



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 10:26 am BST

PDB ID : 1HNW
Title : STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL
SUBUNIT IN COMPLEX WITH TETRACYCLINE
Authors : Brodersen, D.E.; Clemons Jr., W.M.; Carter, A.P.; Morgan-Warren, R.; Wim-
berly, B.T.; Ramakrishnan, V.
Deposited on : 2000-12-08
Resolution : 3.40 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 : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

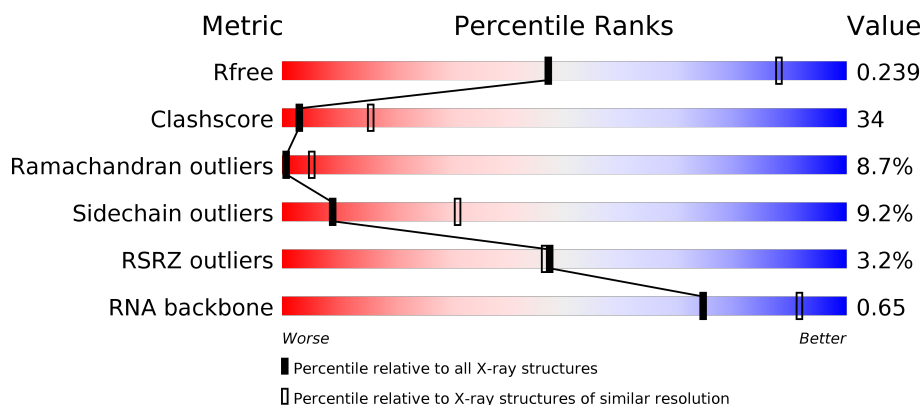
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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 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>5%</div> <div>29%</div> <div>55%</div> <div>12%</div> <div>..</div> </div>
2	X	6	<div> <div>33%</div> <div>100%</div> </div>
3	B	256	<div> <div>4%</div> <div>18%</div> <div>54%</div> <div>16%</div> <div>•</div> <div>9%</div> </div>
4	C	239	<div> <div>23%</div> <div>45%</div> <div>17%</div> <div>•</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
5	D	209	
6	E	162	
7	F	101	
8	G	156	
9	H	138	
10	I	128	
11	J	105	
12	K	129	
13	L	135	
14	M	126	
15	N	61	
16	O	89	
17	P	88	
18	Q	105	
19	R	88	
20	S	93	
21	T	106	
22	V	26	

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	1548	-	-	-	X
23	MG	A	1550	-	-	-	X
23	MG	A	1608	-	-	-	X
23	MG	A	1611	-	-	-	X
23	MG	A	1622	-	-	-	X
23	MG	A	1628	-	-	-	X

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 51934 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	22	0	0
			32391	14418	6002	10465	1506			

- Molecule 2 is a RNA chain called FRAGMENT OF MESSENGER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	6	Total	C	N	O	P	0	0	0
			117	54	14	44	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	88	Total	C	N	O	S	0	0	0
			735	462	147	125	1			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

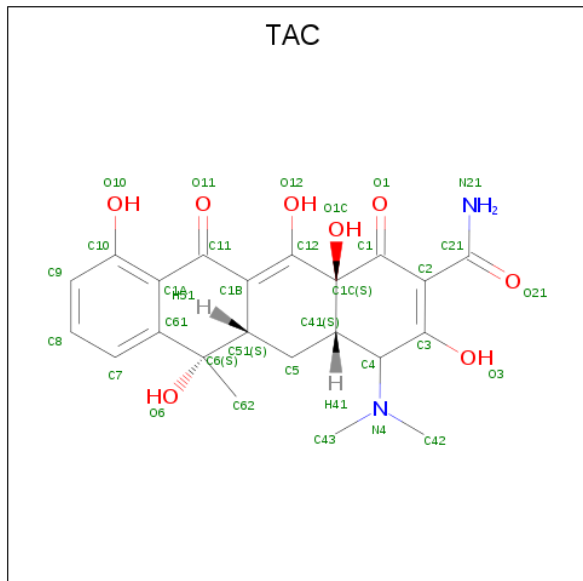
- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	H	1	Total	Mg	0	0
			1	1		
23	A	94	Total	Mg	0	0
			94	94		
23	D	1	Total	Mg	0	0
			1	1		

- Molecule 24 is TETRACYCLINE (three-letter code: TAC) (formula: $C_{22}H_{24}N_2O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			32	22	2	8		
24	A	1	Total	C	N	O	0	0
			32	22	2	8		

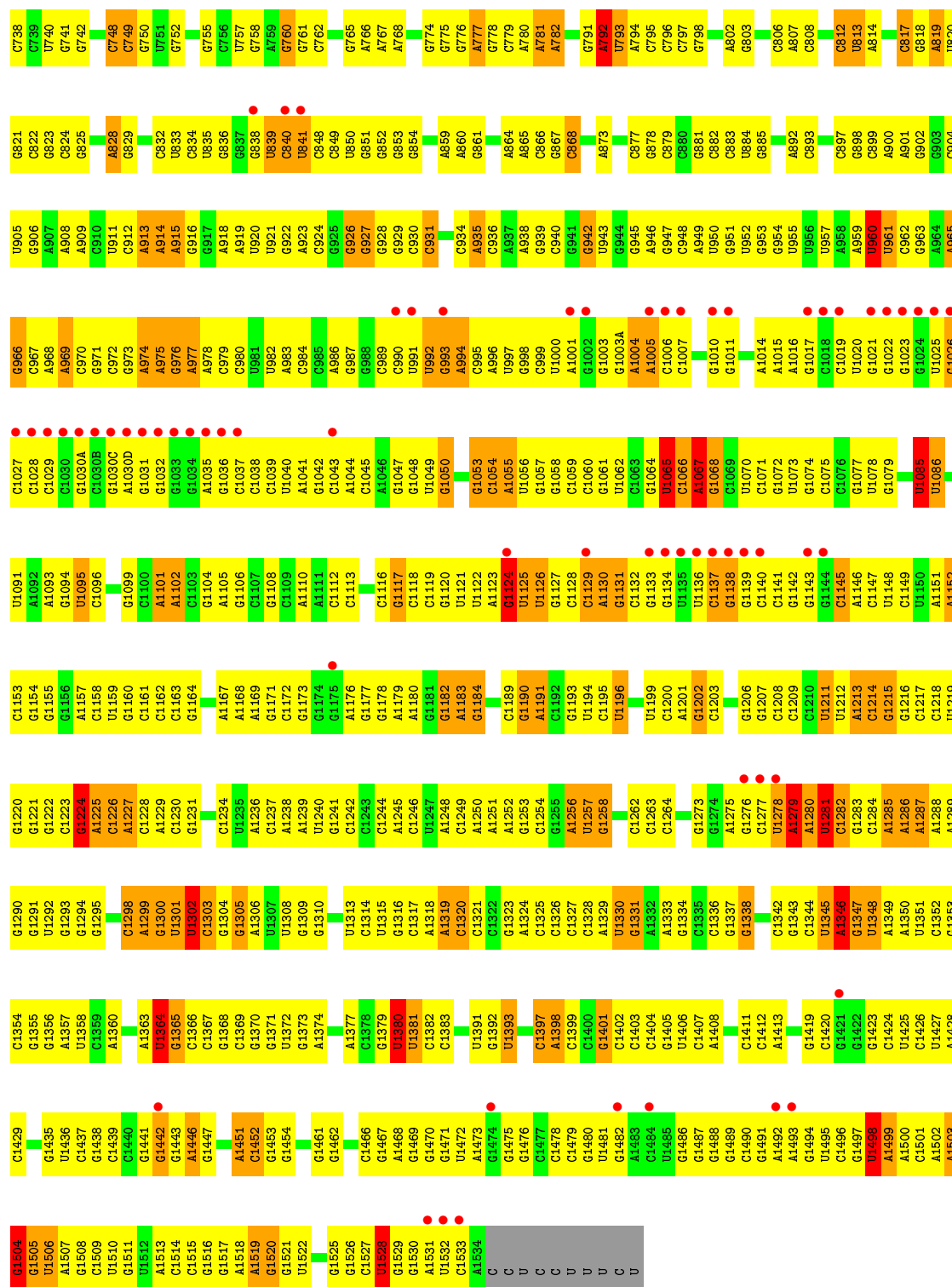
- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

