	1 (0%) 91 93	90, 129, 167, 202	0
5	E	150/162 (92%)	-0.40	0 100 100	79, 107, 143, 204	0
6	F	101/101 (100%)	-0.40	1 (0%) 82 86	111, 155, 184, 234	0
7	G	155/156 (99%)	0.04	12 (7%) 13 15	120, 170, 221, 244	0
8	H	138/138 (100%)	-0.39	0 100 100	73, 99, 132, 167	0
9	I	127/128 (99%)	0.23	8 (6%) 20 22	132, 195, 242, 259	0
10	J	98/105 (93%)	0.84	19 (19%) 1 1	126, 214, 306, 335	0
11	K	116/129 (89%)	-0.36	0 100 100	98, 130, 174, 208	0
12	L	124/135 (91%)	-0.20	2 (1%) 72 74	74, 122, 159, 213	0
13	M	118/126 (93%)	0.02	7 (5%) 22 25	119, 153, 193, 258	0
14	N	60/61 (98%)	0.68	10 (16%) 1 2	149, 175, 241, 282	0
15	O	87/89 (97%)	-0.36	1 (1%) 80 84	82, 117, 154, 175	0
16	P	83/88 (94%)	-0.32	0 100 100	92, 121, 150, 183	0
17	Q	99/105 (94%)	-0.37	1 (1%) 82 86	80, 108, 145, 168	0
18	R	70/88 (79%)	-0.33	0 100 100	100, 131, 181, 209	0
19	S	80/93 (86%)	0.73	10 (12%) 3 4	149, 204, 249, 280	0
20	T	99/106 (93%)	-0.35	1 (1%) 82 86	96, 127, 179, 211	0
21	U	24/27 (88%)	2.04	9 (37%) 0 0	131, 162, 193, 205	0
All	All	3874/4063 (95%)	-0.17	123 (3%) 47 50	73, 137, 230, 372	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	65	ALA	9.9
21	U	25	LYS	8.5
19	S	38	SER	7.4
10	J	34	VAL	7.2
21	U	18	TYR	6.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1541	20/21	0.69	0.52	307,319,331,332	0
1	PSU	A	1540	20/21	0.71	0.72	293,304,328,333	0
1	2MG	A	1207	24/25	0.86	0.27	166,200,208,210	0
1	5MC	A	1407	21/22	0.92	0.17	143,156,168,170	0
1	5MC	A	1404	21/22	0.94	0.20	112,125,133,135	0
1	5MC	A	1400	21/22	0.95	0.16	96,119,128,133	0
1	M2G	A	966	25/26	0.95	0.17	128,130,135,137	0
1	PSU	A	516	20/21	0.95	0.11	114,120,134,135	0
1	5MC	A	967	21/22	0.95	0.15	117,134,142,143	0
1	MA6	A	1518	24/25	0.95	0.16	114,128,149,156	0
1	UR3	A	1498	21/22	0.95	0.20	107,119,127,139	0
1	4OC	A	1402	22/23	0.97	0.19	105,113,122,124	0
1	MA6	A	1519	24/25	0.97	0.13	109,131,137,140	0
1	7MG	A	527	24/25	0.97	0.15	102,107,117,124	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1767	1/1	0.38	0.38	119,119,119,119	0
23	MG	A	1723	1/1	0.42	0.66	111,111,111,111	0
23	MG	A	1801	1/1	0.48	0.31	114,114,114,114	0
23	MG	A	1831	1/1	0.51	0.34	130,130,130,130	0
23	MG	A	1633	1/1	0.59	0.59	122,122,122,122	0
23	MG	A	1807	1/1	0.59	0.81	120,120,120,120	0
