



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:46 PM UTC

PDB ID : 1KOG / pdb_00001kog
Title : Crystal structure of E. coli threonyl-tRNA synthetase interacting with the essential domain of its mRNA operator
Authors : Torres-Larrios, A.; Dock-Bregeon, A.C.; Romby, P.; Rees, B.; Sankaranarayanan, R.; Caillet, J.; Springer, M.; Ehresmann, C.; Ehresmann, B.; Moras, D.
Deposited on : 2001-12-20
Resolution : 3.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

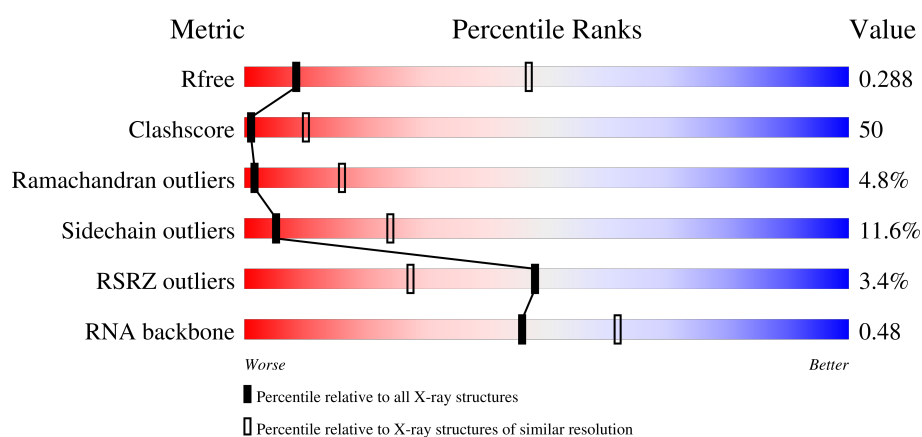
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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 $\leq 5\%$. 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	I	37	11% 32% 38% 22% 8%
1	J	37	5% 16% 54% 16% 14%
1	K	37	35% 14% 54% 16% 16%
1	L	37	3% 27% 43% 19% 11%

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Mol	Chain	Length	Quality of chain
1	M	37	
1	N	37	
1	O	37	
1	P	37	
2	A	401	
2	B	401	
2	C	401	
2	D	401	
2	E	401	
2	F	401	
2	G	401	
2	H	401	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 32922 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 Threonyl-tRNA synthetase mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	J	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	K	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	L	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	M	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	N	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	O	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	P	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			

- Molecule 2 is a protein called Threonyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	B	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	C	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	D	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	E	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	F	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			

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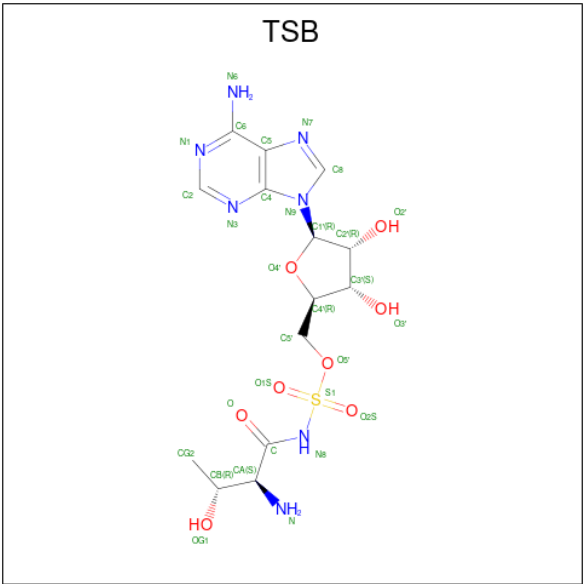
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	H	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 5'-O-(N-(L-THREONYL)-SULFAMOYL)ADENOSINE (CCD ID: TSB) (formula: C₁₄H₂₁N₇O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	B	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	C	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	D	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	E	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	F	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	G	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	H	1	Total 30	C 14	N 7	O 8	S 1	0	0

- Molecule 5 is water.

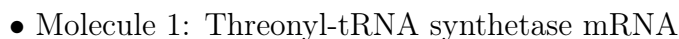
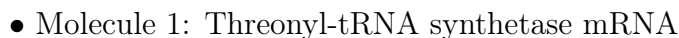
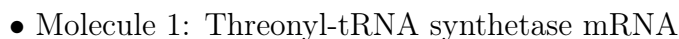
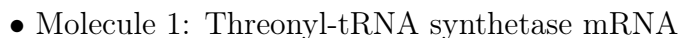
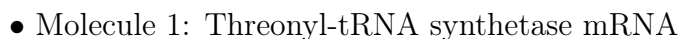
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	11	Total 11	O 11	0	0
5	J	12	Total 12	O 12	0	0
5	K	1	Total 1	O 1	0	0
5	L	8	Total 8	O 8	0	0
5	M	6	Total 6	O 6	0	0
5	N	9	Total 9	O 9	0	0
5	O	11	Total 11	O 11	0	0
5	P	9	Total 9	O 9	0	0
5	A	10	Total 10	O 10	0	0
5	B	15	Total 15	O 15	0	0
5	C	11	Total 11	O 11	0	0
5	D	14	Total 14	O 14	0	0

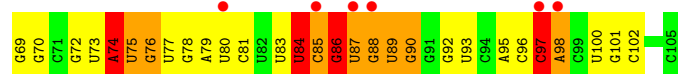
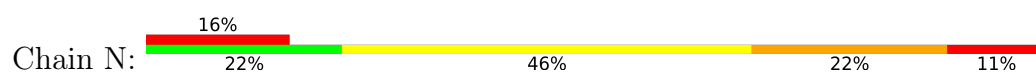
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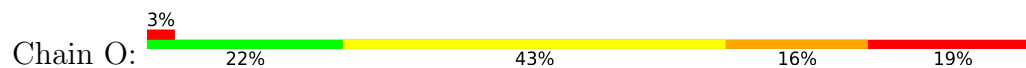
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	11	Total 11	O 11	0	0
5	F	13	Total 13	O 13	0	0
5	G	13	Total 13	O 13	0	0
5	H	16	Total 16	O 16	0	0

- Molecule 1: Threonyl-tRNA synthetase mRNA

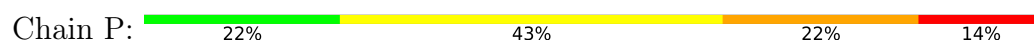




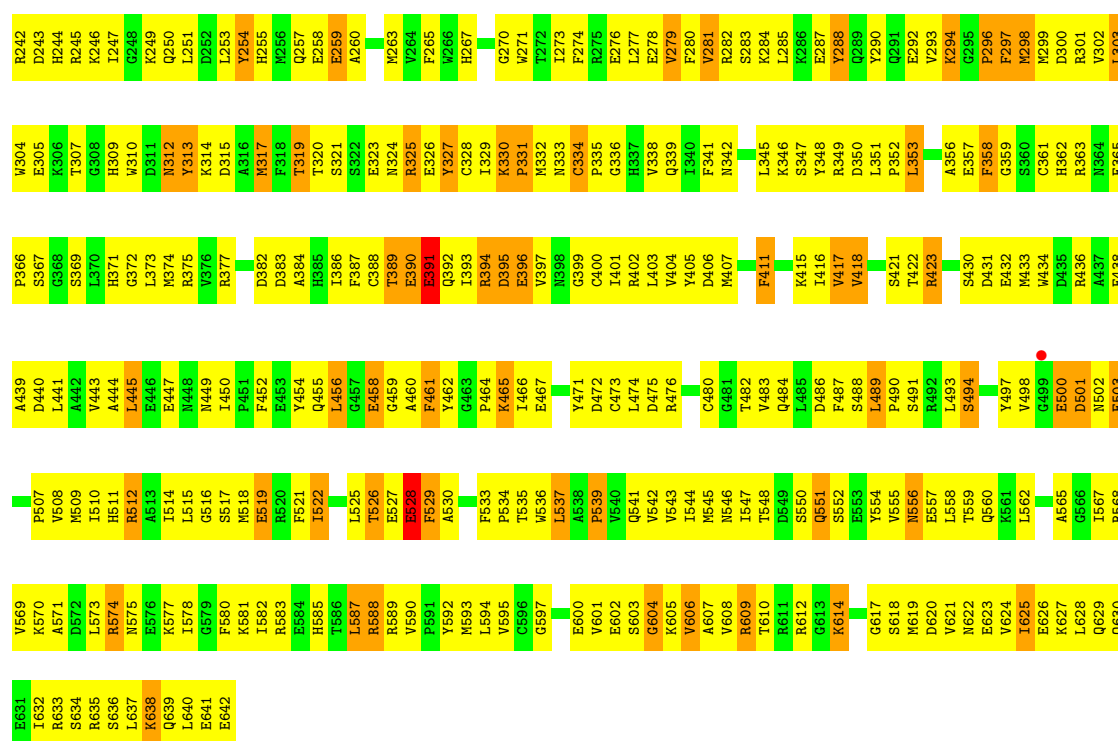
• Molecule 1: Threonyl-tRNA synthetase mRNA