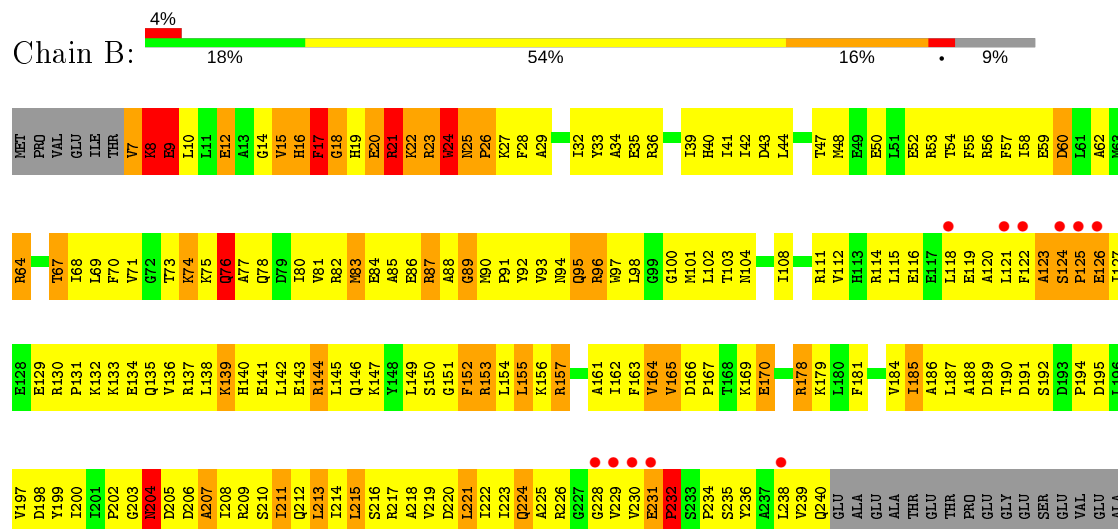
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

Chain A: ■ 5% ■ 29% ■ 55% ■ 12% ■ ..

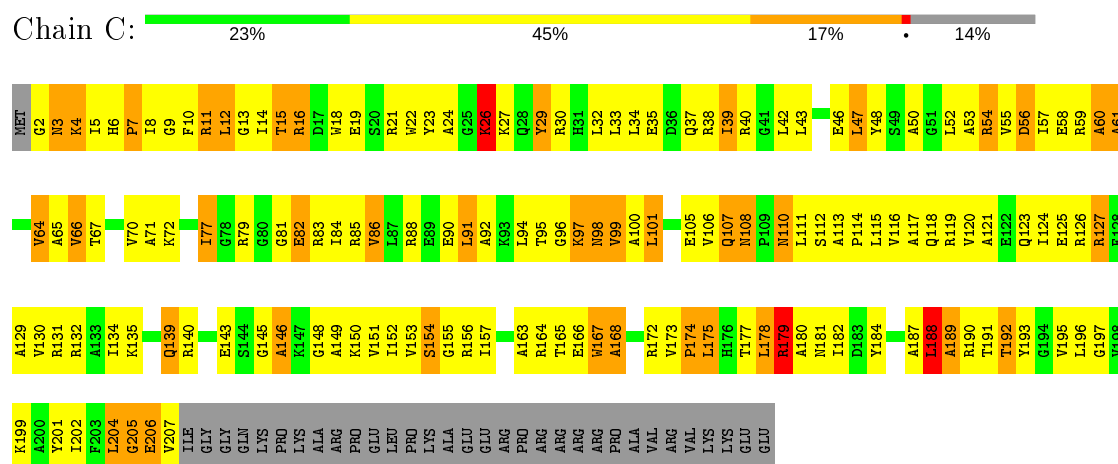
The visualization displays a sequence of 1000 nodes (labeled G650 to G731) arranged in a grid. Each node is a colored square with a 3-letter code. The colors correspond to a probability distribution: 5% red, 29% green, 55% yellow, 12% orange, and a small grey area. The nodes are connected by lines, forming a complex network. The grid is 10 columns wide and 100 rows high. The nodes are labeled with 3-letter codes, such as 'G650' in the top-left and 'G731' in the bottom-right. The colors of the nodes vary, reflecting the probability distribution. For example, the first row contains mostly green and yellow nodes, while the last row contains mostly orange and grey nodes. The connections between nodes are represented by thin black lines, creating a dense web of relationships. The overall structure is a complex, interconnected network of nodes and edges, representing the 'Chain A' data.



