wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 05:17 pm GMT

PDB ID	:	4YHH
Title	:	Crystal structure of the 30S ribosomal subunit from Thermus thermophilus in complex with tigecycline
Authors	:	Schedlbauer, A.; Kaminishi, T.; Ochoa-Lizarralde, B.; Dhimole, N.; Zhou, S.; Lopez-Alonso, J.P.; Connell, S.R.; Fucini, P.
Deposited on	:	2015-02-27
Resolution	:	3.42 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

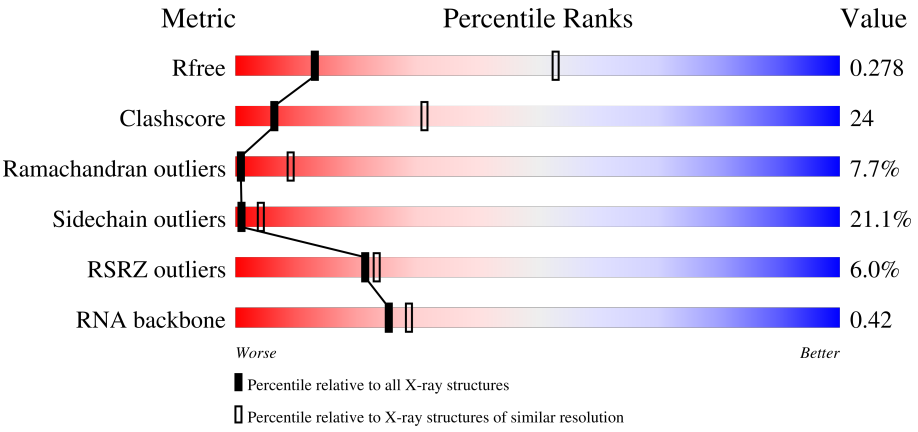
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)
RNA backbone	3102	1012 (3.88-2.96)

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 of 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 <=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	1507	23% 48% 25%
2	B	226	6% 33% 48% 17%
3	C	206	% 39% 49% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	208	5% 28% 53% 16%
5	E	157	13% 34% 45% 20%
6	F	101	5% 27% 45% 27%
7	G	155	5% 49% 44% 6%
8	H	138	3% 30% 47% 21%
9	I	127	6% 50% 38% 12%
10	J	99	18% 45% 48% 6%
11	K	115	8% 46% 43% 10%
12	L	124	19% 42% 47% 10%
13	M	119	22% 49% 41% 9%
14	N	60	3% 32% 50% 18%
15	O	88	33% 51% 16%
16	P	85	11% 40% 51% 9%
17	Q	104	28% 44% 38% 16%
18	R	73	23% 37% 41% 21%
19	S	83	12% 57% 30% 13%
20	T	99	9% 48% 42% 9%
21	V	24	17% 58% 17% 17% 8%

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
23	MG	A	1619	-	-	-	X
23	MG	A	1626	-	-	-	X
23	MG	A	1636	-	-	-	X
23	MG	A	1654	-	-	-	X
23	MG	A	1664	-	-	-	X
23	MG	A	1695	-	-	-	X

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 51732 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1507	32392	14418	6001	10467	1506	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	226	1842	1174	332	331	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1613	1016	314	282	1	0	0	0

- Molecule 4 is a protein called 30S 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 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	157	1199	754	228	213	4	0	0	0

- Molecule 6 is a protein called 30S 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 30S ribosomal protein S7.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	0
			854	531	160	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	119	Total	C	N	O	S	0	0	0
			947	585	195	165	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	85	Total	C	N	O	S	0	0	0
			717	452	144	120	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	83	Total	C	N	O	S	0	0	0
			666	424	124	116	2			

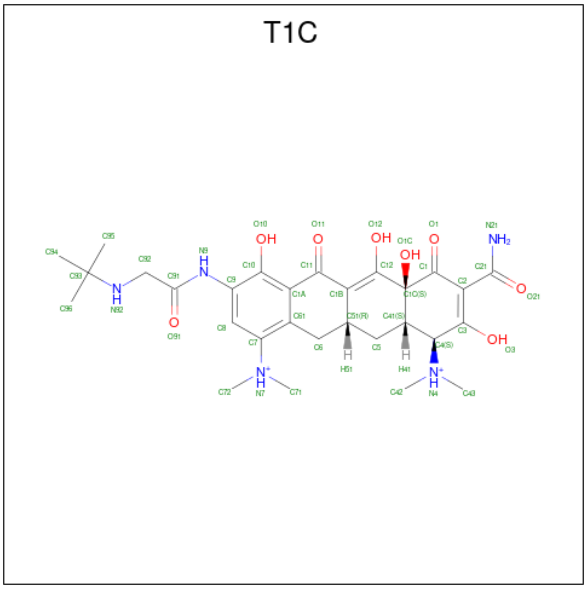
- Molecule 20 is a protein called 30S ribosomal protein S20.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	V	24	Total C N O 209 128 50 31	0	0	0

- Molecule 22 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C N O 42 29 5 8	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	102	Total Mg 102 102	0	0
23	E	1	Total Mg 1 1	0	0

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

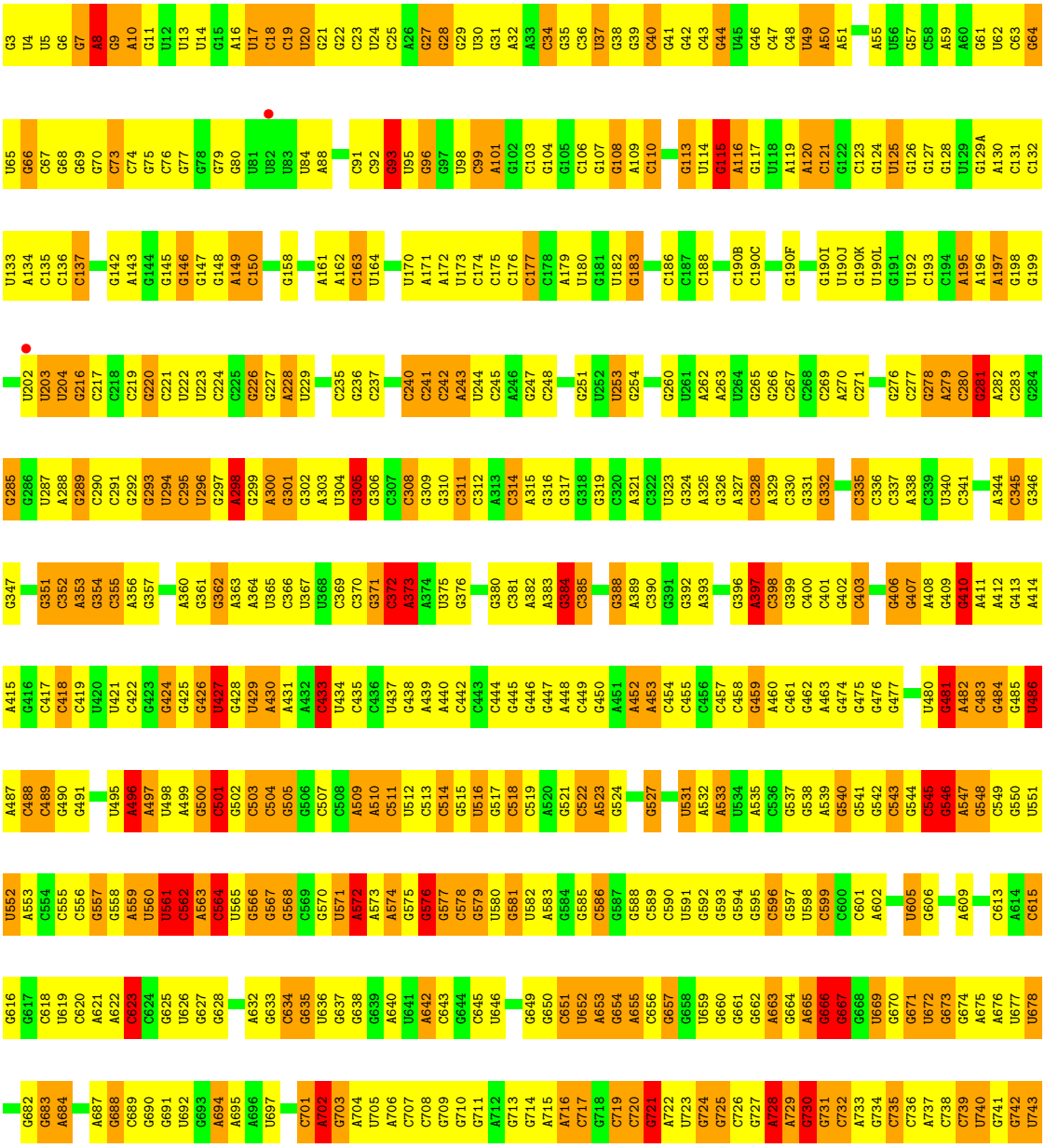
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	D	1	Total Zn 1 1	0	0
24	N	1	Total Zn 1 1	0	0