23	MG	A	1682	1/1	0.60	0.46	106,106,106,106	0
23	MG	A	1787	1/1	0.61	0.58	122,122,122,122	0
23	MG	A	1815	1/1	0.62	0.55	113,113,113,113	0
23	MG	A	1666	1/1	0.63	0.24	133,133,133,133	0
23	MG	A	1638	1/1	0.65	0.35	101,101,101,101	0
23	MG	A	1823	1/1	0.66	2.07	143,143,143,143	0
23	MG	A	1652	1/1	0.66	0.33	118,118,118,118	0
23	MG	A	1777	1/1	0.67	0.20	135,135,135,135	0
23	MG	P	102	1/1	0.67	0.54	125,125,125,125	0
23	MG	L	201	1/1	0.67	0.23	123,123,123,123	0
23	MG	A	1731	1/1	0.67	0.30	126,126,126,126	0
23	MG	Q	202	1/1	0.68	0.36	89,89,89,89	0
23	MG	A	1771	1/1	0.69	0.43	111,111,111,111	0
23	MG	A	1785	1/1	0.70	0.18	154,154,154,154	0
23	MG	A	1679	1/1	0.70	0.41	112,112,112,112	0
23	MG	A	1743	1/1	0.72	0.37	110,110,110,110	0
23	MG	A	1757	1/1	0.73	1.11	123,123,123,123	0
23	MG	A	1822	1/1	0.73	0.45	97,97,97,97	0
23	MG	A	1792	1/1	0.73	0.26	120,120,120,120	0
23	MG	A	1748	1/1	0.74	0.29	117,117,117,117	0
23	MG	P	101	1/1	0.74	0.42	97,97,97,97	0
23	MG	A	1662	1/1	0.75	0.46	126,126,126,126	0
23	MG	A	1802	1/1	0.75	0.59	125,125,125,125	0
23	MG	D	303	1/1	0.76	0.15	104,104,104,104	0
23	MG	Q	201	1/1	0.76	0.24	119,119,119,119	0
23	MG	F	201	1/1	0.76	0.16	112,112,112,112	0
23	MG	A	1800	1/1	0.76	1.05	128,128,128,128	0
23	MG	A	1696	1/1	0.76	0.45	104,104,104,104	0
23	MG	A	1710	1/1	0.77	0.53	115,115,115,115	0
23	MG	K	201	1/1	0.77	0.41	100,100,100,100	0
23	MG	A	1755	1/1	0.78	0.93	116,116,116,116	0
23	MG	A	1709	1/1	0.78	0.21	253,253,253,253	0
23	MG	A	1816	1/1	0.79	0.29	100,100,100,100	0
23	MG	A	1791	1/1	0.80	0.68	155,155,155,155	0
23	MG	A	1631	1/1	0.80	0.52	107,107,107,107	0
23	MG	A	1754	1/1	0.80	0.46	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1747	1/1	0.80	0.28	136,136,136,136	0
23	MG	A	1809	1/1	0.80	0.50	132,132,132,132	0
23	MG	A	1721	1/1	0.81	0.28	77,77,77,77	0
23	MG	A	1717	1/1	0.81	0.33	107,107,107,107	0
23	MG	A	1827	1/1	0.81	0.26	116,116,116,116	0
23	MG	A	1625	1/1	0.81	0.34	134,134,134,134	0
23	MG	A	1659	1/1	0.81	0.25	158,158,158,158	0
23	MG	A	1730	1/1	0.82	0.17	92,92,92,92	0
23	MG	A	1719	1/1	0.82	0.72	117,117,117,117	0
23	MG	A	1828	1/1	0.82	0.38	122,122,122,122	0
23	MG	A	1644	1/1	0.83	0.33	95,95,95,95	0
23	MG	A	1674	1/1	0.83	0.27	128,128,128,128	0
23	MG	A	1768	1/1	0.83	0.29	149,149,149,149	0