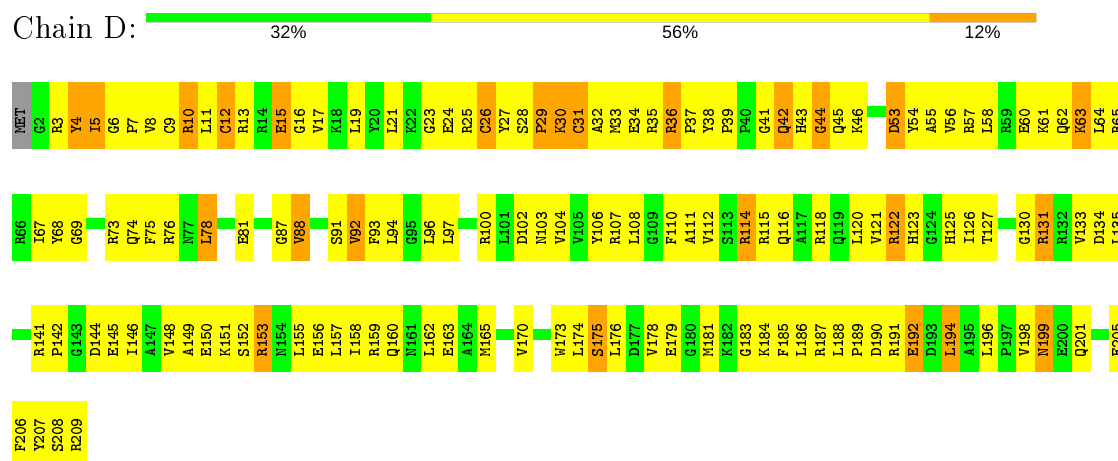
- Molecule 3: 30S RIBOSOMAL PROTEIN S2



● Molecule 4: 30S RIBOSOMAL PROTEIN S3



● Molecule 5: 30S RIBOSOMAL PROTEIN S4



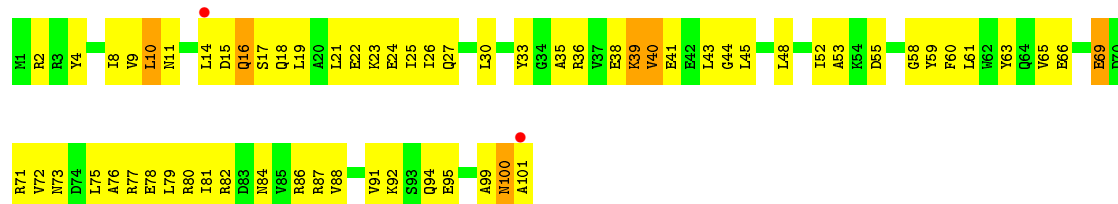
- Molecule 6: 30S RIBOSOMAL PROTEIN S5

Chain E: 




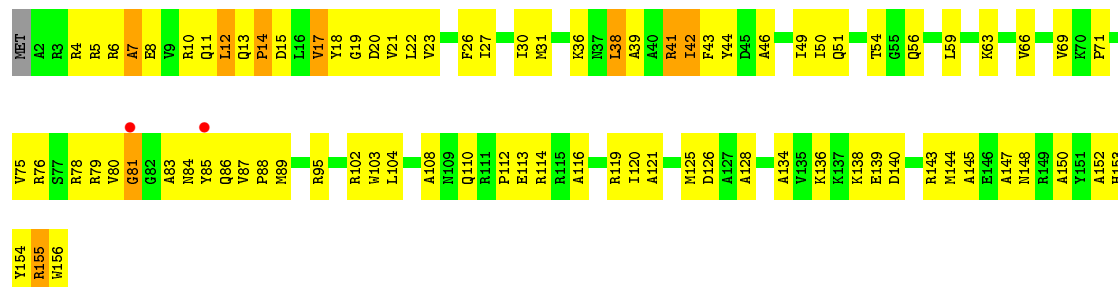
• Molecule 7: 30S RIBOSOMAL PROTEIN S6

Chain F: 



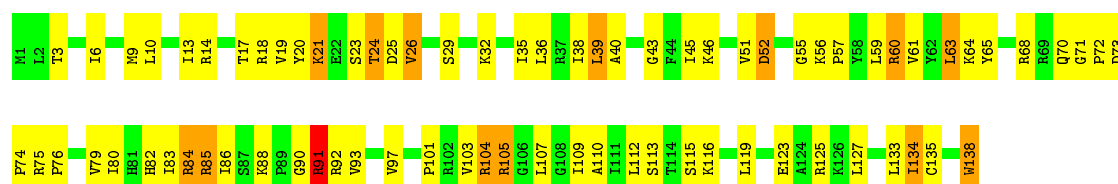
• Molecule 8: 30S RIBOSOMAL PROTEIN S7

Chain G: 



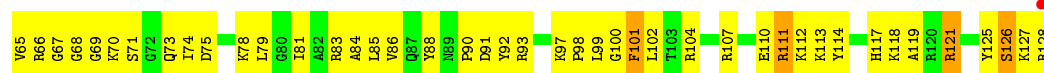
• Molecule 9: 30S RIBOSOMAL PROTEIN S8

Chain H: 

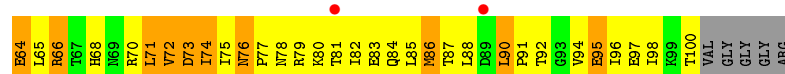
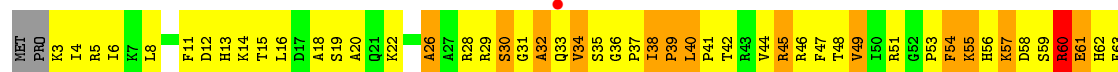
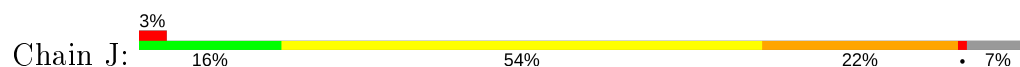


• Molecule 10: 30S RIBOSOMAL PROTEIN S9

Chain I: 



• Molecule 11: 30S RIBOSOMAL PROTEIN S10



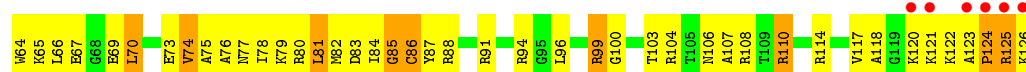
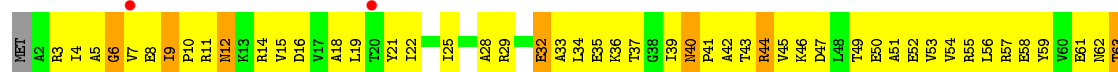
• Molecule 12: 30S RIBOSOMAL PROTEIN S11



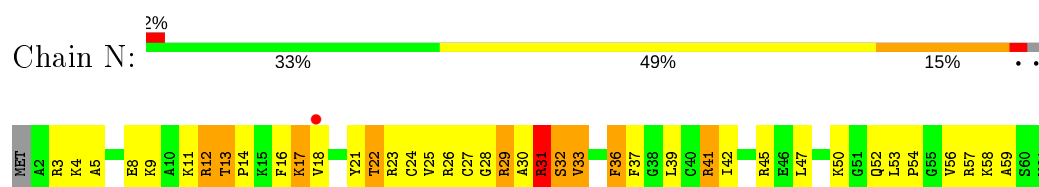
• Molecule 13: 30S RIBOSOMAL PROTEIN S12



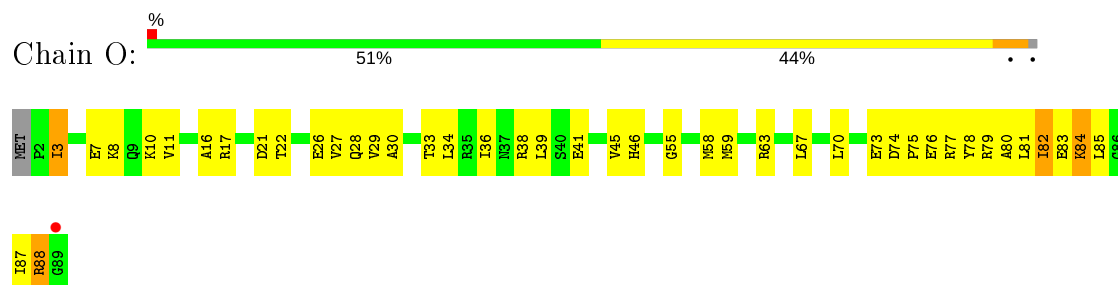
• Molecule 14: 30S RIBOSOMAL PROTEIN S13