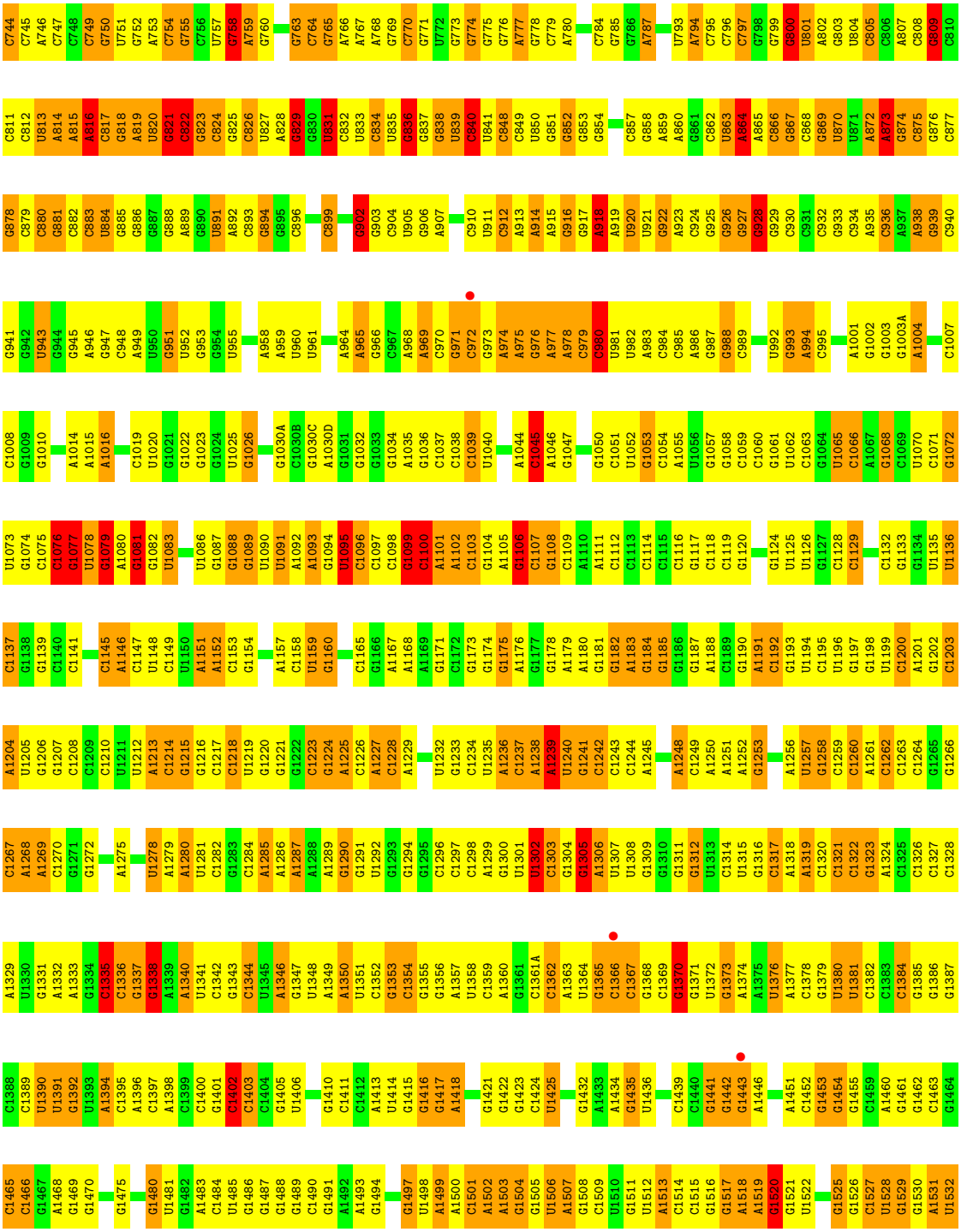
3 Residue-property plots (i)

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.