23	MG	A	1683	1/1	0.83	0.64	117,117,117,117	0
23	MG	A	1639	1/1	0.84	0.24	160,160,160,160	0
23	MG	A	1762	1/1	0.84	0.14	119,119,119,119	0
23	MG	A	1664	1/1	0.84	0.88	96,96,96,96	0
23	MG	A	1814	1/1	0.84	0.34	108,108,108,108	0
23	MG	A	1697	1/1	0.84	0.08	166,166,166,166	0
23	MG	A	1667	1/1	0.84	0.44	97,97,97,97	0
23	MG	A	1776	1/1	0.84	0.27	137,137,137,137	0
23	MG	A	1621	1/1	0.85	0.70	127,127,127,127	0
23	MG	A	1763	1/1	0.85	0.28	146,146,146,146	0
23	MG	A	1733	1/1	0.85	0.14	120,120,120,120	0
23	MG	A	1812	1/1	0.85	0.29	117,117,117,117	0
23	MG	A	1760	1/1	0.86	0.97	116,116,116,116	0
23	MG	A	1813	1/1	0.86	0.42	130,130,130,130	0
23	MG	A	1825	1/1	0.86	0.28	126,126,126,126	0
23	MG	A	1766	1/1	0.86	0.69	73,73,73,73	0
23	MG	A	1778	1/1	0.86	0.16	90,90,90,90	0
23	MG	A	1623	1/1	0.86	0.89	120,120,120,120	0
23	MG	A	1788	1/1	0.86	0.29	124,124,124,124	0
23	MG	A	1729	1/1	0.87	0.25	110,110,110,110	0
23	MG	A	1661	1/1	0.87	0.35	110,110,110,110	0
23	MG	A	1806	1/1	0.87	0.73	96,96,96,96	0
23	MG	A	1627	1/1	0.87	0.36	108,108,108,108	0
23	MG	A	1774	1/1	0.87	0.31	106,106,106,106	0
23	MG	N	102	1/1	0.87	0.40	130,130,130,130	0
23	MG	A	1811	1/1	0.87	0.73	105,105,105,105	0
23	MG	A	1669	1/1	0.87	0.18	133,133,133,133	0
23	MG	A	1810	1/1	0.87	0.50	106,106,106,106	0
23	MG	A	1618	1/1	0.88	0.27	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1799	1/1	0.88	0.17	361,361,361,361	0
23	MG	A	1765	1/1	0.88	0.21	126,126,126,126	0
23	MG	A	1722	1/1	0.88	0.24	106,106,106,106	0
23	MG	A	1678	1/1	0.88	0.19	104,104,104,104	0
23	MG	D	302	1/1	0.88	0.88	105,105,105,105	0
23	MG	A	1779	1/1	0.88	0.14	122,122,122,122	0
23	MG	A	1718	1/1	0.89	0.16	144,144,144,144	0
23	MG	A	1713	1/1	0.89	0.32	109,109,109,109	0
23	MG	A	1753	1/1	0.89	0.25	112,112,112,112	0
23	MG	A	1805	1/1	0.89	0.98	123,123,123,123	0
23	MG	A	1628	1/1	0.89	0.10	165,165,165,165	0
23	MG	A	1808	1/1	0.89	0.42	95,95,95,95	0
23	MG	C	301	1/1	0.89	0.05	92,92,92,92	0
23	MG	A	1741	1/1	0.89	0.25	125,125,125,125	0
23	MG	A	1728	1/1	0.89	0.31	120,120,120,120	0
23	MG	A	1770	1/1	0.89	0.30	114,114,114,114	0
23	MG	A	1817	1/1	0.89	0.17	113,113,113,113	0
23	MG	A	1819	1/1	0.89	0.27	123,123,123,123	0
23	MG	A	1734	1/1	0.90	0.51	112,112,112,112	0
23	MG	A	1675	1/1	0.90	0.35	129,129,129,129	0