• Molecule 1: Threonyl-tRNA synthetase mRNA

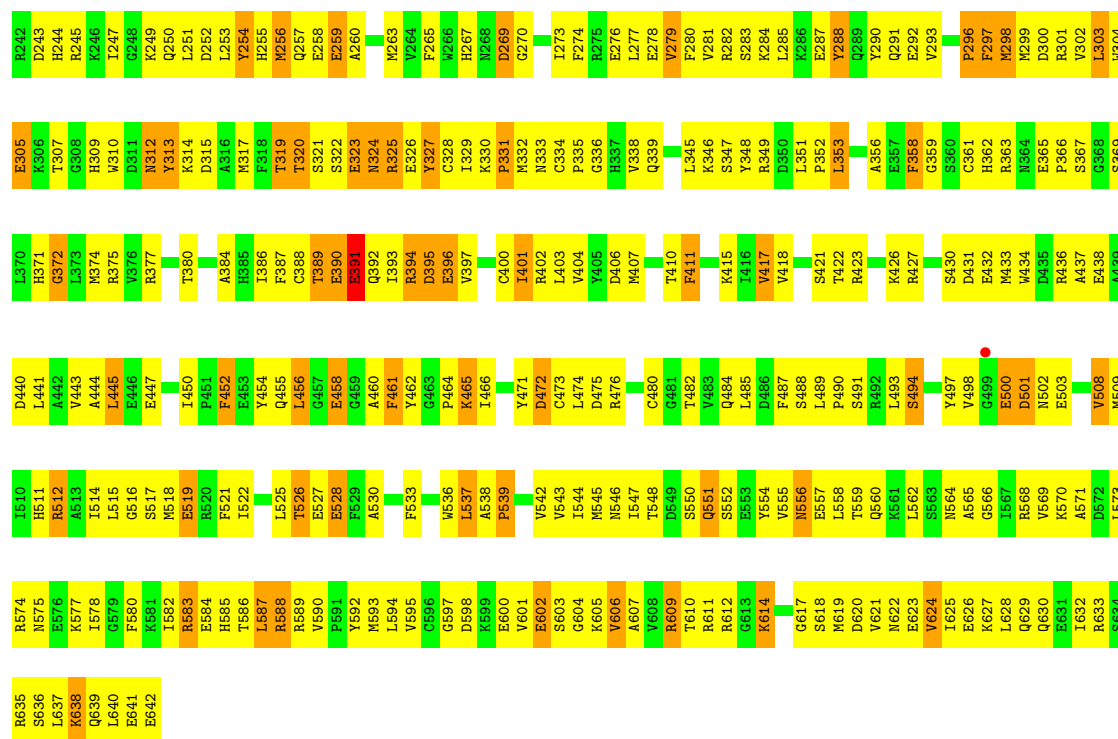


• Molecule 2: Threonyl-tRNA synthetase

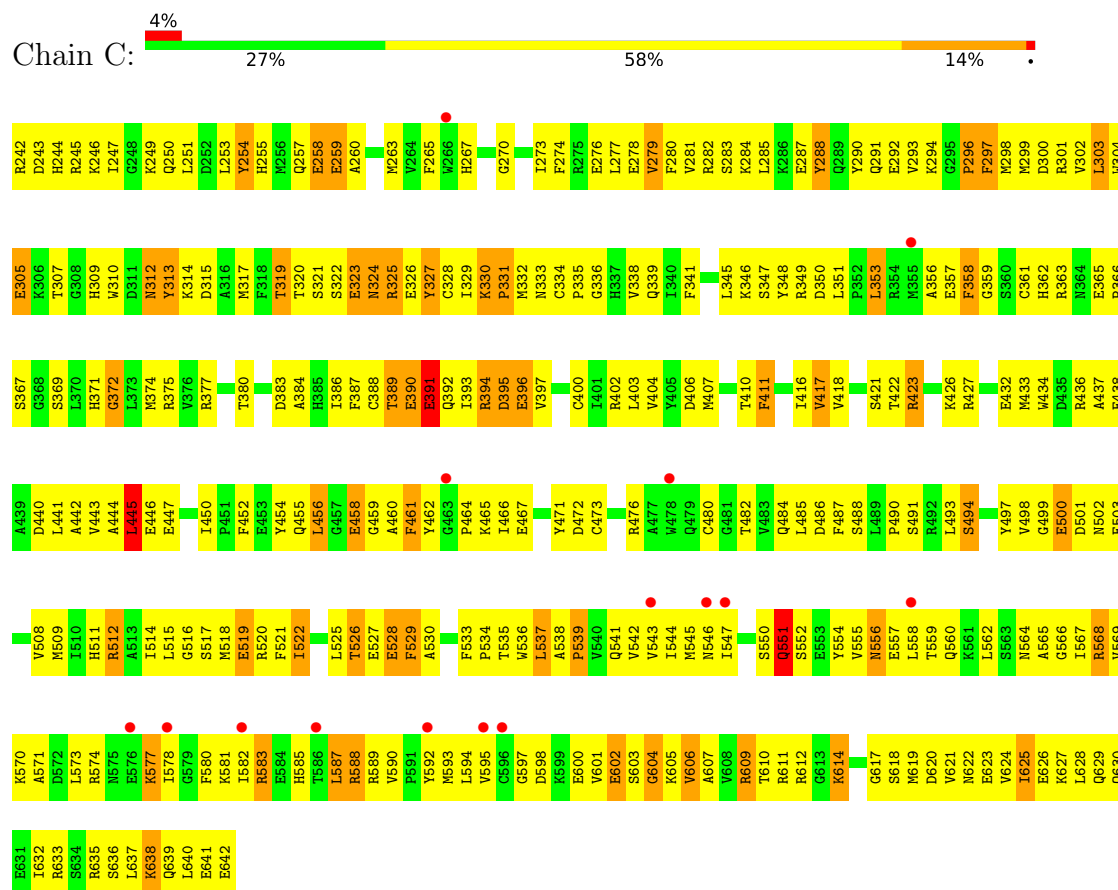


• Molecule 2: Threonyl-tRNA synthetase



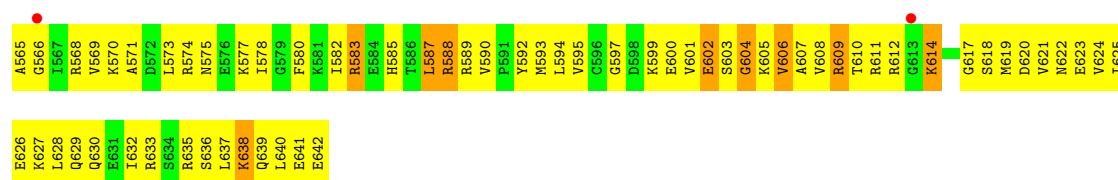


- Molecule 2: Threonyl-tRNA synthetase

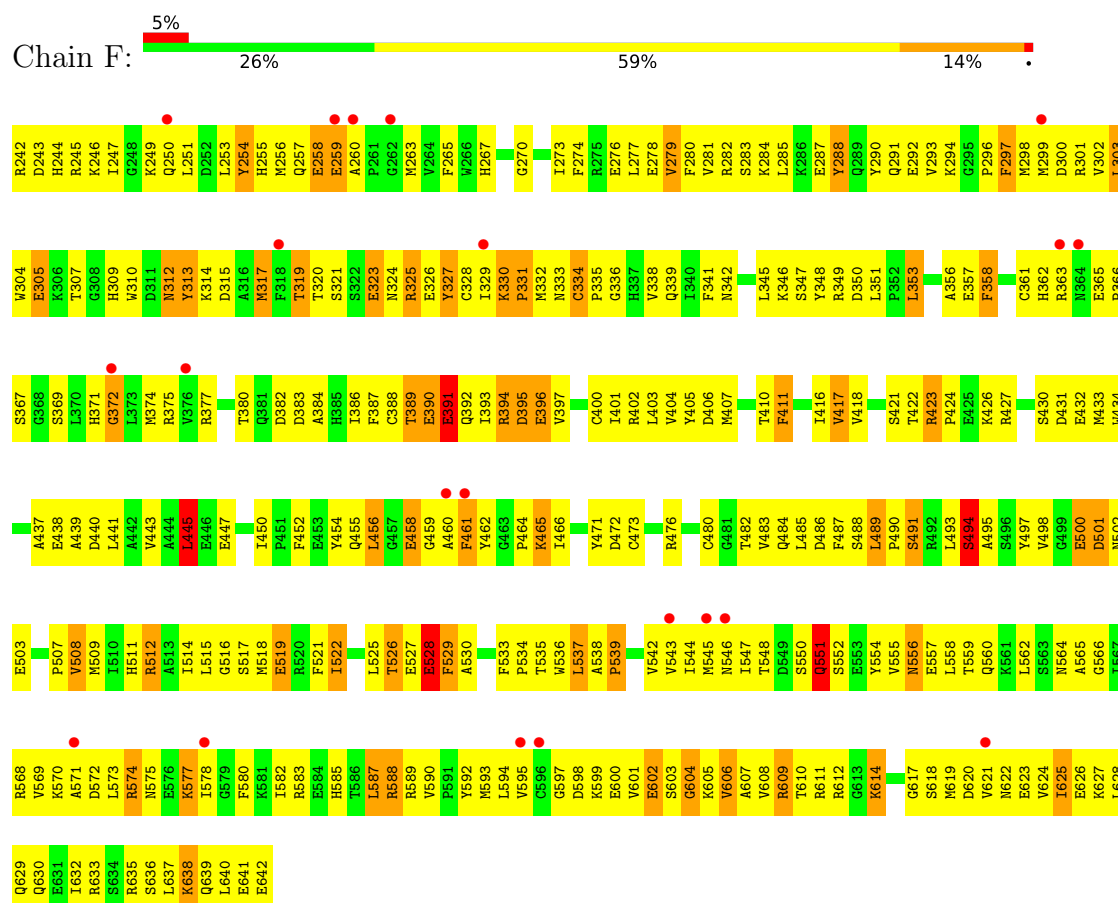


- Molecule 2: Threonyl-tRNA synthetase

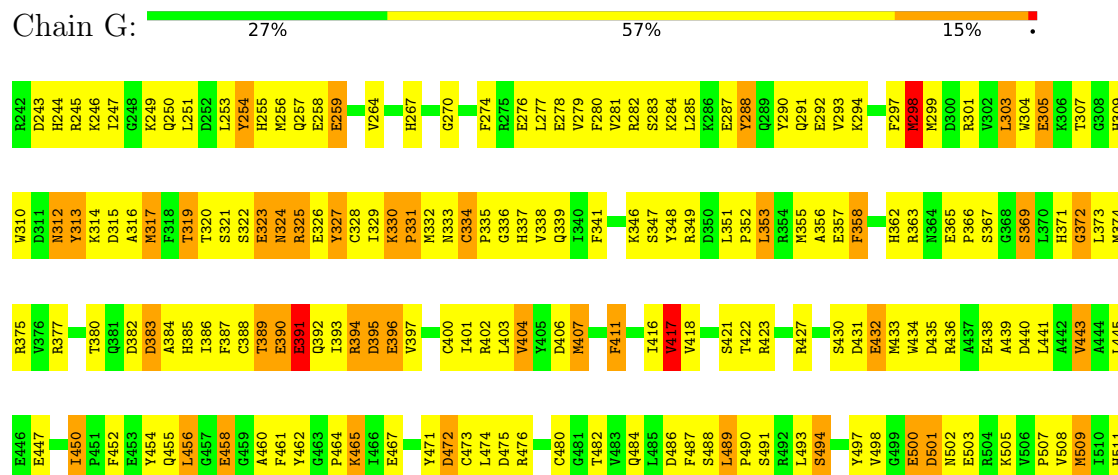


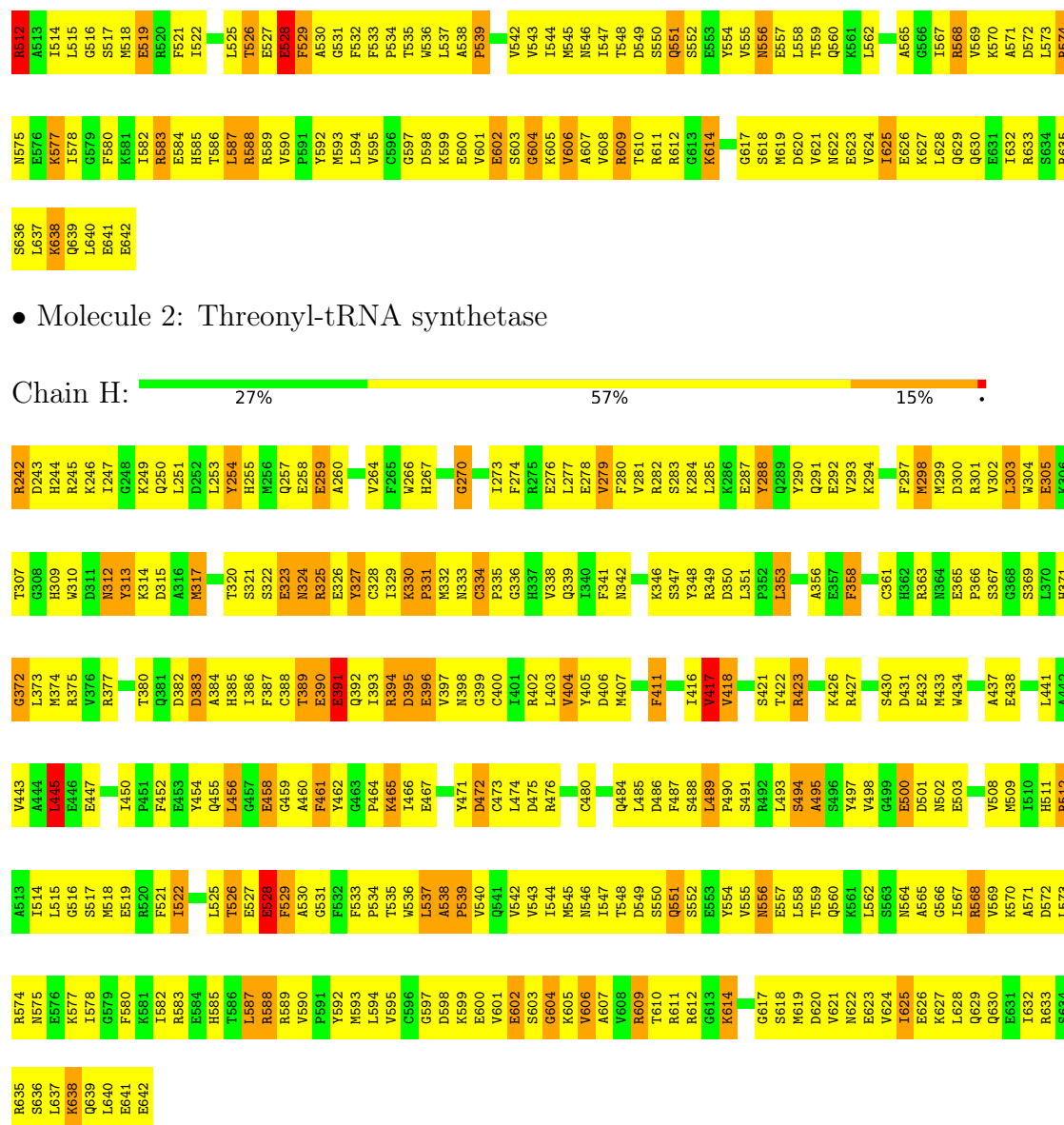


• Molecule 2: Threonyl-tRNA synthetase



• Molecule 2: Threonyl-tRNA synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.45Å 101.74Å 199.34Å 90.00° 114.40° 90.00°	Depositor
Resolution (Å)	29.80 – 3.50 29.80 – 3.50	Depositor EDS
% Data completeness (in resolution range)	90.0 (29.80-3.50) 94.2 (29.80-3.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 3.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.287 0.256 , 0.288	Depositor DCC
R_{free} test set	8671 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å ²)	96.2	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 114.3	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	32922	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, TSB

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	I	0.49	0/874	0.99	7/1358 (0.5%)
1	J	0.56	0/874	1.00	7/1358 (0.5%)
1	K	0.66	0/874	0.98	7/1358 (0.5%)
1	L	0.46	0/874	0.95	6/1358 (0.4%)
1	M	0.53	0/874	1.00	7/1358 (0.5%)
1	N	0.47	0/874	0.88	6/1358 (0.4%)
1	O	0.67	0/874	1.08	9/1358 (0.7%)
1	P	0.51	0/874	1.01	8/1358 (0.6%)
2	A	0.78	2/3349 (0.1%)	1.13	23/4508 (0.5%)
2	B	0.85	3/3349 (0.1%)	1.12	24/4508 (0.5%)
2	C	0.59	0/3349	1.06	21/4508 (0.5%)
2	D	0.55	0/3349	1.06	21/4508 (0.5%)
2	E	0.55	0/3349	1.06	22/4508 (0.5%)
2	F	0.61	0/3349	1.09	23/4508 (0.5%)
2	G	0.97	3/3349 (0.1%)	1.19	24/4508 (0.5%)
2	H	0.78	1/3349 (0.0%)	1.14	29/4508 (0.6%)
All	All	0.69	9/33784 (0.0%)	1.08	244/46928 (0.5%)

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	I	0	2
1	J	0	4
1	K	0	1
1	L	0	3
1	M	0	2
1	N	0	2