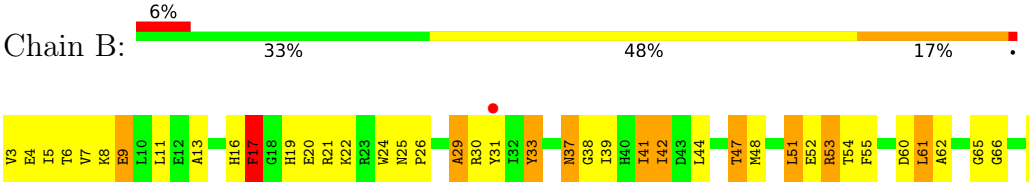
- Molecule 1: 16S ribosomal RNA

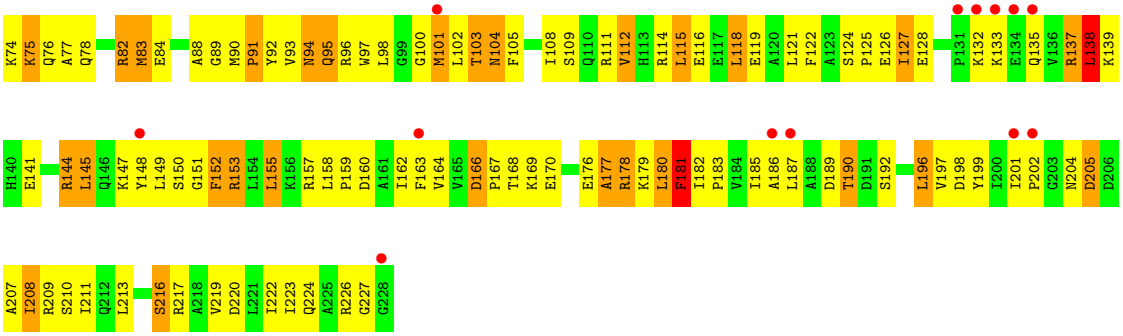
Chain A: 23% 48% 25%





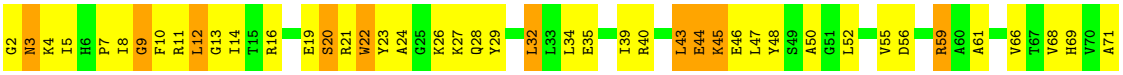
• Molecule 2: 30S ribosomal protein S2

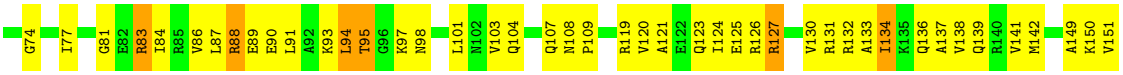


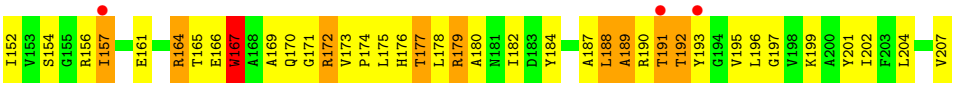


• Molecule 3: 30S ribosomal protein S3

Chain C:

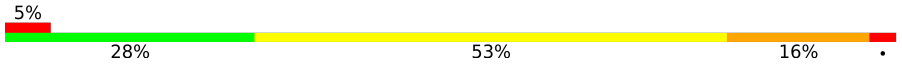


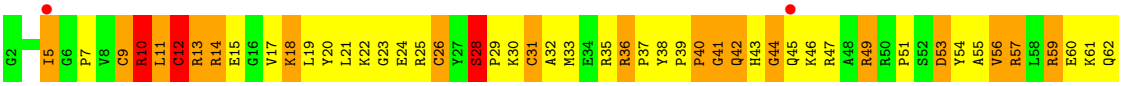


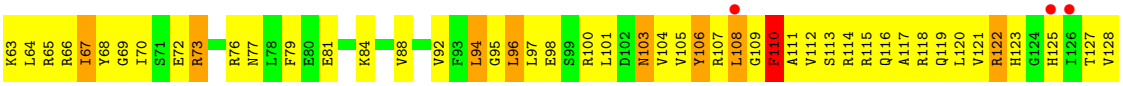


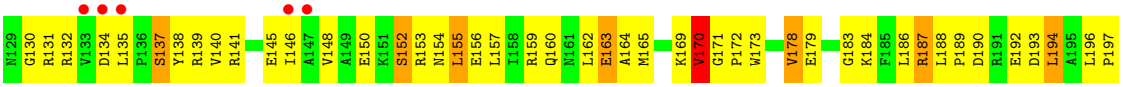
• Molecule 4: 30S ribosomal protein S4

Chain D:



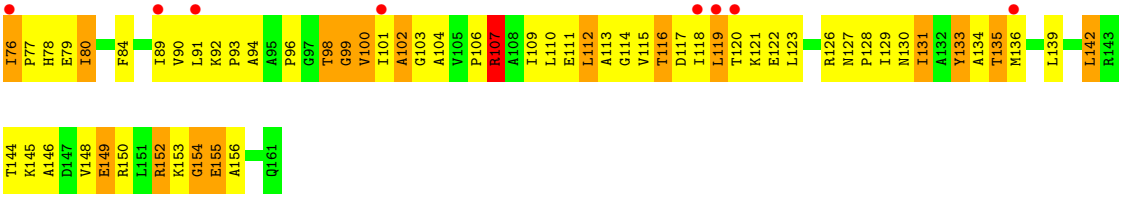




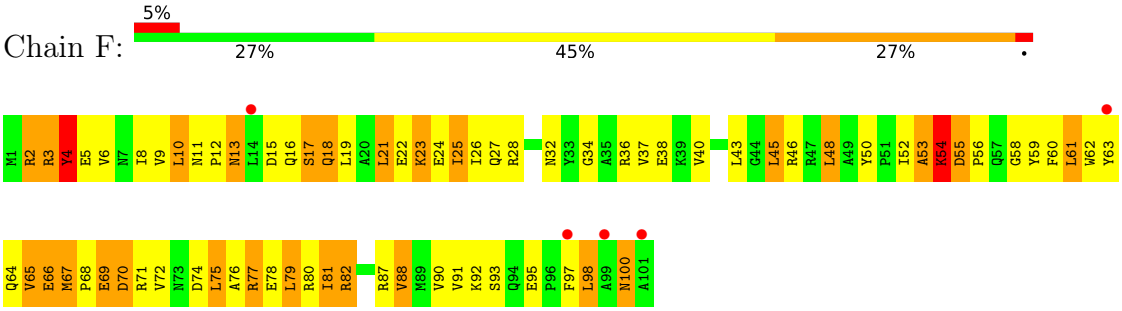


• Molecule 5: 30S ribosomal protein S5

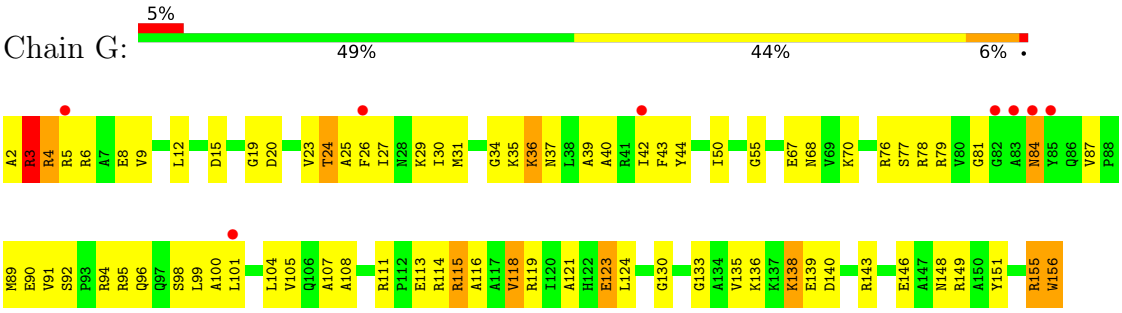
Chain E:



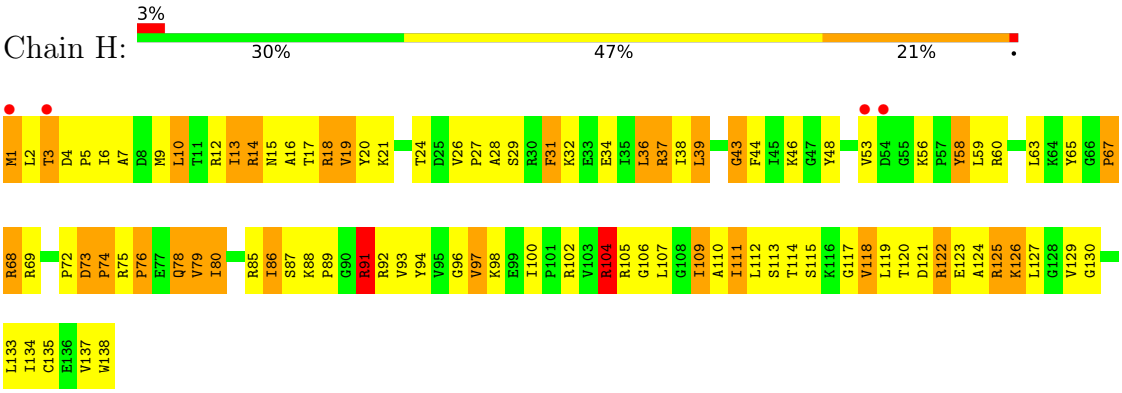
• Molecule 6: 30S ribosomal protein S6



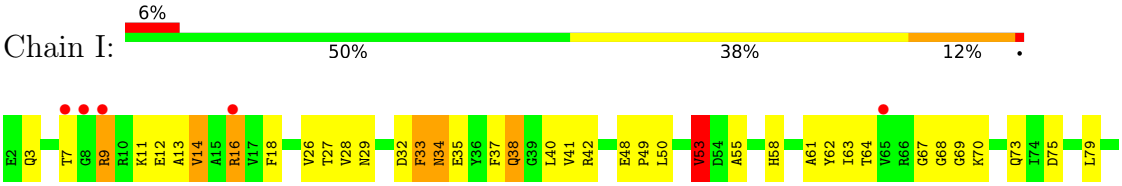
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

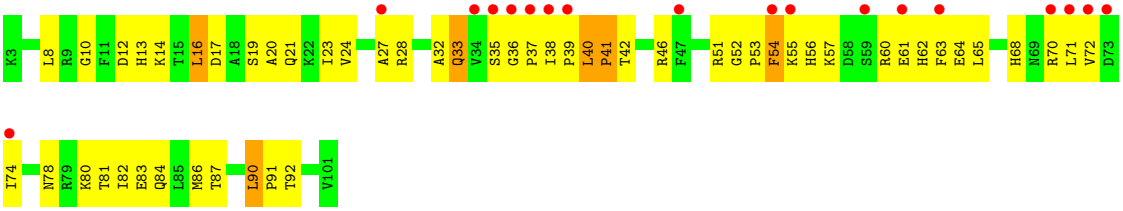


• Molecule 9: 30S ribosomal protein S9



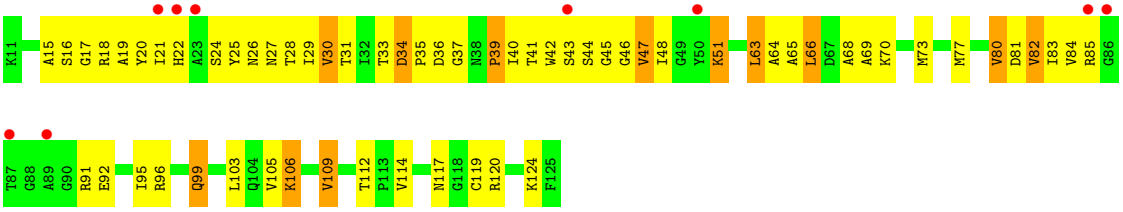
• Molecule 10: 30S ribosomal protein S10

Chain J:



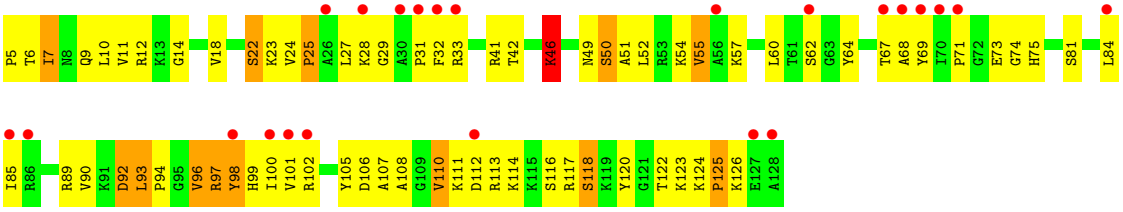
• Molecule 11: 30S ribosomal protein S11

Chain K:



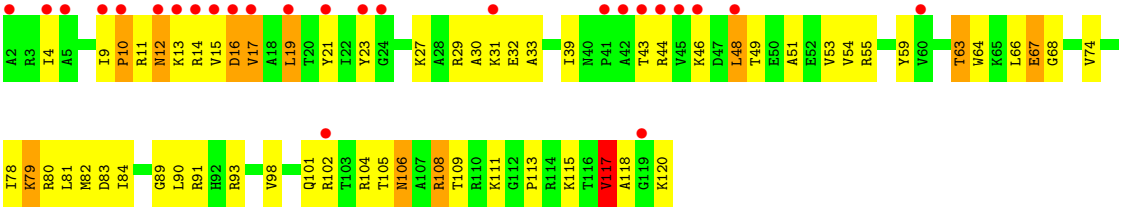
• Molecule 12: 30S ribosomal protein S12

Chain L:



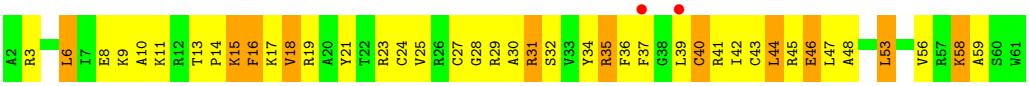
• Molecule 13: 30S ribosomal protein S13

Chain M:

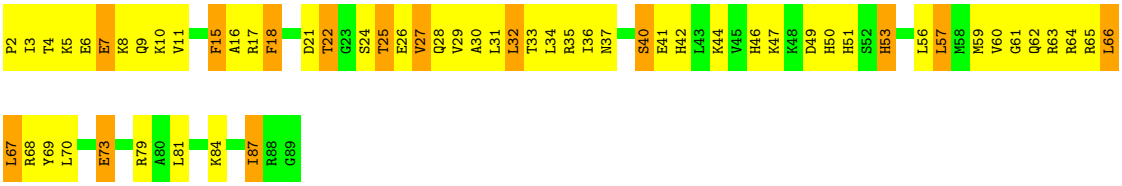


• Molecule 14: 30S ribosomal protein S14 type Z

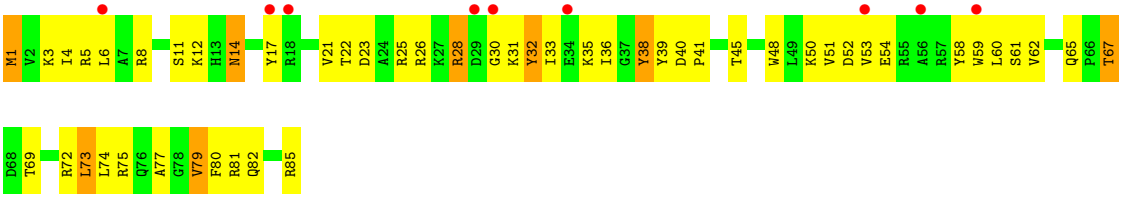
Chain N:



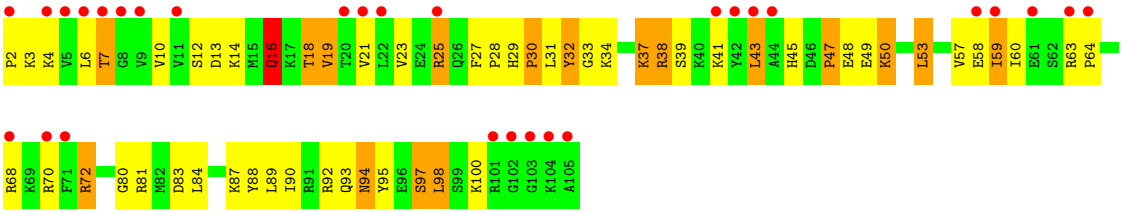
• Molecule 15: 30S ribosomal protein S15



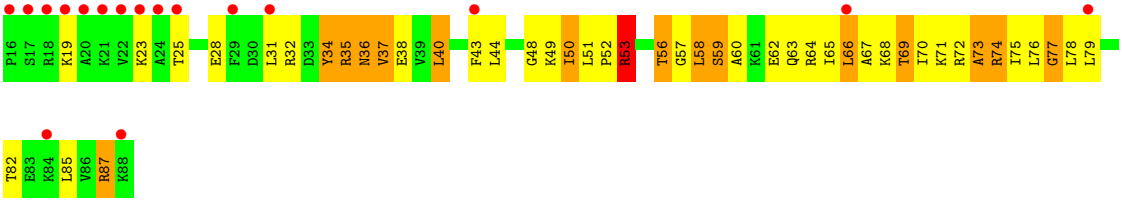
• Molecule 16: 30S ribosomal protein S16



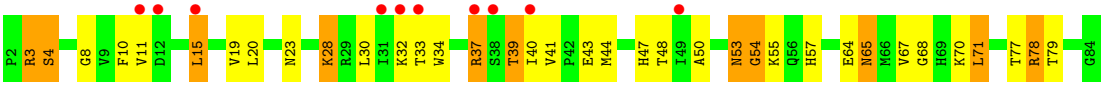
• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

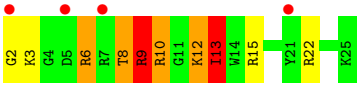


• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20

• Molecule 21: 30S ribosomal protein Thx



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	409.59Å 409.59Å 171.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 3.42 49.60 – 3.42	Depositor EDS
% Data completeness (in resolution range)	87.5 (48.72-3.42) 87.6 (49.60-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.228 , 0.287 0.221 , 0.278	Depositor DCC
R_{free} test set	8627 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	147.3	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 105.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	51732	wwPDB-VP
Average B, all atoms (Å^2)	212.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, T1C, ZN

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	0.77	14/36260 (0.0%)	1.43	658/56595 (1.2%)
2	B	0.56	0/1874	0.80	1/2522 (0.0%)
3	C	0.57	0/1637	0.81	0/2205
4	D	0.72	2/1733 (0.1%)	0.94	5/2318 (0.2%)
5	E	0.76	0/1216	1.01	1/1636 (0.1%)
6	F	0.67	0/856	0.94	2/1154 (0.2%)
7	G	0.46	0/1276	0.66	0/1709
8	H	0.74	2/1136 (0.2%)	1.02	3/1527 (0.2%)
9	I	0.47	0/1029	0.67	0/1379
10	J	0.50	0/815	0.73	0/1095
11	K	0.46	0/869	0.68	0/1173
12	L	0.50	0/987	0.78	0/1320
13	M	0.42	0/957	0.67	0/1281
14	N	0.47	0/501	0.79	2/664 (0.3%)
15	O	0.68	2/745 (0.3%)	0.83	0/992
16	P	0.48	0/733	0.75	0/984
17	Q	0.55	0/870	0.80	0/1159
18	R	0.63	0/604	1.04	1/801 (0.1%)
19	S	0.45	0/681	0.63	0/915
20	T	0.44	0/765	0.72	0/1007
21	V	0.51	0/213	0.79	0/277
All	All	0.71	20/55757 (0.0%)	1.27	673/82713 (0.8%)

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
4	D	0	2
6	F	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
17	Q	0	2
All	All	0	7

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	12	CYS	CB-SG	7.79	1.95	1.82
1	A	758	G	N7-C5	-7.24	1.34	1.39
1	A	728	A	N9-C4	6.34	1.41	1.37
1	A	410	G	N9-C4	6.21	1.43	1.38
8	H	123	GLU	CG-CD	6.14	1.61	1.51

The worst 5 of 673 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	578	C	N3-C4-C5	-16.18	115.43	121.90
1	A	578	C	C4-C5-C6	14.72	124.76	117.40
1	A	764	C	C6-N1-C2	-13.75	114.80	120.30
1	A	758	G	C8-N9-C4	-13.19	101.12	106.40
1	A	581	G	N1-C6-O6	13.04	127.72	119.90

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	28	SER	Peptide
4	D	31	CYS	Peptide
6	F	2	ARG	Peptide
6	F	46	ARG	Peptide
12	L	126	LYS	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	32392	0	16349	1113	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1842	0	1894	118	0
3	C	1613	0	1677	107	0
4	D	1703	0	1763	135	0
5	E	1199	0	1251	100	0
6	F	843	0	857	78	0
7	G	1257	0	1296	52	0
8	H	1116	0	1177	94	0
9	I	1010	0	1037	52	0
10	J	802	0	849	47	0
11	K	854	0	868	42	0
12	L	971	0	1057	67	0
13	M	947	0	1008	36	0
14	N	492	0	532	34	0
15	O	734	0	771	46	0
16	P	717	0	738	38	0
17	Q	857	0	928	47	0
18	R	598	0	670	46	0
19	S	666	0	686	28	0
20	T	763	0	861	39	0
21	V	209	0	221	7	0
22	A	42	0	38	1	0
23	A	102	0	0	0	0
23	E	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
All	All	51732	0	36528	2073	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 24.