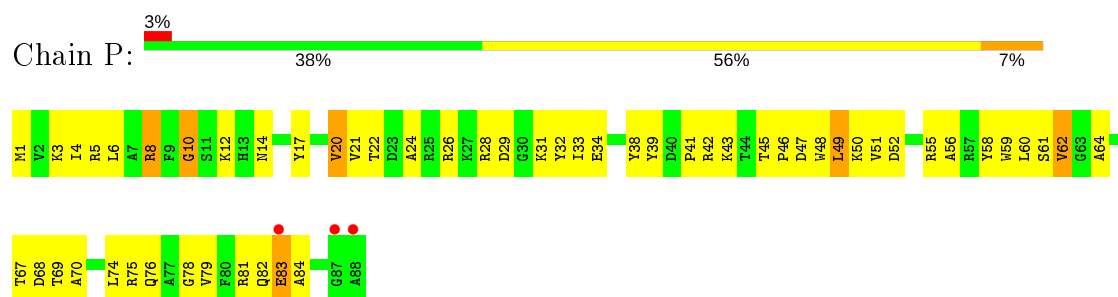
• Molecule 15: 30S RIBOSOMAL PROTEIN S14



• Molecule 16: 30S RIBOSOMAL PROTEIN S15



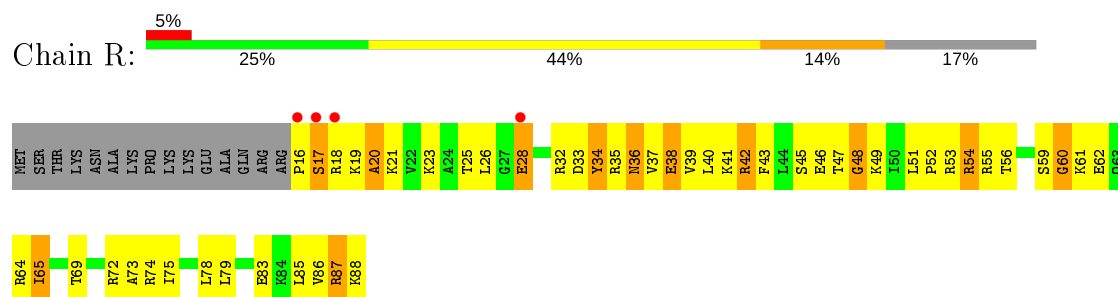
• Molecule 17: 30S RIBOSOMAL PROTEIN S16



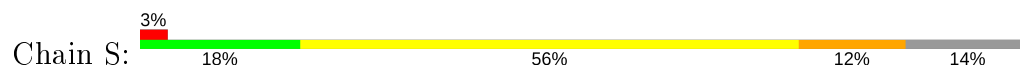
• Molecule 18: 30S RIBOSOMAL PROTEIN S17

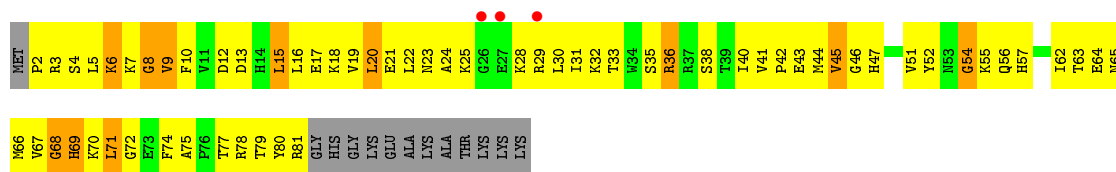


• Molecule 19: 30S RIBOSOMAL PROTEIN S18

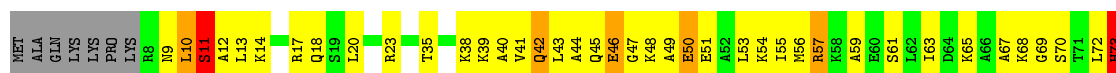


• Molecule 20: 30S RIBOSOMAL PROTEIN S19

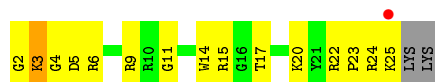




• Molecule 21: 30S RIBOSOMAL PROTEIN S20



• Molecule 22: 30S 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	401.16Å 401.16Å 176.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.40 29.64 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.75-3.40) 83.7 (29.64-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.264 0.197 , 0.239	Depositor DCC
R_{free} test set	12235 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	51934	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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, MG, TAC

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	0/36259	0.76	47/56593 (0.1%)
2	X	0.54	0/128	0.69	0/196
3	B	0.38	0/1935	0.68	0/2609
4	C	0.38	0/1636	0.67	0/2205
5	D	0.42	0/1733	0.68	1/2318 (0.0%)
6	E	0.47	0/1162	0.78	1/1564 (0.1%)
7	F	0.34	0/856	0.64	0/1154
8	G	0.37	0/1276	0.63	0/1709
9	H	0.46	0/1136	0.75	0/1527
10	I	0.36	0/1029	0.65	0/1378
11	J	0.38	0/805	0.70	0/1082
12	K	0.39	0/900	0.71	0/1213
13	L	0.44	0/986	0.78	1/1320 (0.1%)
14	M	0.35	0/1008	0.64	0/1347
15	N	0.44	0/501	0.76	0/664
16	O	0.36	0/745	0.62	0/992
17	P	0.44	0/751	0.76	0/1008
18	Q	0.47	0/870	0.78	0/1159
19	R	0.38	0/603	0.64	0/799
20	S	0.34	0/661	0.72	1/890 (0.1%)
21	T	0.40	0/764	0.73	0/1006
22	V	0.47	0/212	0.73	0/277
All	All	0.47	0/55956	0.74	51/83010 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	50

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	10.26	132.07	109.50
1	A	1085	U	C2'-C3'-O3'	9.36	130.08	109.50
1	A	559	A	C2'-C3'-O3'	9.22	129.78	109.50
1	A	181	G	C2'-C3'-O3'	9.18	129.70	109.50
1	A	1528	U	C2'-C3'-O3'	8.97	129.24	109.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1085	U	C3'
1	A	1498	U	C3'
1	A	1528	U	C3'

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	G	Sidechain
1	A	108	G	Sidechain
1	A	12	U	Sidechain
1	A	37	U	Sidechain
1	A	77	G	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32391	0	16349	1178	0
2	X	117	0	64	0	0
3	B	1900	0	1951	258	1
4	C	1612	0	1677	236	0
5	D	1703	0	1764	173	0
6	E	1146	0	1207	120	0
7	F	843	0	857	80	0
8	G	1257	0	1296	90	0
9	H	1116	0	1177	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	1011	0	1043	135	0
11	J	792	0	835	138	0
12	K	885	0	904	60	0
13	L	970	0	1057	98	0
14	M	997	0	1072	119	0
15	N	492	0	529	62	0
16	O	734	0	771	52	0
17	P	735	0	752	71	0
18	Q	857	0	930	72	0
19	R	597	0	668	89	0
20	S	647	0	673	89	0
21	T	762	0	859	80	0
22	V	208	0	221	22	0
23	A	94	0	0	0	0
23	D	1	0	0	0	0
23	H	1	0	0	0	0
24	A	64	0	45	4	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
All	All	51934	0	36701	3016	1

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 34.