1	O	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	3
All	All	0	20

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	407	MET	SD-CE	10.25	2.05	1.79
2	G	509	MET	SD-CE	6.77	1.96	1.79
2	B	256	MET	SD-CE	6.49	1.95	1.79
2	G	355	MET	SD-CE	6.45	1.95	1.79
2	B	269	ASP	CG-OD1	-6.06	1.13	1.25

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	74	A	N9-C1'-C2'	10.28	129.42	114.00
2	B	391	GLU	N-CA-C	-9.50	101.11	112.89
1	L	74	A	N9-C1'-C2'	9.36	126.04	112.00
1	N	74	A	N9-C1'-C2'	9.18	125.77	112.00
1	I	74	A	N9-C1'-C2'	9.18	125.76	112.00

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	74	A	Sidechain
1	I	86	G	Sidechain
1	J	74	A	Sidechain
1	J	86	G	Sidechain
1	J	89	U	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	I	785	0	397	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	785	0	397	53	0
1	K	785	0	397	78	0
1	L	785	0	397	42	0
1	M	785	0	397	73	0
1	N	785	0	397	43	0
1	O	785	0	397	55	0
1	P	785	0	397	65	0
2	A	3278	0	3208	364	0
2	B	3278	0	3208	341	0
2	C	3278	0	3208	356	0
2	D	3278	0	3208	359	0
2	E	3278	0	3208	355	0
2	F	3278	0	3208	367	0
2	G	3278	0	3208	343	0
2	H	3278	0	3208	335	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	30	0	21	3	0
4	B	30	0	20	4	0
4	C	30	0	21	3	0
4	D	30	0	21	4	0
4	E	30	0	21	4	0
4	F	30	0	21	5	0
4	G	30	0	21	4	0
4	H	30	0	21	4	0
5	A	10	0	0	0	0
5	B	15	0	0	8	0
5	C	11	0	0	3	0
5	D	14	0	0	4	0
5	E	11	0	0	5	0
5	F	13	0	0	2	0
5	G	13	0	0	4	0
5	H	16	0	0	3	0
5	I	11	0	0	10	0
5	J	12	0	0	8	0
5	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	8	0	0	3	0
5	M	6	0	0	10	0
5	N	9	0	0	2	0
5	O	11	0	0	9	0
5	P	9	0	0	14	0
All	All	32922	0	29007	3085	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 50.

The worst 5 of 3085 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)
2:G:407:MET:CE	2:G:407:MET:SD	2.05	1.44
2:D:559:THR:HG21	2:D:571:ALA:HB2	1.29	1.15
2:G:559:THR:HG21	2:G:571:ALA:HB2	1.27	1.12
2:E:559:THR:HG21	2:E:571:ALA:HB2	1.30	1.12
2:A:559:THR:HG21	2:A:571:ALA:HB2	1.27	1.11