23	MG	A	1629	1/1	0.90	0.29	103,103,103,103	0
23	MG	A	1736	1/1	0.90	0.40	114,114,114,114	0
23	MG	A	1681	1/1	0.90	0.30	146,146,146,146	0
23	MG	A	1794	1/1	0.90	0.30	120,120,120,120	0
23	MG	H	201	1/1	0.90	0.17	107,107,107,107	0
23	MG	A	1673	1/1	0.91	0.26	148,148,148,148	0
23	MG	A	1705	1/1	0.91	0.10	82,82,82,82	0
23	MG	A	1761	1/1	0.91	0.18	117,117,117,117	0
23	MG	A	1665	1/1	0.91	0.40	117,117,117,117	0
23	MG	A	1797	1/1	0.91	0.34	126,126,126,126	0
23	MG	A	1698	1/1	0.91	0.12	136,136,136,136	0
23	MG	A	1605	1/1	0.92	0.51	118,118,118,118	0
23	MG	A	1660	1/1	0.92	0.14	154,154,154,154	0
23	MG	A	1824	1/1	0.92	0.85	118,118,118,118	0
23	MG	A	1783	1/1	0.92	0.29	319,319,319,319	0
23	MG	A	1720	1/1	0.92	0.11	165,165,165,165	0
23	MG	A	1804	1/1	0.92	1.12	116,116,116,116	0
23	MG	A	1737	1/1	0.92	0.20	128,128,128,128	0
23	MG	A	1685	1/1	0.93	0.31	173,173,173,173	0
23	MG	A	1781	1/1	0.93	0.17	200,200,200,200	0
23	MG	A	1603	1/1	0.93	0.13	126,126,126,126	0
23	MG	A	1769	1/1	0.93	0.21	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1677	1/1	0.93	0.18	244,244,244,244	0
23	MG	A	1782	1/1	0.93	0.20	264,264,264,264	0
23	MG	A	1751	1/1	0.93	0.10	89,89,89,89	0
23	MG	A	1650	1/1	0.93	0.21	107,107,107,107	0
23	MG	A	1707	1/1	0.93	0.23	131,131,131,131	0
23	MG	A	1830	1/1	0.93	0.42	107,107,107,107	0
23	MG	A	1798	1/1	0.93	0.28	129,129,129,129	0
23	MG	B	302	1/1	0.93	0.27	168,168,168,168	0
23	MG	A	1640	1/1	0.93	0.12	67,67,67,67	0
23	MG	E	201	1/1	0.93	0.07	140,140,140,140	0
23	MG	A	1746	1/1	0.93	0.17	85,85,85,85	0
23	MG	A	1642	1/1	0.94	0.17	113,113,113,113	0
23	MG	A	1663	1/1	0.94	0.14	113,113,113,113	0
23	MG	A	1727	1/1	0.94	0.41	91,91,91,91	0
23	MG	A	1657	1/1	0.94	0.20	88,88,88,88	0
23	MG	A	1764	1/1	0.94	0.10	123,123,123,123	0
23	MG	A	1773	1/1	0.94	0.12	109,109,109,109	0
23	MG	A	1725	1/1	0.94	0.71	120,120,120,120	0
23	MG	A	1820	1/1	0.94	0.38	92,92,92,92	0
23	MG	A	1630	1/1	0.94	0.54	102,102,102,102	0
23	MG	A	1694	1/1	0.94	0.29	116,116,116,116	0
23	MG	A	1786	1/1	0.94	0.26	115,115,115,115	0
23	MG	A	1711	1/1	0.95	0.15	103,103,103,103	0
23	MG	A	1680	1/1	0.95	0.14	125,125,125,125	0
23	MG	A	1671	1/1	0.95	0.28	115,115,115,115	0
23	MG	A	1790	1/1	0.95	0.24	142,142,142,142	0
23	MG	A	1832	1/1	0.95	0.17	132,132,132,132	0