The worst 5 of 3016 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)
4:C:94:LEU:HD23	4:C:95:THR:HG23	1.27	1.16
1:A:1443:G:H5''	1:A:1446:A:H5'	1.21	1.12
13:L:41:ARG:HG2	13:L:42:THR:H	1.03	1.12
5:D:36:ARG:H	5:D:37:PRO:HD3	1.09	1.11
3:B:77:ALA:HB2	3:B:211:ILE:HD13	1.26	1.11

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:157:ARG:NH1	3:B:157:ARG:NH1[7_555]	1.76	0.44

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	232/256 (91%)	161 (69%)	41 (18%)	30 (13%)	0	2
4	C	204/239 (85%)	131 (64%)	45 (22%)	28 (14%)	0	1
5	D	206/209 (99%)	158 (77%)	30 (15%)	18 (9%)	1	5
6	E	148/162 (91%)	131 (88%)	13 (9%)	4 (3%)	5	26
7	F	99/101 (98%)	82 (83%)	15 (15%)	2 (2%)	7	30
8	G	153/156 (98%)	105 (69%)	37 (24%)	11 (7%)	1	7
9	H	136/138 (99%)	115 (85%)	18 (13%)	3 (2%)	6	29
10	I	125/128 (98%)	87 (70%)	29 (23%)	9 (7%)	1	7
11	J	96/105 (91%)	57 (59%)	23 (24%)	16 (17%)	0	0
12	K	117/129 (91%)	84 (72%)	19 (16%)	14 (12%)	0	3
13	L	122/135 (90%)	94 (77%)	18 (15%)	10 (8%)	1	5
14	M	123/126 (98%)	84 (68%)	27 (22%)	12 (10%)	0	4
15	N	58/61 (95%)	41 (71%)	10 (17%)	7 (12%)	0	2
16	O	86/89 (97%)	69 (80%)	13 (15%)	4 (5%)	2	15
17	P	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	21
18	Q	102/105 (97%)	81 (79%)	13 (13%)	8 (8%)	1	6
19	R	71/88 (81%)	47 (66%)	19 (27%)	5 (7%)	1	7
20	S	78/93 (84%)	56 (72%)	15 (19%)	7 (9%)	1	4
21	T	97/106 (92%)	62 (64%)	22 (23%)	13 (13%)	0	1
22	V	22/26 (85%)	18 (82%)	3 (14%)	1 (4%)	2	16
All	All	2361/2540 (93%)	1728 (73%)	428 (18%)	205 (9%)	1	5

5 of 205 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	8	LYS

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Mol	Chain	Res	Type
3	B	15	VAL
3	B	16	HIS
3	B	17	PHE
3	B	21	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	
3	B	202/220 (92%)	173 (86%)	29 (14%)	3	13
4	C	160/188 (85%)	137 (86%)	23 (14%)	3	13
5	D	180/181 (99%)	168 (93%)	12 (7%)	16	46
6	E	115/123 (94%)	99 (86%)	16 (14%)	3	13
7	F	90/90 (100%)	86 (96%)	4 (4%)	28	58
8	G	126/127 (99%)	120 (95%)	6 (5%)	25	56
9	H	119/119 (100%)	103 (87%)	16 (13%)	4	15
10	I	98/99 (99%)	87 (89%)	11 (11%)	6	22
11	J	87/92 (95%)	77 (88%)	10 (12%)	5	20
12	K	90/99 (91%)	84 (93%)	6 (7%)	16	46
13	L	104/111 (94%)	96 (92%)	8 (8%)	13	40
14	M	100/101 (99%)	91 (91%)	9 (9%)	9	32
15	N	49/50 (98%)	45 (92%)	4 (8%)	11	37
16	O	79/80 (99%)	77 (98%)	2 (2%)	47	72
17	P	74/74 (100%)	70 (95%)	4 (5%)	22	52
18	Q	96/97 (99%)	91 (95%)	5 (5%)	23	53
19	R	64/77 (83%)	57 (89%)	7 (11%)	6	23
20	S	71/80 (89%)	68 (96%)	3 (4%)	30	59
21	T	76/82 (93%)	67 (88%)	9 (12%)	5	19
22	V	19/21 (90%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1999/2111 (95%)	1815 (91%)	184 (9%)	9 31

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	F	100	ASN
9	H	105	ARG
19	R	54	ARG
8	G	11	GLN
9	H	52	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
7	F	57	GLN
8	G	106	GLN
18	Q	26	GLN
7	F	73	ASN
7	F	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	218 (14%)	89 (5%)
2	X	5/6 (83%)	0	0
All	All	1512/1528 (98%)	218 (14%)	89 (5%)

5 of 218 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A

5 of 89 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C

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Mol	Chain	Res	Type
1	A	960	U
1	A	1364	U
1	A	733	A
1	A	819	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 98 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	TAC	A	1633	-	33,35,35	4.51	26 (78%)	42,58,58	1.22	5 (11%)
24	TAC	A	1632	23	33,35,35	2.66	18 (54%)	42,58,58	0.99	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	TAC	A	1633	-	-	4/8/74/74	0/4/4/4
24	TAC	A	1632	23	-	0/8/74/74	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1633	TAC	C1C-C12	10.96	1.61	1.52
24	A	1633	TAC	C6-C61	10.45	1.61	1.53
24	A	1633	TAC	C1C-C41	8.60	1.60	1.53
24	A	1633	TAC	C4-C3	5.95	1.63	1.51
24	A	1633	TAC	C4-N4	5.92	1.60	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1633	TAC	C42-N4-C4	3.41	122.11	114.09
24	A	1633	TAC	O21-C21-N21	-2.73	116.50	122.88
24	A	1633	TAC	O1C-C1C-C1	-2.40	99.37	106.40
24	A	1632	TAC	C21-C2-C1	2.28	123.66	120.97
24	A	1633	TAC	O21-C21-C2	2.27	124.57	120.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1633	TAC	C3-C4-N4-C42
24	A	1633	TAC	C3-C4-N4-C43
24	A	1633	TAC	C41-C4-N4-C43
24	A	1633	TAC	C41-C4-N4-C42