The worst 5 of 2073 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:559:A:OP1	5:E:126:ARG:NH2	1.92	1.01
17:Q:29:HIS:HB3	17:Q:33:GLY:H	1.27	0.98
1:A:447:G:H2'	1:A:485:G:H22	1.28	0.97
1:A:663:A:H2'	1:A:664:G:H8	1.29	0.96
2:B:100:GLY:O	2:B:102:LEU:N	2.00	0.95

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	224/226 (99%)	154 (69%)	45 (20%)	25 (11%)	0 5
3	C	204/206 (99%)	142 (70%)	45 (22%)	17 (8%)	1 8
4	D	206/208 (99%)	147 (71%)	34 (16%)	25 (12%)	0 4
5	E	155/157 (99%)	109 (70%)	30 (19%)	16 (10%)	0 6
6	F	99/101 (98%)	79 (80%)	11 (11%)	9 (9%)	1 7
7	G	153/155 (99%)	113 (74%)	32 (21%)	8 (5%)	2 16
8	H	136/138 (99%)	98 (72%)	26 (19%)	12 (9%)	1 7
9	I	125/127 (98%)	96 (77%)	23 (18%)	6 (5%)	2 18
10	J	97/99 (98%)	78 (80%)	15 (16%)	4 (4%)	3 22
11	K	113/115 (98%)	90 (80%)	16 (14%)	7 (6%)	1 13
12	L	122/124 (98%)	85 (70%)	28 (23%)	9 (7%)	1 10
13	M	117/119 (98%)	90 (77%)	19 (16%)	8 (7%)	1 11
14	N	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	9 40
15	O	86/88 (98%)	63 (73%)	21 (24%)	2 (2%)	6 34
16	P	83/85 (98%)	60 (72%)	20 (24%)	3 (4%)	3 25
17	Q	102/104 (98%)	78 (76%)	14 (14%)	10 (10%)	0 6
18	R	71/73 (97%)	49 (69%)	15 (21%)	7 (10%)	0 6
19	S	81/83 (98%)	66 (82%)	11 (14%)	4 (5%)	2 18
20	T	97/99 (98%)	74 (76%)	18 (19%)	5 (5%)	2 16
21	V	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	1 7
All	All	2351/2391 (98%)	1736 (74%)	435 (18%)	180 (8%)	1 9

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	29	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	30	ARG
2	B	78	GLN
2	B	82	ARG
2	B	101	MET

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	195/195 (100%)	147 (75%)	48 (25%)	0 3
3	C	160/160 (100%)	130 (81%)	30 (19%)	1 6
4	D	180/180 (100%)	139 (77%)	41 (23%)	1 3
5	E	119/119 (100%)	85 (71%)	34 (29%)	0 2
6	F	90/90 (100%)	60 (67%)	30 (33%)	0 1
7	G	126/126 (100%)	109 (86%)	17 (14%)	4 19
8	H	119/119 (100%)	90 (76%)	29 (24%)	0 3
9	I	98/98 (100%)	79 (81%)	19 (19%)	1 6
10	J	89/89 (100%)	79 (89%)	10 (11%)	6 26
11	K	87/87 (100%)	70 (80%)	17 (20%)	1 5
12	L	104/104 (100%)	87 (84%)	17 (16%)	2 12
13	M	95/95 (100%)	78 (82%)	17 (18%)	2 8
14	N	49/49 (100%)	35 (71%)	14 (29%)	0 2
15	O	79/79 (100%)	62 (78%)	17 (22%)	1 4
16	P	73/73 (100%)	58 (80%)	15 (20%)	1 5
17	Q	96/96 (100%)	78 (81%)	18 (19%)	1 6
18	R	64/64 (100%)	49 (77%)	15 (23%)	1 3
19	S	72/72 (100%)	60 (83%)	12 (17%)	2 10
20	T	76/76 (100%)	64 (84%)	12 (16%)	2 13
21	V	19/19 (100%)	12 (63%)	7 (37%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1990/1990 (100%)	1571 (79%)	419 (21%)	1 4

5 of 419 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	9	ARG
12	L	97	ARG
19	S	79	THR
9	I	50	LEU
11	K	30	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	56	HIS
12	L	49	ASN
19	S	47	HIS
15	O	46	HIS
15	O	62	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1507 (99%)	396 (26%)	7 (0%)

5 of 396 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	G
1	A	8	A
1	A	9	G
1	A	10	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	793	U
1	A	1145	C
1	A	1529	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1183	A
1	A	702	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 106 ligands modelled in this entry, 105 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	T1C	A	1601	23	44,45,45	1.27	4 (9%)	53,72,72	1.24	4 (7%)

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	T1C	A	1601	23	-	9/22/80/80	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	T1C	C8-C7	4.31	1.46	1.39
22	A	1601	T1C	C4-N4	3.60	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	T1C	C4-C3	3.14	1.58	1.51
22	A	1601	T1C	C7-N7	2.54	1.49	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1601	T1C	C8-C9-C10	-4.44	116.08	120.49
22	A	1601	T1C	C92-N92-C93	4.30	121.22	115.84
22	A	1601	T1C	C41-C1C-C1	2.81	114.27	111.05
22	A	1601	T1C	C8-C7-N7	-2.08	118.12	120.91

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1601	T1C	C94-C93-N92-C92
22	A	1601	T1C	C95-C93-N92-C92
22	A	1601	T1C	C96-C93-N92-C92
22	A	1601	T1C	C3-C2-C21-O21
22	A	1601	T1C	C3-C2-C21-N21

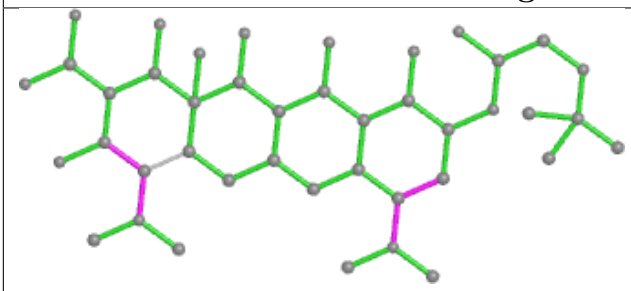
There are no ring outliers.

1 monomer is involved in 1 short contact:

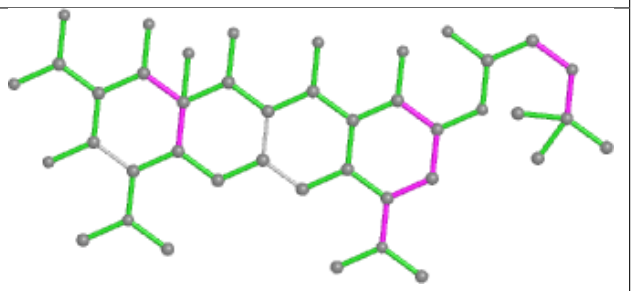
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	T1C	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