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	A	399/401 (100%)	327 (82%)	53 (13%)	19 (5%)	2	16
2	B	399/401 (100%)	325 (82%)	57 (14%)	17 (4%)	2	18
2	C	399/401 (100%)	327 (82%)	52 (13%)	20 (5%)	1	15
2	D	399/401 (100%)	327 (82%)	54 (14%)	18 (4%)	2	17
2	E	399/401 (100%)	327 (82%)	55 (14%)	17 (4%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	399/401 (100%)	327 (82%)	52 (13%)	20 (5%)	1	15
2	G	399/401 (100%)	323 (81%)	55 (14%)	21 (5%)	1	14
2	H	399/401 (100%)	323 (81%)	55 (14%)	21 (5%)	1	14
All	All	3192/3208 (100%)	2606 (82%)	433 (14%)	153 (5%)	2	16

5 of 153 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	313	TYR
2	A	324	ASN
2	A	456	LEU
2	A	528	GLU
2	A	574	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	A	356/356 (100%)	313 (88%)	43 (12%)	5	22
2	B	356/356 (100%)	314 (88%)	42 (12%)	5	23
2	C	356/356 (100%)	317 (89%)	39 (11%)	6	26
2	D	356/356 (100%)	314 (88%)	42 (12%)	5	23
2	E	356/356 (100%)	316 (89%)	40 (11%)	6	25
2	F	356/356 (100%)	314 (88%)	42 (12%)	5	23
2	G	356/356 (100%)	315 (88%)	41 (12%)	5	24
2	H	356/356 (100%)	314 (88%)	42 (12%)	5	23
All	All	2848/2848 (100%)	2517 (88%)	331 (12%)	5	24

5 of 331 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	494	SER

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Mol	Chain	Res	Type
2	G	609	ARG
2	F	537	LEU
2	G	334	CYS
2	H	323	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	267	HIS
2	H	585	HIS
2	F	268	ASN
2	H	575	ASN
2	H	257	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	36/37 (97%)	6 (16%)	4 (11%)
1	J	36/37 (97%)	9 (25%)	5 (13%)
1	K	36/37 (97%)	11 (30%)	4 (11%)
1	L	36/37 (97%)	7 (19%)	4 (11%)
1	M	36/37 (97%)	8 (22%)	5 (13%)
1	N	36/37 (97%)	8 (22%)	4 (11%)
1	O	36/37 (97%)	9 (25%)	5 (13%)
1	P	36/37 (97%)	8 (22%)	5 (13%)
All	All	288/296 (97%)	66 (22%)	36 (12%)

5 of 66 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	76	G
1	I	85	C
1	I	86	G
1	I	89	U
1	I	90	G

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	O	84	U

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Continued from previous page...