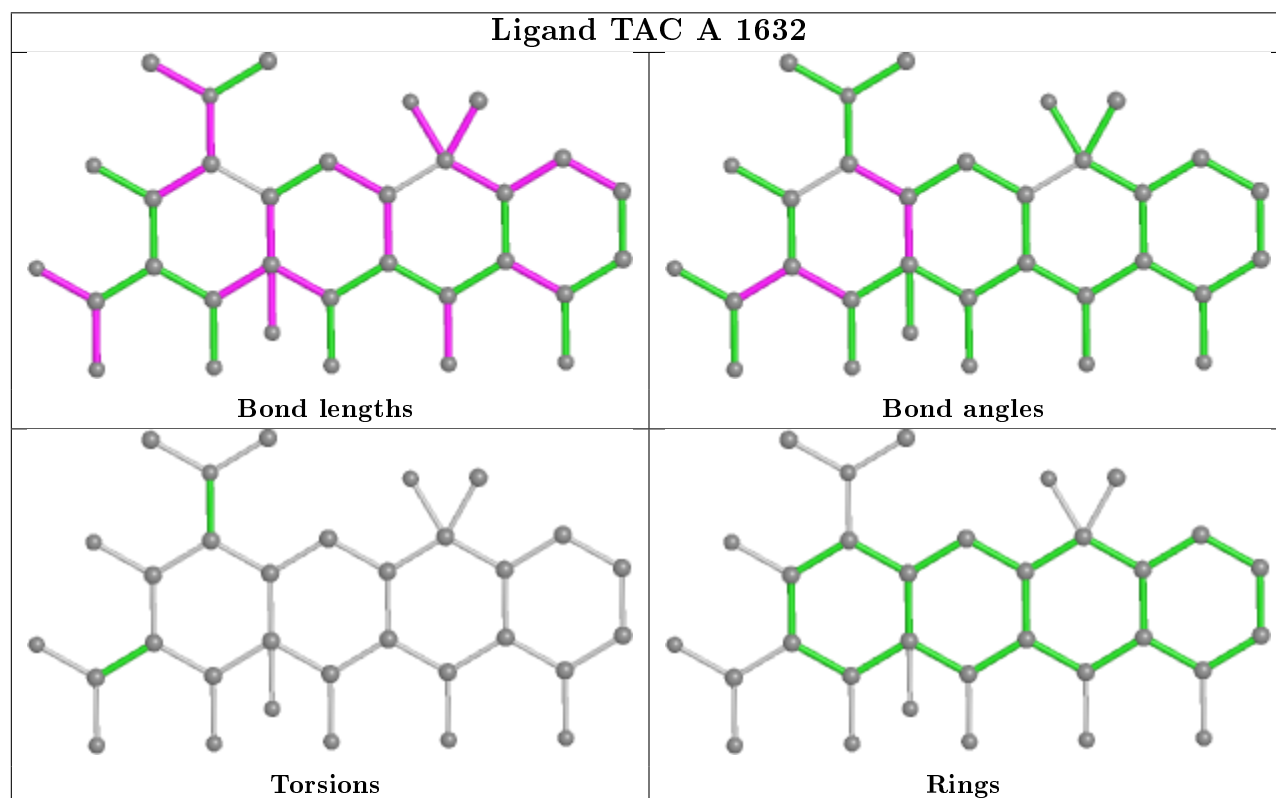
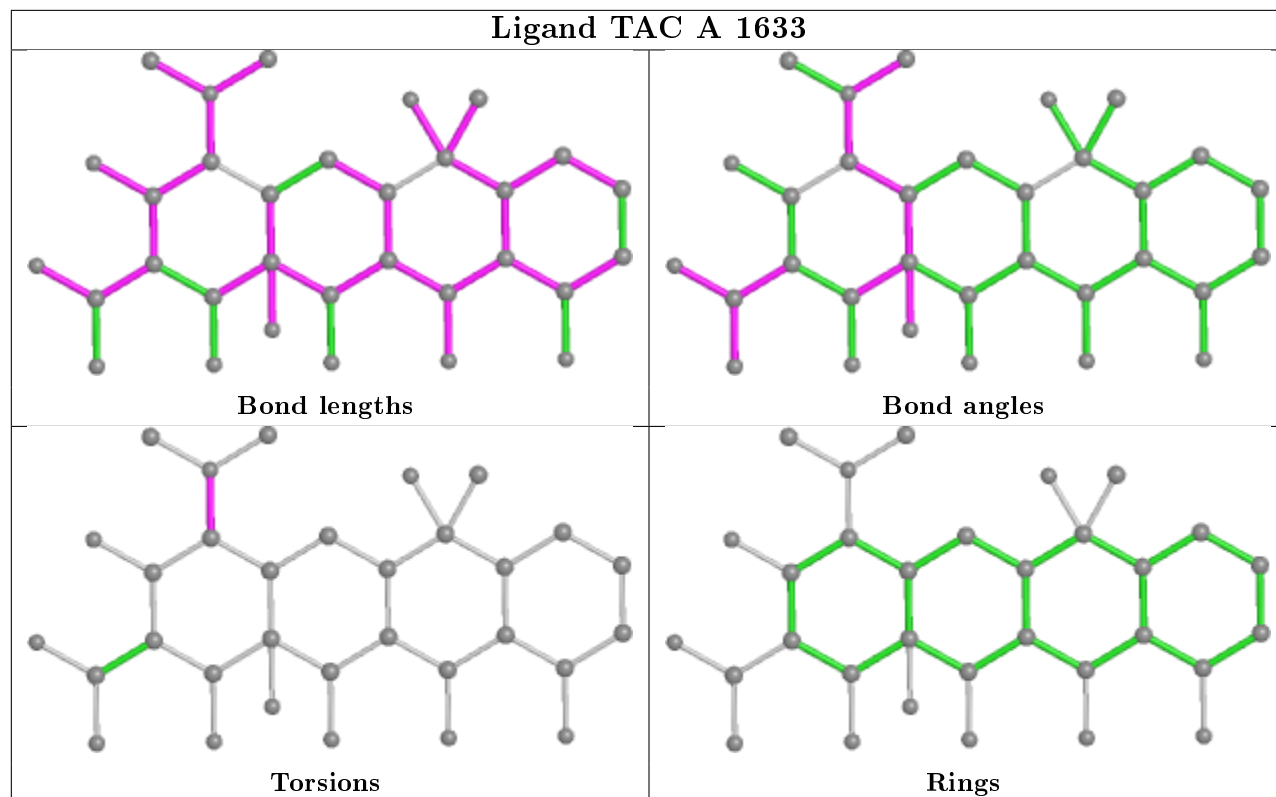
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1633	TAC	3	0
24	A	1632	TAC	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 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	1506/1522 (98%)	0.32	75 (4%) 28 29	28, 61, 137, 198	0
2	X	6/6 (100%)	1.06	2 (33%) 0 0	49, 60, 101, 115	0
3	B	234/256 (91%)	-0.06	11 (4%) 31 31	29, 83, 142, 189	0
4	C	206/239 (86%)	-0.21	0 100 100	41, 81, 136, 152	0
5	D	208/209 (99%)	-0.26	0 100 100	34, 65, 117, 161	0
6	E	150/162 (92%)	-0.37	0 100 100	30, 52, 100, 154	0
7	F	101/101 (100%)	-0.13	2 (1%) 65 64	52, 87, 135, 168	0
8	G	155/156 (99%)	-0.22	2 (1%) 77 76	34, 75, 132, 187	0
9	H	138/138 (100%)	-0.37	0 100 100	22, 48, 84, 137	0
10	I	127/128 (99%)	-0.19	1 (0%) 86 85	37, 86, 126, 152	0
11	J	98/105 (93%)	0.08	3 (3%) 49 48	47, 106, 168, 186	0
12	K	119/129 (92%)	-0.29	2 (1%) 70 68	33, 64, 111, 178	0
13	L	124/135 (91%)	-0.22	1 (0%) 86 85	17, 64, 108, 156	0
14	M	125/126 (99%)	0.16	8 (6%) 19 20	43, 80, 146, 194	0
15	N	60/61 (98%)	-0.08	1 (1%) 70 68	47, 77, 127, 153	0
16	O	88/89 (98%)	-0.25	1 (1%) 80 79	32, 66, 126, 186	0
17	P	88/88 (100%)	-0.08	3 (3%) 45 44	32, 55, 144, 198	0
18	Q	104/105 (99%)	0.11	5 (4%) 30 31	29, 58, 126, 198	0
19	R	73/88 (82%)	0.00	4 (5%) 25 25	42, 69, 143, 187	0
20	S	80/93 (86%)	0.18	3 (3%) 40 39	64, 100, 151, 189	0
21	T	99/106 (93%)	-0.22	1 (1%) 82 81	36, 65, 110, 161	0
22	V	24/26 (92%)	-0.28	1 (4%) 36 35	36, 71, 104, 118	0
All	All	3913/4068 (96%)	0.03	126 (3%) 47 46	17, 67, 138, 198	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Q	103	GLY	13.4
18	Q	105	ALA	13.1
18	Q	104	LYS	12.0
18	Q	102	GLY	9.8
14	M	124	PRO	9.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
23	MG	A	1550	1/1	0.35	0.84	35,35,35,35	1
23	MG	A	211	1/1	0.53	0.36	35,35,35,35	0
23	MG	A	1623	1/1	0.67	0.20	35,35,35,35	1
23	MG	A	1612	1/1	0.69	0.40	35,35,35,35	1
23	MG	A	1608	1/1	0.70	0.76	35,35,35,35	1
23	MG	A	1622	1/1	0.70	0.71	35,35,35,35	1
23	MG	A	1584	1/1	0.71	0.33	35,35,35,35	1
23	MG	A	1613	1/1	0.71	0.30	35,35,35,35	1
23	MG	A	1566	1/1	0.75	0.23	35,35,35,35	0
23	MG	A	1617	1/1	0.77	0.30	35,35,35,35	1
23	MG	A	1549	1/1	0.77	0.15	35,35,35,35	1
23	MG	A	1548	1/1	0.77	0.47	35,35,35,35	0
23	MG	A	1603	1/1	0.77	0.18	35,35,35,35	1
23	MG	A	210	1/1	0.80	0.32	35,35,35,35	1
23	MG	A	1628	1/1	0.80	0.73	35,35,35,35	1
23	MG	A	1611	1/1	0.80	0.41	35,35,35,35	1
23	MG	H	213	1/1	0.81	0.59	35,35,35,35	1
23	MG	A	1580	1/1	0.83	0.26	35,35,35,35	0
23	MG	A	1610	1/1	0.83	0.12	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	D	215	1/1	0.83	0.17	35,35,35,35	1
24	TAC	A	1633	32/32	0.84	0.37	19,19,19,19	0
23	MG	A	1596	1/1	0.86	0.16	35,35,35,35	0
23	MG	A	1609	1/1	0.86	0.34	35,35,35,35	1
23	MG	A	1563	1/1	0.88	0.09	35,35,35,35	0
23	MG	A	1581	1/1	0.88	0.50	35,35,35,35	1
23	MG	A	1591	1/1	0.88	0.17	35,35,35,35	0
23	MG	A	1568	1/1	0.89	0.35	35,35,35,35	0
23	MG	A	1607	1/1	0.89	0.35	35,35,35,35	0
23	MG	A	1575	1/1	0.89	0.30	35,35,35,35	1
23	MG	A	1560	1/1	0.90	0.17	35,35,35,35	0
23	MG	A	1618	1/1	0.90	0.17	35,35,35,35	1
23	MG	A	212	1/1	0.90	1.45	35,35,35,35	1
23	MG	A	1559	1/1	0.91	0.20	35,35,35,35	0
23	MG	A	1589	1/1	0.91	0.16	35,35,35,35	0
23	MG	A	1598	1/1	0.91	0.12	35,35,35,35	0
23	MG	A	1605	1/1	0.92	0.14	35,35,35,35	0
23	MG	A	1555	1/1	0.92	0.66	35,35,35,35	0
23	MG	A	1614	1/1	0.92	1.37	35,35,35,35	1
24	TAC	A	1632	32/32	0.92	0.26	19,19,19,19	0
23	MG	A	1619	1/1	0.92	0.26	35,35,35,35	0
23	MG	A	1600	1/1	0.92	0.26	35,35,35,35	1
23	MG	A	1551	1/1	0.92	0.72	35,35,35,35	0
23	MG	A	1545	1/1	0.92	0.12	35,35,35,35	1
23	MG	A	1570	1/1	0.92	0.18	35,35,35,35	1
23	MG	A	1554	1/1	0.92	0.62	35,35,35,35	0
23	MG	A	1567	1/1	0.93	0.36	35,35,35,35	0
23	MG	A	1579	1/1	0.93	0.22	35,35,35,35	0
23	MG	A	71	1/1	0.93	0.20	35,35,35,35	0
23	MG	A	1626	1/1	0.93	0.34	35,35,35,35	1
23	MG	A	1586	1/1	0.94	0.17	35,35,35,35	0
23	MG	A	1621	1/1	0.94	0.60	35,35,35,35	1
23	MG	A	1602	1/1	0.94	0.39	35,35,35,35	0
23	MG	A	1562	1/1	0.94	0.42	35,35,35,35	0
23	MG	A	1595	1/1	0.94	0.28	35,35,35,35	1
23	MG	A	1588	1/1	0.95	0.26	35,35,35,35	0
23	MG	A	1561	1/1	0.95	0.24	35,35,35,35	0
23	MG	A	1587	1/1	0.95	0.31	35,35,35,35	0
23	MG	A	1593	1/1	0.95	0.40	35,35,35,35	0
23	MG	A	1625	1/1	0.95	0.33	35,35,35,35	0
23	MG	A	1556	1/1	0.95	0.28	35,35,35,35	1
23	MG	A	1572	1/1	0.95	0.47	35,35,35,35	0