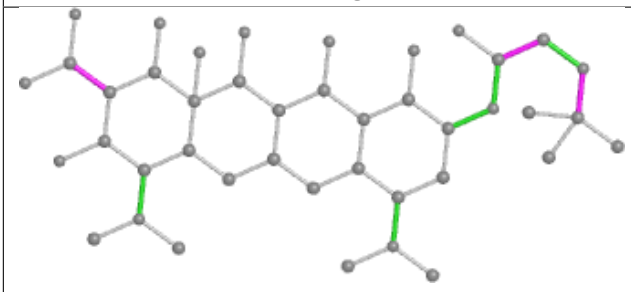
Ligand T1C A 1601



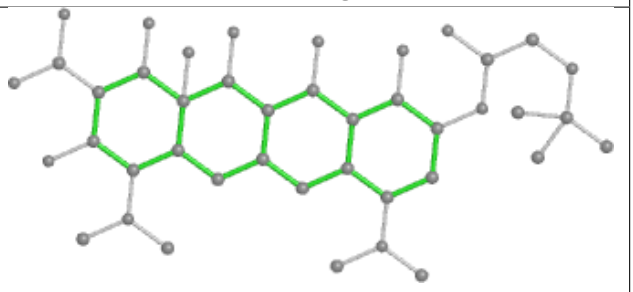
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1507/1507 (100%)	-0.63	5 (0%) 94 93	141, 212, 294, 438	0
2	B	226/226 (100%)	-0.03	14 (6%) 20 22	113, 192, 235, 265	0
3	C	206/206 (100%)	-0.46	3 (1%) 73 72	137, 204, 238, 266	0
4	D	208/208 (100%)	0.23	10 (4%) 30 31	125, 184, 221, 235	0
5	E	157/157 (100%)	0.54	20 (12%) 3 5	115, 165, 225, 272	0
6	F	101/101 (100%)	-0.13	5 (4%) 28 29	136, 190, 228, 264	0
7	G	155/155 (100%)	-0.21	8 (5%) 27 28	162, 226, 265, 299	0
8	H	138/138 (100%)	-0.03	4 (2%) 51 50	104, 167, 200, 223	0
9	I	127/127 (100%)	0.08	8 (6%) 20 21	144, 230, 273, 295	0
10	J	99/99 (100%)	0.79	18 (18%) 1 2	159, 222, 278, 287	0
11	K	115/115 (100%)	0.25	9 (7%) 13 16	155, 210, 239, 245	0
12	L	124/124 (100%)	0.87	23 (18%) 1 2	139, 201, 228, 293	0
13	M	119/119 (100%)	0.91	26 (21%) 0 1	194, 235, 259, 271	0
14	N	60/60 (100%)	0.23	2 (3%) 46 46	156, 212, 240, 247	0
15	O	88/88 (100%)	-0.42	0 100 100	107, 185, 225, 256	0
16	P	85/85 (100%)	0.71	9 (10%) 6 9	156, 198, 238, 282	0
17	Q	104/104 (100%)	1.20	29 (27%) 0 0	147, 196, 234, 331	0
18	R	73/73 (100%)	1.24	17 (23%) 0 1	121, 187, 281, 319	0
19	S	83/83 (100%)	0.40	10 (12%) 4 6	168, 250, 281, 295	0
20	T	99/99 (100%)	0.47	9 (9%) 9 12	184, 219, 267, 292	0
21	V	24/24 (100%)	0.90	4 (16%) 1 2	178, 205, 231, 244	0
All	All	3898/3898 (100%)	-0.07	233 (5%) 21 23	104, 206, 274, 438	0

The worst 5 of 233 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	105	ALA	11.5
17	Q	104	LYS	11.4
17	Q	103	GLY	10.0
10	J	35	SER	8.7
10	J	34	VAL	8.5

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

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

6.3 Carbohydrates (i)

There are no 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1664	1/1	0.39	0.85	136,136,136,136	0
23	MG	A	1619	1/1	0.60	0.55	143,143,143,143	0
23	MG	A	1695	1/1	0.74	0.56	124,124,124,124	0
23	MG	A	1647	1/1	0.75	0.31	109,109,109,109	0
23	MG	A	1686	1/1	0.77	0.15	146,146,146,146	0
23	MG	A	1617	1/1	0.77	0.26	130,130,130,130	0
23	MG	A	1701	1/1	0.77	0.37	124,124,124,124	0
23	MG	A	1636	1/1	0.79	0.52	105,105,105,105	0
23	MG	A	1626	1/1	0.79	0.48	125,125,125,125	0
23	MG	A	1654	1/1	0.80	1.37	117,117,117,117	0
23	MG	A	1608	1/1	0.81	0.49	128,128,128,128	0
23	MG	A	1696	1/1	0.81	0.93	121,121,121,121	0
23	MG	A	1612	1/1	0.81	0.48	117,117,117,117	0
23	MG	A	1623	1/1	0.82	0.50	113,113,113,113	0
23	MG	A	1616	1/1	0.82	0.08	125,125,125,125	0
23	MG	A	1610	1/1	0.83	0.30	144,144,144,144	0
23	MG	A	1606	1/1	0.83	0.70	117,117,117,117	0
23	MG	A	1687	1/1	0.83	0.20	145,145,145,145	0
23	MG	A	1650	1/1	0.84	0.10	131,131,131,131	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1693	1/1	0.84	0.16	128,128,128,128	0
23	MG	A	1613	1/1	0.84	0.38	136,136,136,136	0
23	MG	A	1622	1/1	0.84	0.86	133,133,133,133	0
23	MG	A	1648	1/1	0.84	0.35	152,152,152,152	0
23	MG	A	1625	1/1	0.85	0.62	109,109,109,109	0
23	MG	A	1662	1/1	0.85	0.09	138,138,138,138	0
23	MG	A	1607	1/1	0.85	0.77	98,98,98,98	0
23	MG	A	1657	1/1	0.86	0.25	112,112,112,112	0
23	MG	A	1604	1/1	0.87	0.12	120,120,120,120	0
23	MG	A	1603	1/1	0.87	0.44	127,127,127,127	0
23	MG	A	1649	1/1	0.88	0.30	159,159,159,159	0
23	MG	A	1646	1/1	0.88	0.80	122,122,122,122	0
23	MG	A	1668	1/1	0.88	0.74	123,123,123,123	0
23	MG	A	1621	1/1	0.89	0.32	126,126,126,126	0
23	MG	A	1669	1/1	0.90	0.98	128,128,128,128	0
23	MG	A	1635	1/1	0.90	0.26	97,97,97,97	0
23	MG	A	1658	1/1	0.90	0.26	120,120,120,120	0
23	MG	A	1652	1/1	0.90	0.49	145,145,145,145	0
23	MG	A	1663	1/1	0.90	0.25	97,97,97,97	0
23	MG	A	1653	1/1	0.90	0.81	114,114,114,114	0
23	MG	A	1634	1/1	0.90	0.84	104,104,104,104	0
23	MG	E	201	1/1	0.90	0.19	109,109,109,109	0
23	MG	A	1680	1/1	0.91	0.20	99,99,99,99	0
23	MG	A	1655	1/1	0.91	0.23	112,112,112,112	0
23	MG	A	1642	1/1	0.91	0.81	114,114,114,114	0
23	MG	A	1673	1/1	0.91	0.35	129,129,129,129	0
23	MG	A	1637	1/1	0.92	0.23	105,105,105,105	0
23	MG	A	1602	1/1	0.92	0.38	99,99,99,99	0
23	MG	A	1681	1/1	0.92	0.20	131,131,131,131	0
23	MG	A	1694	1/1	0.92	0.29	176,176,176,176	0
23	MG	A	1624	1/1	0.93	0.20	122,122,122,122	0
23	MG	A	1660	1/1	0.93	0.11	141,141,141,141	0
23	MG	A	1682	1/1	0.93	0.19	109,109,109,109	0
23	MG	A	1674	1/1	0.93	0.20	125,125,125,125	0
23	MG	A	1698	1/1	0.93	0.42	95,95,95,95	0
23	MG	A	1678	1/1	0.93	0.56	117,117,117,117	0
23	MG	A	1689	1/1	0.93	0.52	118,118,118,118	0
23	MG	A	1645	1/1	0.94	0.29	173,173,173,173	0
23	MG	A	1615	1/1	0.94	0.30	152,152,152,152	0
23	MG	A	1697	1/1	0.94	0.61	113,113,113,113	0
23	MG	A	1609	1/1	0.94	0.08	151,151,151,151	0
22	T1C	A	1601	42/42	0.94	0.20	173,207,227,233	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1684	1/1	0.94	0.31	138,138,138,138	0
23	MG	A	1643	1/1	0.95	0.23	127,127,127,127	0
23	MG	A	1644	1/1	0.95	0.18	132,132,132,132	0
23	MG	A	1676	1/1	0.95	0.75	136,136,136,136	0
23	MG	A	1641	1/1	0.95	0.30	98,98,98,98	0
23	MG	A	1679	1/1	0.95	0.18	130,130,130,130	0
23	MG	A	1631	1/1	0.95	0.09	118,118,118,118	0
23	MG	A	1691	1/1	0.95	0.27	121,121,121,121	0
23	MG	A	1692	1/1	0.95	0.23	172,172,172,172	0
23	MG	A	1640	1/1	0.96	0.34	97,97,97,97	0
23	MG	A	1632	1/1	0.96	0.47	95,95,95,95	0
23	MG	A	1671	1/1	0.96	0.22	120,120,120,120	0
23	MG	A	1620	1/1	0.96	0.14	106,106,106,106	0
23	MG	A	1627	1/1	0.96	0.35	93,93,93,93	0
23	MG	A	1630	1/1	0.96	0.42	127,127,127,127	0
23	MG	A	1618	1/1	0.96	0.10	120,120,120,120	0
23	MG	A	1690	1/1	0.96	0.17	114,114,114,114	0
23	MG	A	1639	1/1	0.96	0.14	132,132,132,132	0
23	MG	A	1670	1/1	0.97	0.68	123,123,123,123	0
23	MG	A	1651	1/1	0.97	0.43	115,115,115,115	0
23	MG	A	1659	1/1	0.97	0.33	106,106,106,106	0
23	MG	A	1629	1/1	0.97	0.56	113,113,113,113	0
23	MG	A	1675	1/1	0.97	0.31	135,135,135,135	0
23	MG	A	1611	1/1	0.97	0.11	131,131,131,131	0
23	MG	A	1677	1/1	0.97	0.20	132,132,132,132	0
23	MG	A	1614	1/1	0.97	0.11	108,108,108,108	0
23	MG	A	1605	1/1	0.97	0.62	135,135,135,135	0
23	MG	A	1665	1/1	0.97	0.19	101,101,101,101	0
23	MG	A	1666	1/1	0.97	0.41	89,89,89,89	0
23	MG	A	1656	1/1	0.97	0.21	104,104,104,104	0
23	MG	A	1700	1/1	0.97	0.16	137,137,137,137	0
23	MG	A	1683	1/1	0.97	0.09	115,115,115,115	0
23	MG	A	1628	1/1	0.97	0.21	139,139,139,139	0
23	MG	A	1633	1/1	0.98	0.55	106,106,106,106	0
23	MG	A	1667	1/1	0.98	0.20	111,111,111,111	0
23	MG	A	1661	1/1	0.98	0.54	119,119,119,119	0
23	MG	A	1672	1/1	0.98	0.41	111,111,111,111	0
23	MG	A	1703	1/1	0.98	0.15	116,116,116,116	0
23	MG	A	1685	1/1	0.98	0.19	109,109,109,109	0
23	MG	A	1688	1/1	0.99	0.18	140,140,140,140	0
23	MG	A	1702	1/1	0.99	0.12	127,127,127,127	0
23	MG	A	1699	1/1	0.99	0.18	121,121,121,121	0