Mol	Chain	Res	Type
1	P	97	C
1	O	88	G
1	P	75	U
1	K	97	C

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
4	TSB	F	7002	3	32,32,32	1.83	3 (9%)	46,48,48	0.93	5 (10%)
4	TSB	D	5002	3	32,32,32	2.30	4 (12%)	46,48,48	0.75	1 (2%)
4	TSB	E	6002	3	32,32,32	2.43	5 (15%)	46,48,48	0.87	2 (4%)
4	TSB	H	9002	3	32,32,32	2.03	3 (9%)	46,48,48	0.96	3 (6%)
4	TSB	G	8002	3	32,32,32	2.24	3 (9%)	46,48,48	1.18	3 (6%)
4	TSB	B	3002	3	32,32,32	2.69	4 (12%)	46,48,48	0.81	3 (6%)
4	TSB	A	2002	3	32,32,32	1.77	4 (12%)	46,48,48	0.93	3 (6%)
4	TSB	C	4002	3	32,32,32	2.06	4 (12%)	46,48,48	0.87	3 (6%)

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
4	TSB	F	7002	3	-	3/22/39/39	0/3/3/3
4	TSB	D	5002	3	-	4/22/39/39	0/3/3/3
4	TSB	E	6002	3	-	5/22/39/39	0/3/3/3
4	TSB	H	9002	3	-	3/22/39/39	0/3/3/3
4	TSB	G	8002	3	-	3/22/39/39	0/3/3/3
4	TSB	B	3002	3	-	5/22/39/39	0/3/3/3
4	TSB	A	2002	3	-	4/22/39/39	0/3/3/3
4	TSB	C	4002	3	-	3/22/39/39	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3002	TSB	O1S-S1	10.94	1.52	1.42
4	E	6002	TSB	O1S-S1	9.90	1.51	1.42
4	G	8002	TSB	O2S-S1	9.44	1.50	1.42
4	B	3002	TSB	O2S-S1	9.17	1.50	1.42
4	D	5002	TSB	O1S-S1	8.94	1.50	1.42

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	8002	TSB	O-C-CA	-4.64	116.99	120.66
4	G	8002	TSB	C-CA-N	-4.14	104.23	110.31
4	E	6002	TSB	C-CA-N	-4.03	104.40	110.31
4	H	9002	TSB	O-C-CA	-3.69	117.75	120.66
4	B	3002	TSB	C-CA-N	-3.31	105.45	110.31

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

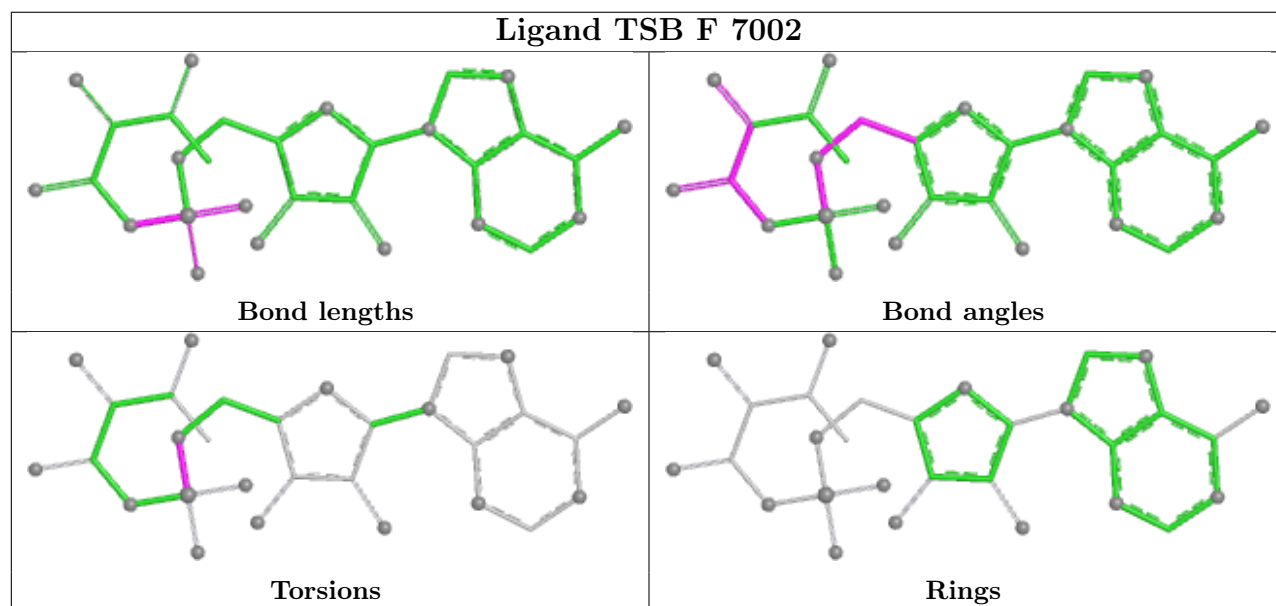
Mol	Chain	Res	Type	Atoms
4	A	2002	TSB	C5'-O5'-S1-N8
4	B	3002	TSB	C5'-O5'-S1-N8
4	C	4002	TSB	C5'-O5'-S1-N8
4	D	5002	TSB	C5'-O5'-S1-N8
4	E	6002	TSB	C5'-O5'-S1-N8