23	MG	A	1803	1/1	0.95	0.39	110,110,110,110	0
23	MG	A	1688	1/1	0.95	0.20	120,120,120,120	0
23	MG	A	1622	1/1	0.95	0.16	94,94,94,94	0
23	MG	A	1651	1/1	0.95	0.25	76,76,76,76	0
23	MG	A	1758	1/1	0.95	0.17	111,111,111,111	0
23	MG	A	1706	1/1	0.95	0.30	159,159,159,159	0
23	MG	A	1742	1/1	0.95	0.27	94,94,94,94	0
23	MG	A	1829	1/1	0.95	0.52	114,114,114,114	0
23	MG	A	1818	1/1	0.95	0.13	134,134,134,134	0
23	MG	A	1643	1/1	0.95	0.28	77,77,77,77	0
23	MG	A	1687	1/1	0.96	0.59	179,179,179,179	0
23	MG	B	301	1/1	0.96	0.29	125,125,125,125	0
23	MG	A	1732	1/1	0.96	0.35	87,87,87,87	0
23	MG	A	1744	1/1	0.96	0.30	99,99,99,99	0
23	MG	A	1784	1/1	0.96	0.13	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1726	1/1	0.96	0.24	120,120,120,120	0
23	MG	A	1646	1/1	0.96	0.27	103,103,103,103	0
23	MG	A	1795	1/1	0.96	0.64	79,79,79,79	0
24	ZN	N	101	1/1	0.96	0.19	166,166,166,166	0
23	MG	A	1789	1/1	0.96	0.10	125,125,125,125	0
23	MG	A	1752	1/1	0.96	0.20	87,87,87,87	0
23	MG	A	1690	1/1	0.96	0.33	151,151,151,151	0
23	MG	A	1612	1/1	0.96	0.14	127,127,127,127	0
23	MG	A	1821	1/1	0.96	0.44	135,135,135,135	0
23	MG	A	1672	1/1	0.96	0.08	134,134,134,134	0
23	MG	A	1649	1/1	0.96	0.16	106,106,106,106	0
23	MG	A	1604	1/1	0.96	0.21	107,107,107,107	0
23	MG	A	1796	1/1	0.97	0.25	98,98,98,98	0
23	MG	A	1772	1/1	0.97	0.40	101,101,101,101	0
22	SRY	A	1601	40/40	0.97	0.22	93,111,127,129	0
23	MG	A	1702	1/1	0.97	0.10	138,138,138,138	0
23	MG	A	1701	1/1	0.97	0.15	113,113,113,113	0
23	MG	A	1645	1/1	0.97	0.09	88,88,88,88	0
23	MG	A	1699	1/1	0.97	0.10	108,108,108,108	0
23	MG	A	1756	1/1	0.97	0.08	153,153,153,153	0
23	MG	A	1684	1/1	0.97	0.10	114,114,114,114	0
23	MG	A	1712	1/1	0.97	0.15	194,194,194,194	0
23	MG	A	1759	1/1	0.97	0.51	88,88,88,88	0
23	MG	A	1648	1/1	0.97	0.36	117,117,117,117	0
23	MG	A	1613	1/1	0.97	0.11	105,105,105,105	0
23	MG	A	1780	1/1	0.97	0.06	122,122,122,122	0
23	MG	A	1610	1/1	0.97	0.13	85,85,85,85	0
23	MG	A	1647	1/1	0.97	0.24	143,143,143,143	0
23	MG	A	1617	1/1	0.97	0.31	112,112,112,112	0
23	MG	A	1745	1/1	0.97	0.19	100,100,100,100	0
23	MG	A	1656	1/1	0.97	0.14	174,174,174,174	0
23	MG	A	1826	1/1	0.97	0.21	82,82,82,82	0
23	MG	A	1624	1/1	0.97	0.59	64,64,64,64	0
23	MG	A	1609	1/1	0.97	0.14	106,106,106,106	0
23	MG	A	1715	1/1	0.97	0.16	116,116,116,116	0