Continued on next page...

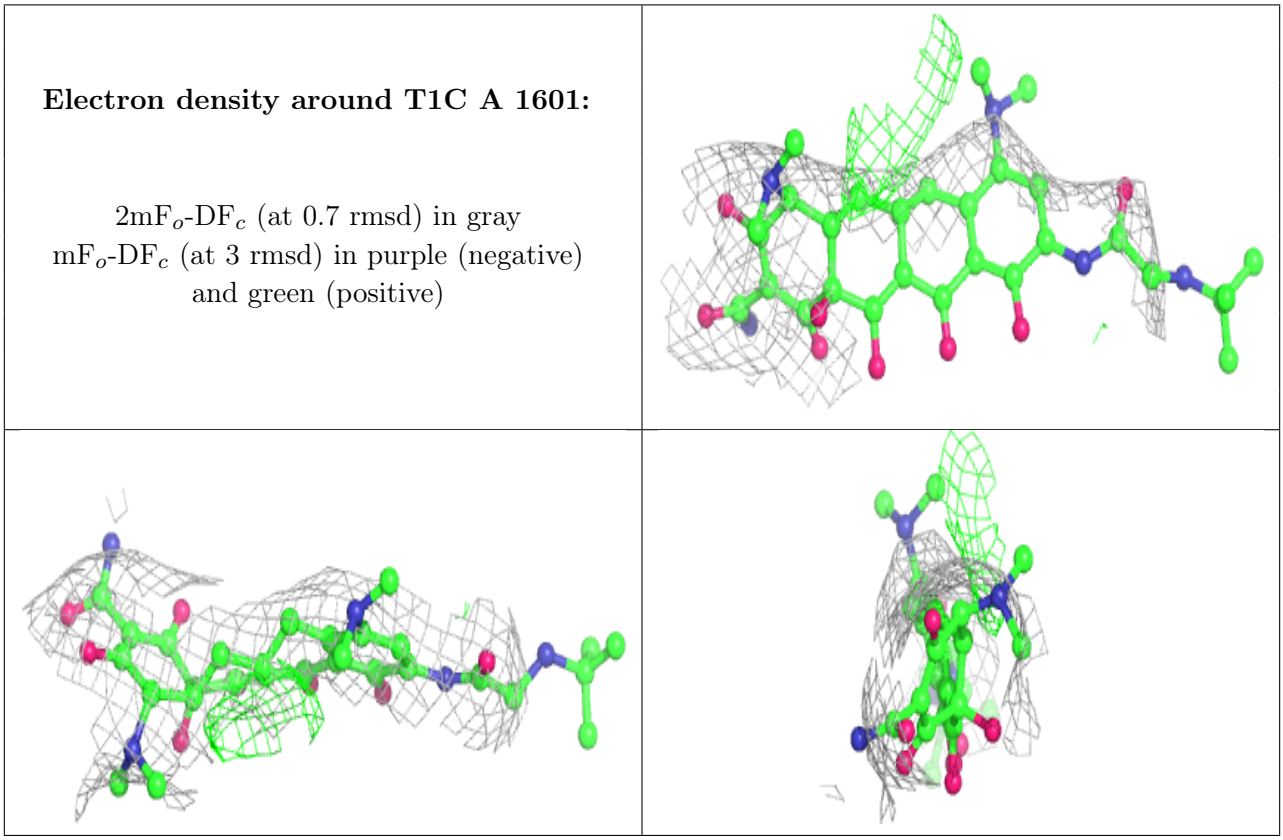
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1638	1/1	0.99	0.28	93,93,93,93	0
24	ZN	D	301	1/1	0.99	0.39	175,175,175,175	0
24	ZN	N	101	1/1	0.99	0.23	209,209,209,209	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around T1C A 1601:

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



6.5 Other polymers

There are no such residues in this entry.