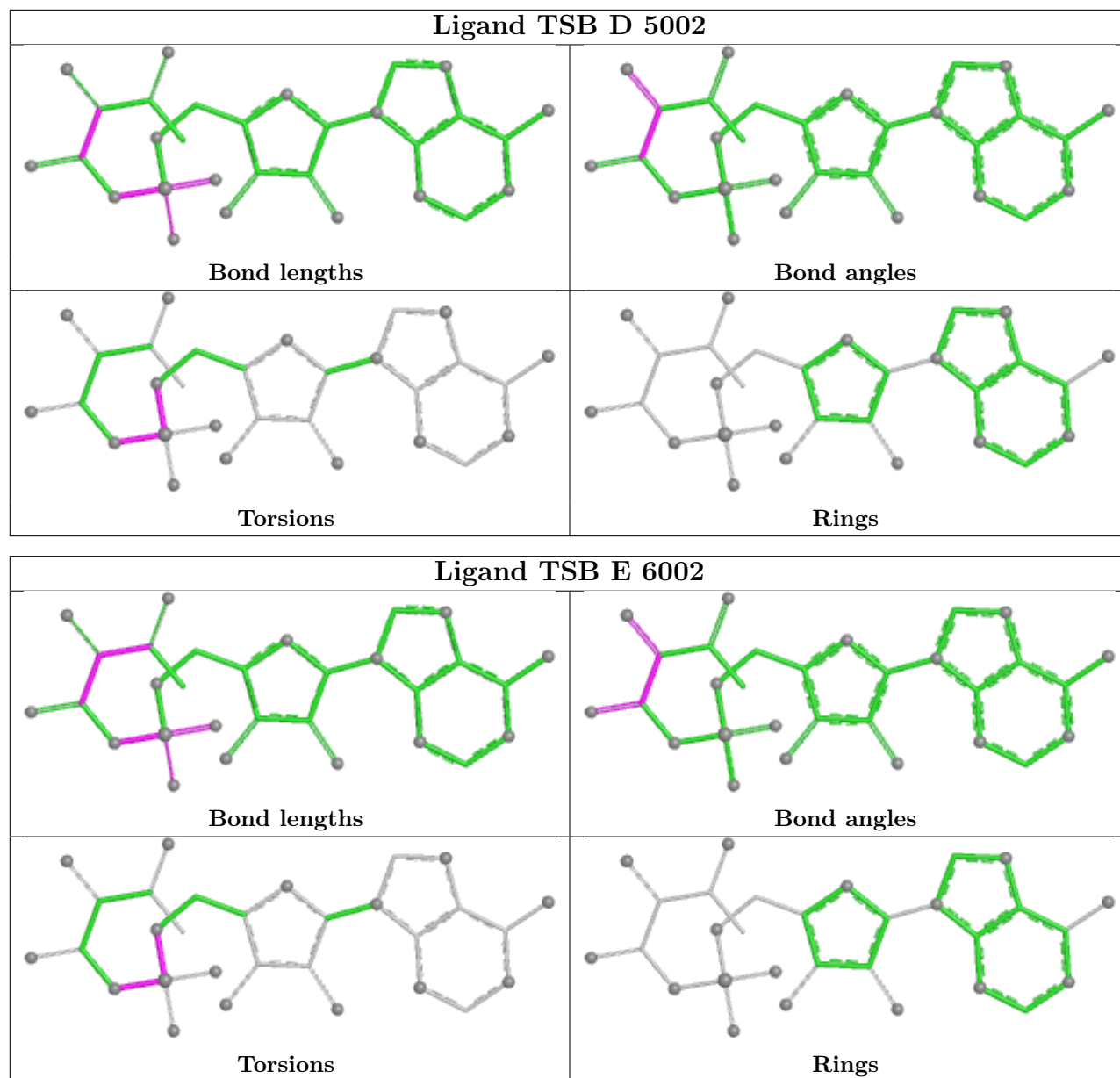
There are no ring outliers.

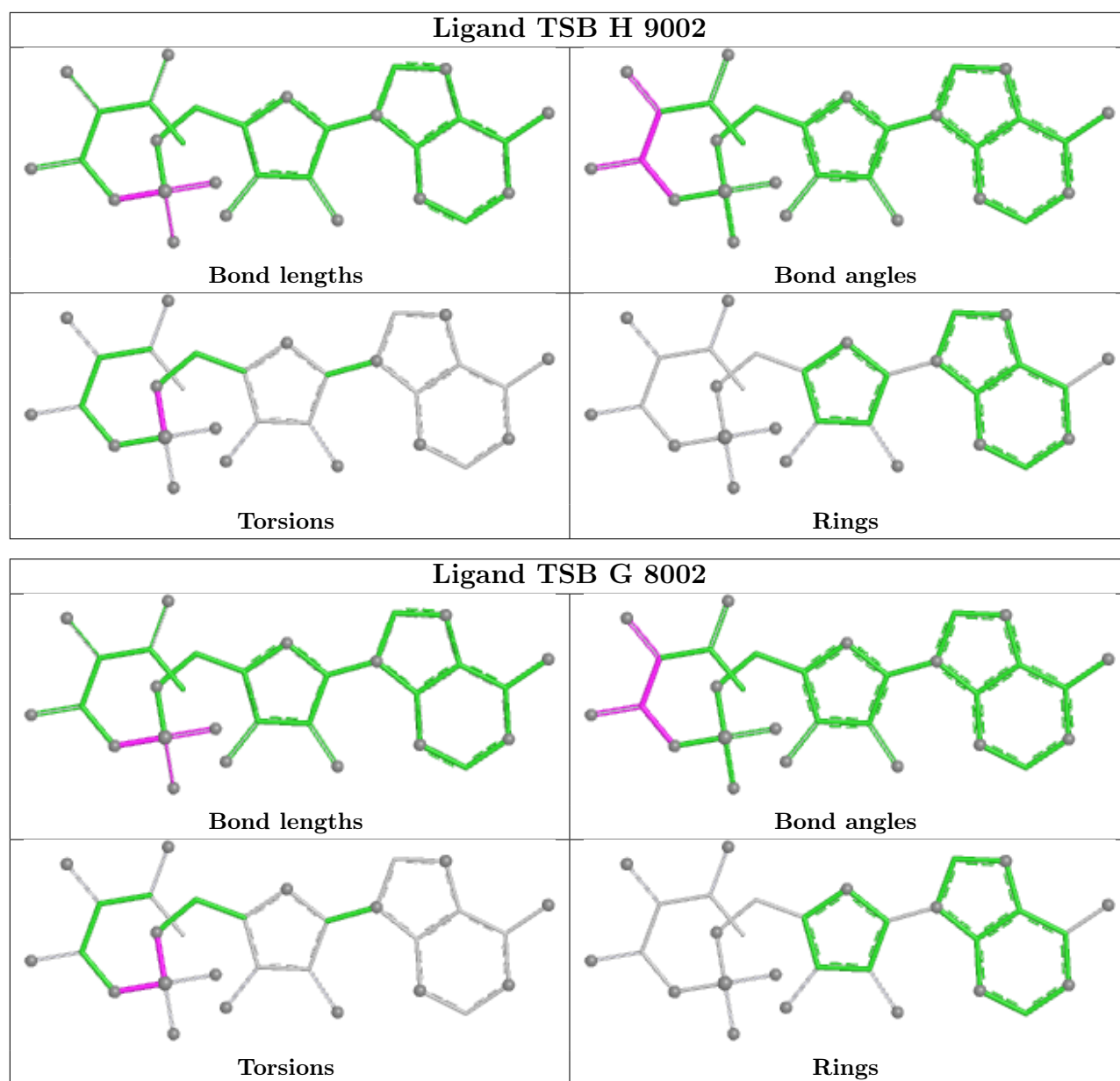
8 monomers are involved in 31 short contacts:

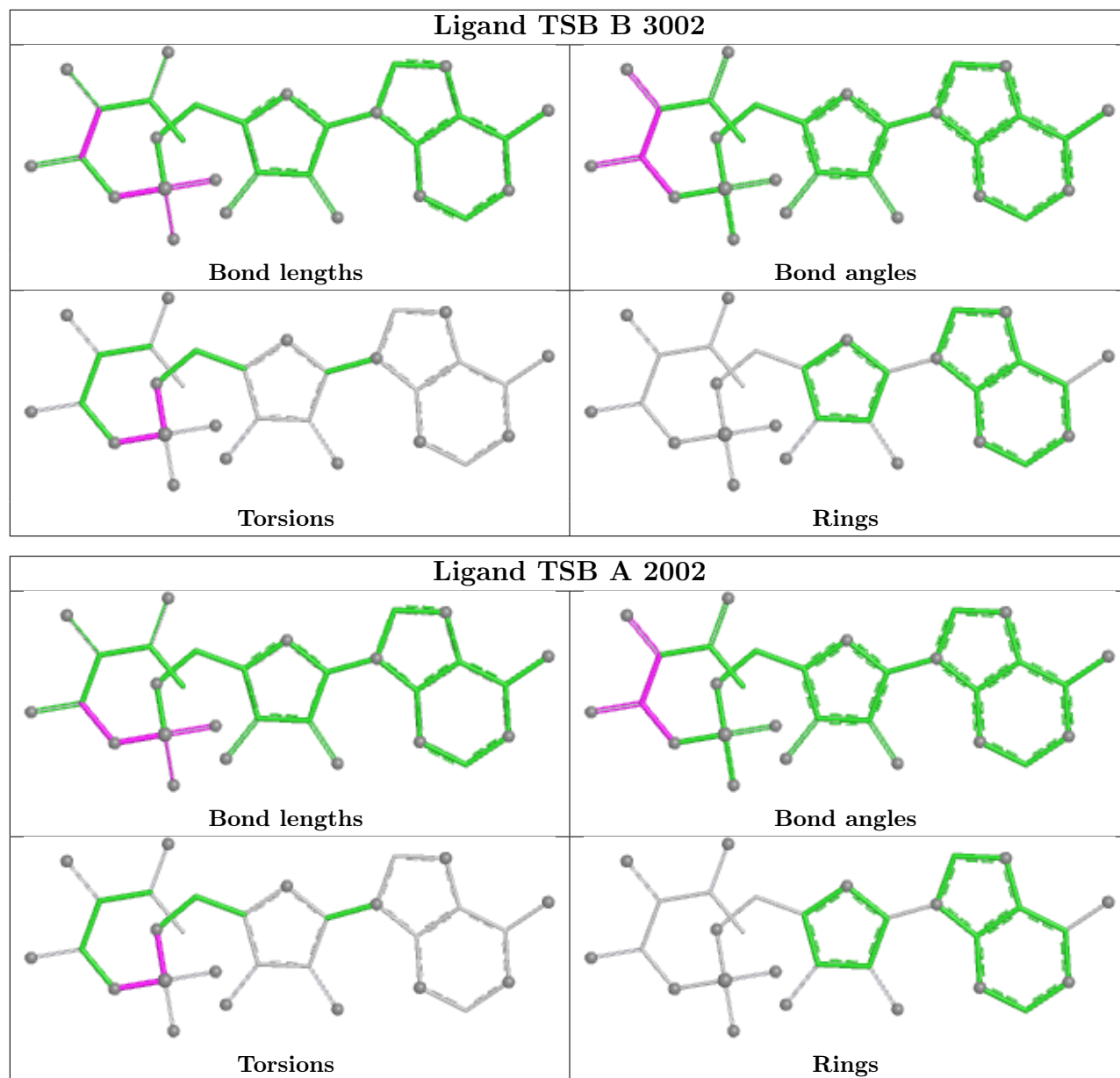
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	7002	TSB	5	0
4	D	5002	TSB	4	0
4	E	6002	TSB	4	0
4	H	9002	TSB	4	0
4	G	8002	TSB	4	0
4	B	3002	TSB	4	0
4	A	2002	TSB	3	0
4	C	4002	TSB	3	0

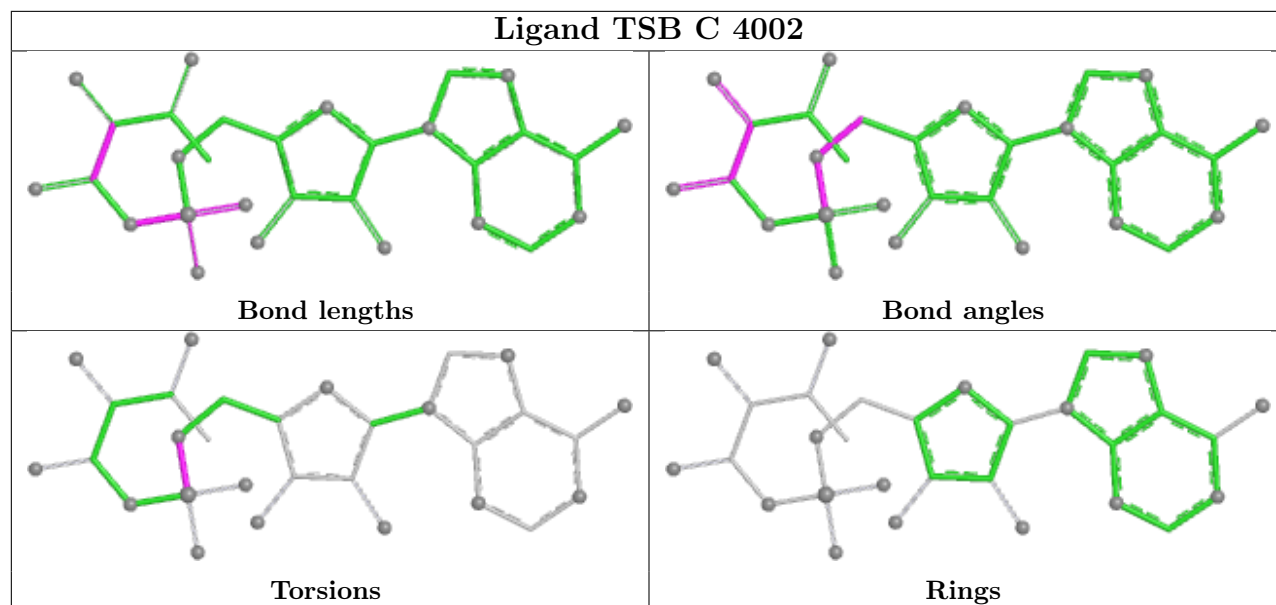
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	I	37/37 (100%)	1.02	4 (10%) 11 8	82, 115, 150, 153	0
1	J	37/37 (100%)	0.45	2 (5%) 31 18	55, 88, 135, 152	0
1	K	37/37 (100%)	1.62	13 (35%) 1 1	119, 148, 168, 184	0
1	L	37/37 (100%)	0.76	1 (2%) 56 33	110, 134, 170, 180	0
1	M	37/37 (100%)	0.49	3 (8%) 18 12	60, 86, 153, 166	0
1	N	37/37 (100%)	1.44	6 (16%) 4 4	140, 163, 181, 184	0
1	O	37/37 (100%)	0.39	1 (2%) 56 33	45, 67, 115, 124	0
1	P	37/37 (100%)	0.49	0 100 100	46, 104, 155, 159	0
2	A	401/401 (100%)	-0.09	1 (0%) 91 82	15, 68, 109, 136	0
2	B	401/401 (100%)	-0.16	1 (0%) 91 82	17, 62, 105, 137	0
2	C	401/401 (100%)	0.38	15 (3%) 45 25	55, 101, 146, 160	0
2	D	401/401 (100%)	0.52	19 (4%) 36 20	80, 123, 147, 158	0
2	E	401/401 (100%)	0.80	31 (7%) 19 13	75, 126, 150, 168	0
2	F	401/401 (100%)	0.51	21 (5%) 33 19	47, 105, 148, 168	0
2	G	401/401 (100%)	-0.31	0 100 100	7, 48, 98, 132	0
2	H	401/401 (100%)	-0.16	0 100 100	14, 68, 105, 135	0
All	All	3504/3504 (100%)	0.24	118 (3%) 48 27	7, 91, 147, 184	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	482	THR	5.5
2	F	260	ALA	5.2
2	E	356	ALA	4.9
2	C	595	VAL	4.7
2	C	578	ILE	4.6