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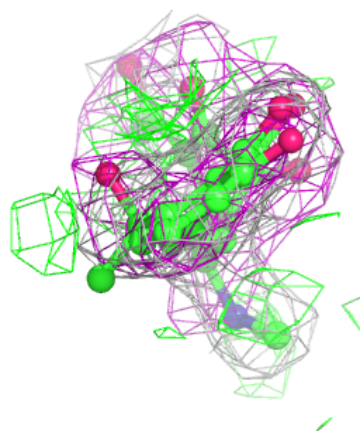
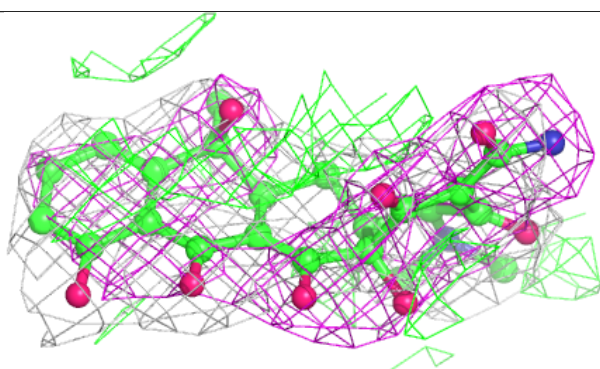
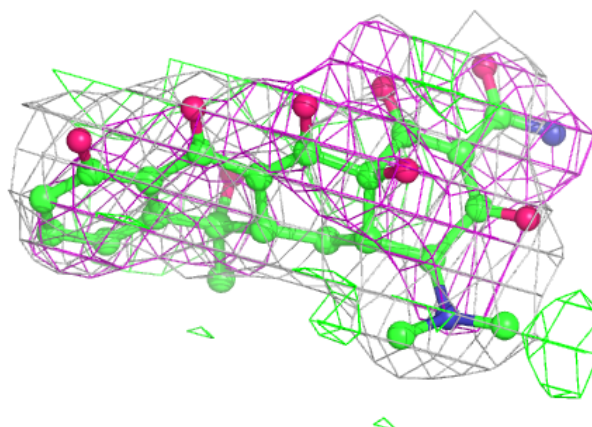
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1577	1/1	0.95	0.24	35,35,35,35	0
23	MG	A	214	1/1	0.95	0.21	35,35,35,35	0
23	MG	A	1631	1/1	0.95	0.06	23,23,23,23	0
23	MG	A	1590	1/1	0.96	0.45	35,35,35,35	0
23	MG	A	1597	1/1	0.96	0.16	35,35,35,35	1
23	MG	A	1585	1/1	0.96	0.29	35,35,35,35	0
23	MG	A	1564	1/1	0.96	0.16	35,35,35,35	0
23	MG	A	1616	1/1	0.96	0.20	35,35,35,35	1
23	MG	A	1592	1/1	0.96	0.31	35,35,35,35	0
23	MG	A	1601	1/1	0.96	0.55	35,35,35,35	0
23	MG	A	1558	1/1	0.96	0.41	35,35,35,35	0
23	MG	A	1576	1/1	0.96	0.43	35,35,35,35	0
23	MG	A	1547	1/1	0.97	0.61	35,35,35,35	0
23	MG	A	1578	1/1	0.97	0.13	35,35,35,35	0
23	MG	A	1582	1/1	0.97	0.23	35,35,35,35	0
23	MG	A	1606	1/1	0.97	0.82	35,35,35,35	0
23	MG	A	1630	1/1	0.97	0.64	35,35,35,35	1
23	MG	A	1546	1/1	0.97	0.50	35,35,35,35	0
23	MG	A	1557	1/1	0.97	0.53	35,35,35,35	0
23	MG	A	87	1/1	0.97	0.32	35,35,35,35	1
23	MG	A	1615	1/1	0.97	0.30	35,35,35,35	0
23	MG	A	1553	1/1	0.97	0.58	35,35,35,35	0
23	MG	A	1574	1/1	0.97	0.29	35,35,35,35	0
23	MG	A	1569	1/1	0.97	0.34	35,35,35,35	1
23	MG	A	1599	1/1	0.97	0.71	35,35,35,35	0
23	MG	A	1571	1/1	0.97	0.54	35,35,35,35	0
23	MG	A	86	1/1	0.98	0.52	35,35,35,35	0
23	MG	A	1565	1/1	0.98	0.44	35,35,35,35	0
23	MG	A	1573	1/1	0.98	0.28	35,35,35,35	0
23	MG	A	1604	1/1	0.98	0.47	35,35,35,35	0
23	MG	A	1629	1/1	0.98	0.74	35,35,35,35	1
23	MG	A	1552	1/1	0.98	0.20	35,35,35,35	0
23	MG	A	1594	1/1	0.98	0.30	35,35,35,35	0
25	ZN	D	300	1/1	0.99	0.30	44,44,44,44	0
23	MG	A	1627	1/1	0.99	0.24	35,35,35,35	1
23	MG	A	1620	1/1	0.99	0.12	35,35,35,35	1
23	MG	A	1583	1/1	0.99	0.40	35,35,35,35	0
25	ZN	N	190	1/1	0.99	0.14	44,44,44,44	1
23	MG	A	1624	1/1	0.99	0.24	35,35,35,35	1