23	MG	A	1626	1/1	0.97	0.90	75,75,75,75	0
23	MG	A	1724	1/1	0.97	0.10	140,140,140,140	0
23	MG	A	1676	1/1	0.97	0.17	106,106,106,106	0
23	MG	A	1635	1/1	0.97	0.15	119,119,119,119	0
23	MG	A	1654	1/1	0.98	0.27	71,71,71,71	0
23	MG	A	1615	1/1	0.98	0.21	83,83,83,83	0
23	MG	A	1653	1/1	0.98	0.10	99,99,99,99	0

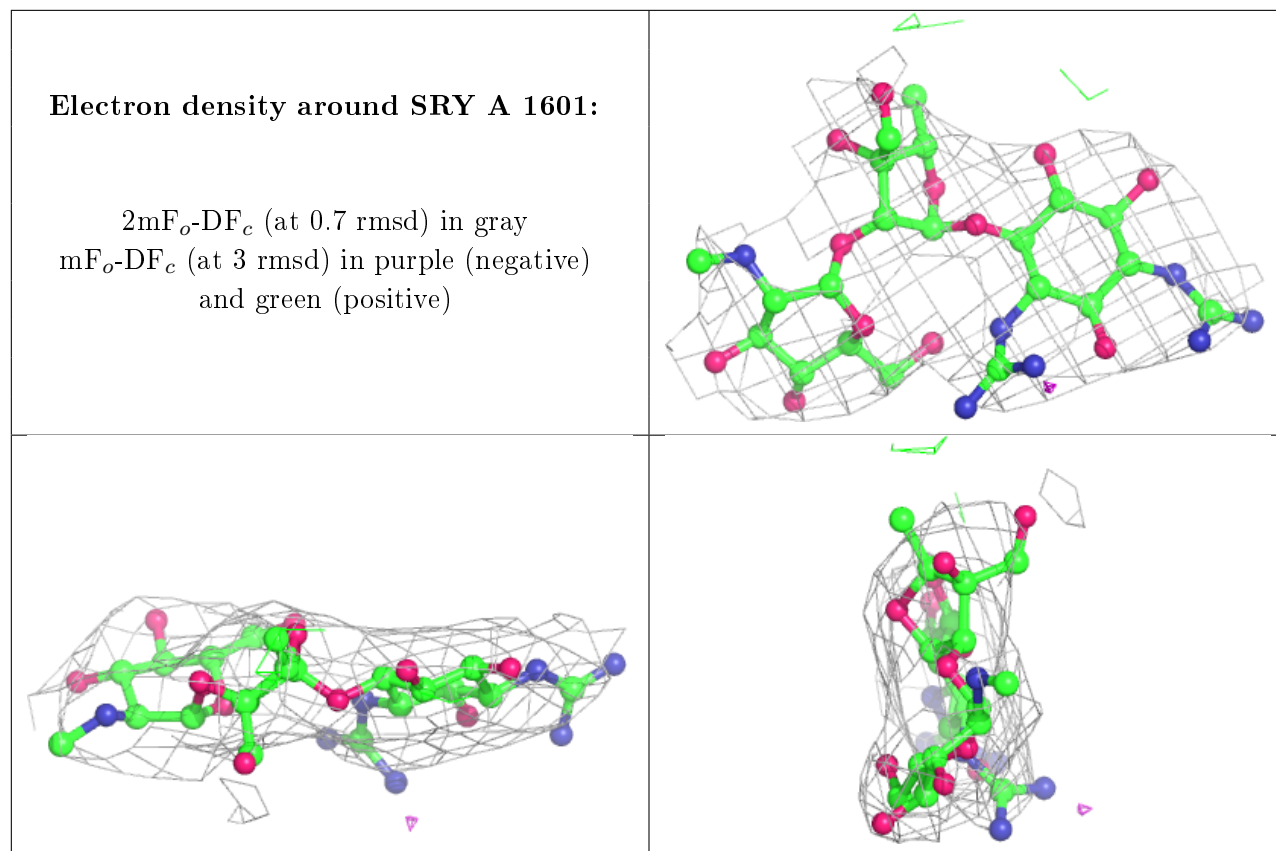
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1708	1/1	0.98	0.26	325,325,325,325	0
23	MG	A	1793	1/1	0.98	0.27	92,92,92,92	0
23	MG	A	1693	1/1	0.98	0.12	108,108,108,108	0
24	ZN	D	301	1/1	0.98	0.34	102,102,102,102	0
23	MG	A	1738	1/1	0.98	0.11	91,91,91,91	0
23	MG	A	1641	1/1	0.98	0.11	101,101,101,101	0
23	MG	A	1716	1/1	0.98	0.11	102,102,102,102	0
23	MG	A	1611	1/1	0.98	0.10	179,179,179,179	0
23	MG	A	1607	1/1	0.98	0.45	111,111,111,111	0
23	MG	A	1686	1/1	0.98	0.18	146,146,146,146	0
23	MG	A	1608	1/1	0.98	0.06	114,114,114,114	0
23	MG	A	1689	1/1	0.98	0.22	202,202,202,202	0
23	MG	A	1700	1/1	0.98	0.16	226,226,226,226	0
23	MG	A	1749	1/1	0.98	0.27	127,127,127,127	0
23	MG	A	1775	1/1	0.98	0.14	108,108,108,108	0
23	MG	A	1703	1/1	0.98	0.17	141,141,141,141	0
23	MG	A	1619	1/1	0.98	0.39	117,117,117,117	0
23	MG	A	1668	1/1	0.98	0.16	116,116,116,116	0
23	MG	A	1695	1/1	0.98	0.12	144,144,144,144	0
23	MG	A	1735	1/1	0.98	0.11	110,110,110,110	0
23	MG	A	1620	1/1	0.98	0.20	128,128,128,128	0
23	MG	A	1750	1/1	0.98	0.24	120,120,120,120	0
23	MG	A	1616	1/1	0.98	0.19	61,61,61,61	0
23	MG	A	1739	1/1	0.98	0.17	106,106,106,106	0
23	MG	A	1740	1/1	0.99	0.14	126,126,126,126	0
23	MG	A	1606	1/1	0.99	0.09	89,89,89,89	0
23	MG	A	1632	1/1	0.99	0.12	85,85,85,85	0
23	MG	A	1691	1/1	0.99	0.14	136,136,136,136	0
23	MG	A	1670	1/1	0.99	0.11	105,105,105,105	0
23	MG	A	1634	1/1	0.99	0.33	133,133,133,133	0
23	MG	A	1714	1/1	0.99	0.20	54,54,54,54	0
23	MG	A	1704	1/1	0.99	0.37	112,112,112,112	0
23	MG	A	1658	1/1	0.99	0.14	98,98,98,98	0
23	MG	A	1636	1/1	0.99	0.12	97,97,97,97	0
23	MG	A	1692	1/1	0.99	0.21	112,112,112,112	0
23	MG	A	1637	1/1	0.99	0.28	99,99,99,99	0
23	MG	A	1602	1/1	0.99	0.21	109,109,109,109	0
23	MG	A	1614	1/1	0.99	0.10	98,98,98,98	0
23	MG	A	1655	1/1	1.00	0.09	93,93,93,93	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 ⓘ

There are no such residues in this entry.