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.

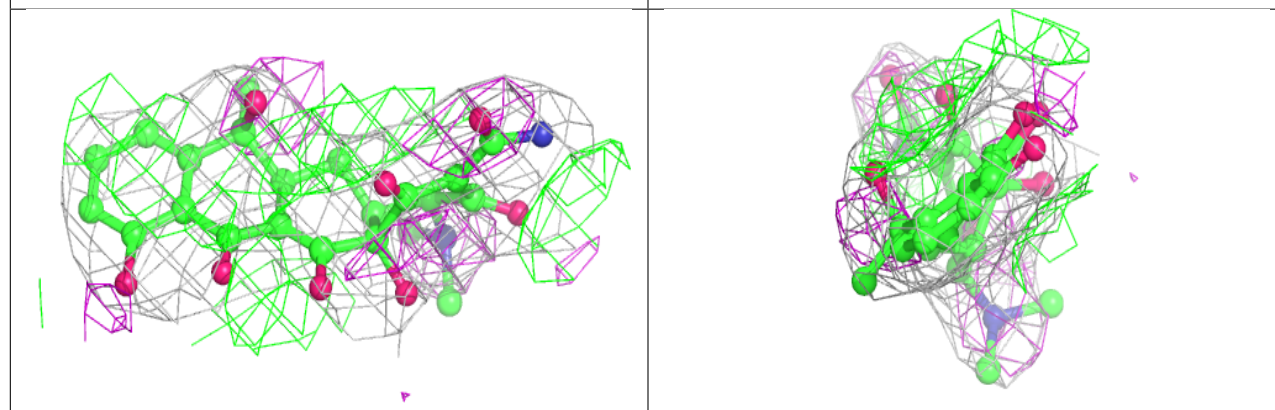
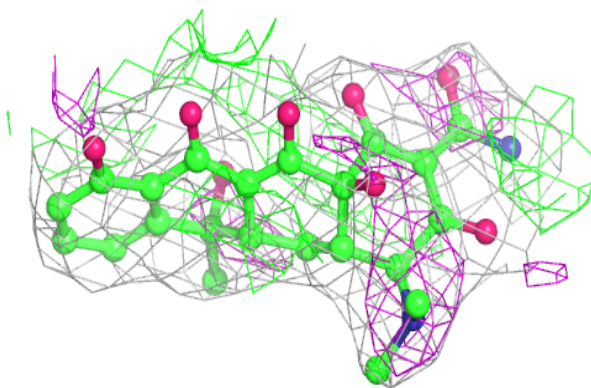
Electron density around TAC A 1633:

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



Electron density around TAC A 1632:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.