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

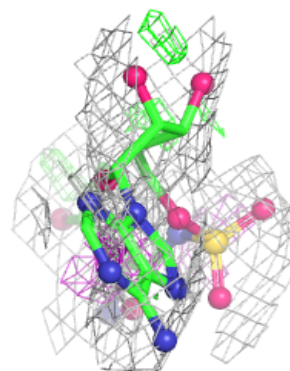
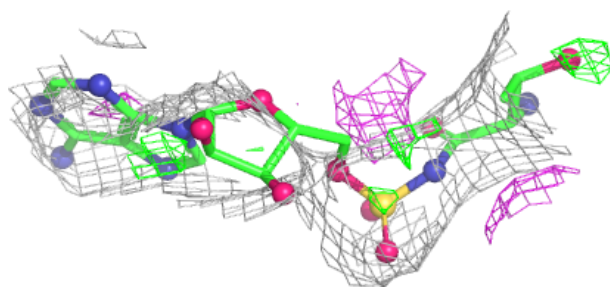
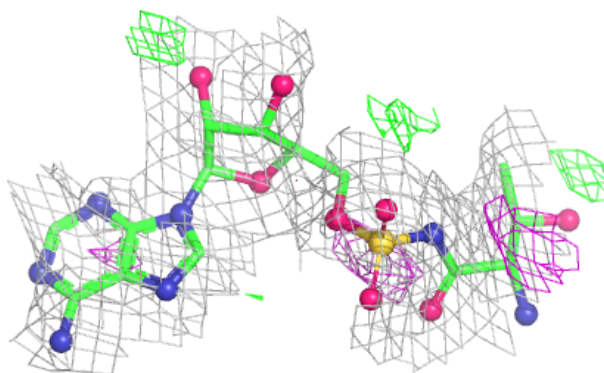
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TSB	E	6002	30/30	0.71	0.14	86,122,126,127	0
4	TSB	D	5002	30/30	0.81	0.13	94,112,119,120	0
4	TSB	F	7002	30/30	0.86	0.14	89,103,111,112	0
4	TSB	C	4002	30/30	0.91	0.12	73,88,100,102	0
4	TSB	H	9002	30/30	0.93	0.11	30,48,71,72	0
3	ZN	E	1	1/1	0.94	0.06	185,185,185,185	0
3	ZN	D	1	1/1	0.95	0.05	135,135,135,135	0
4	TSB	A	2002	30/30	0.96	0.09	31,44,58,65	0
4	TSB	G	8002	30/30	0.96	0.09	0,18,49,50	0
3	ZN	F	1	1/1	0.96	0.04	101,101,101,101	0
4	TSB	B	3002	30/30	0.97	0.08	32,50,57,58	0
3	ZN	C	1	1/1	0.98	0.03	95,95,95,95	0
3	ZN	H	1	1/1	0.99	0.04	54,54,54,54	0
3	ZN	B	1	1/1	0.99	0.06	52,52,52,52	0
3	ZN	G	1	1/1	0.99	0.02	27,27,27,27	0
3	ZN	A	1	1/1	1.00	0.03	42,42,42,42	0

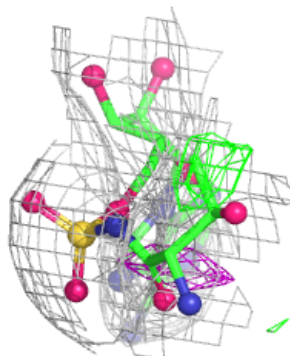
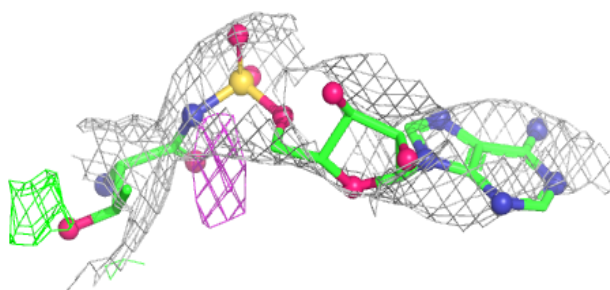
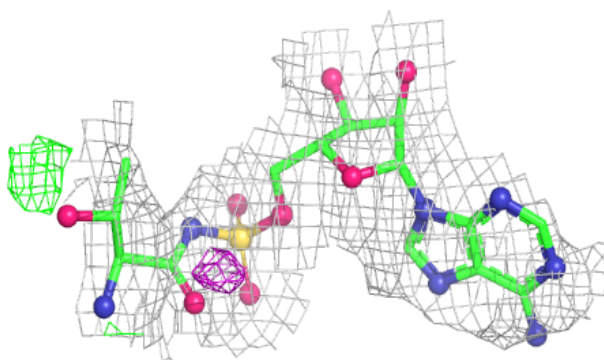
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TSB E 6002:

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

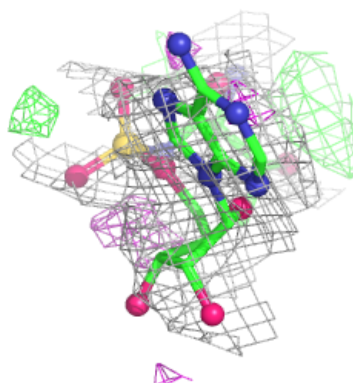
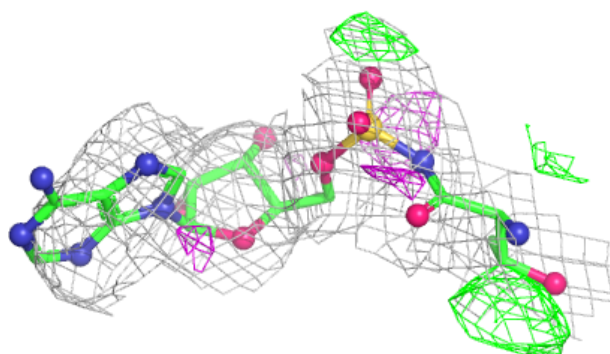
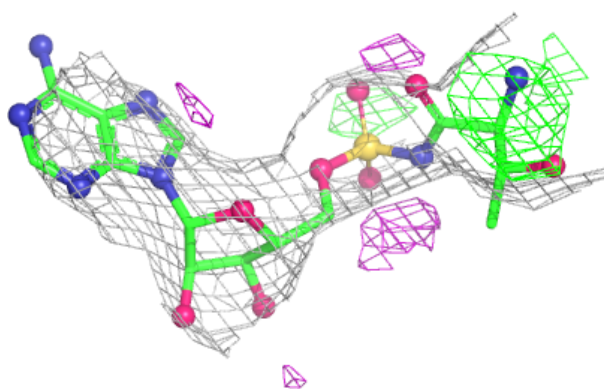
**Electron density around TSB D 5002:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

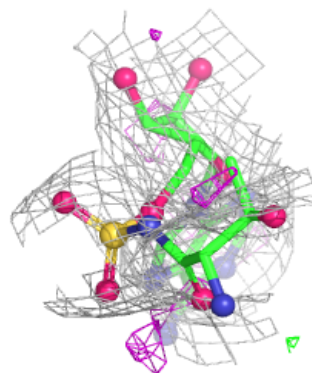
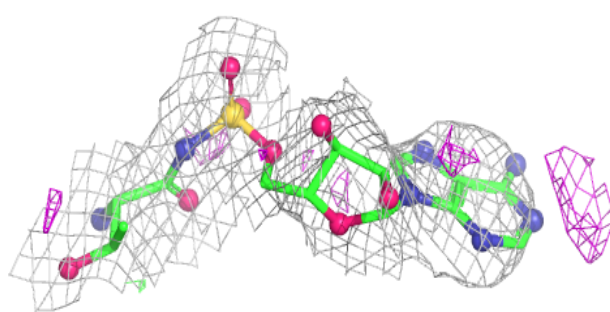
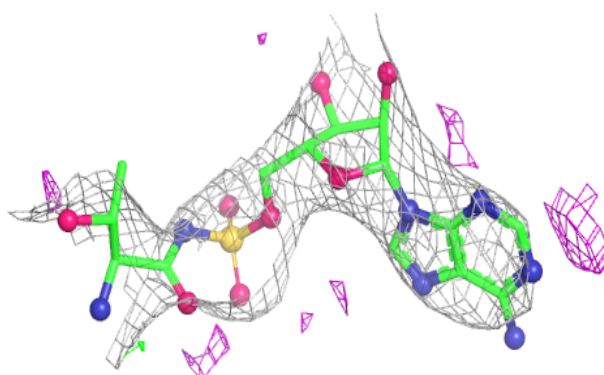


Electron density around TSB F 7002:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

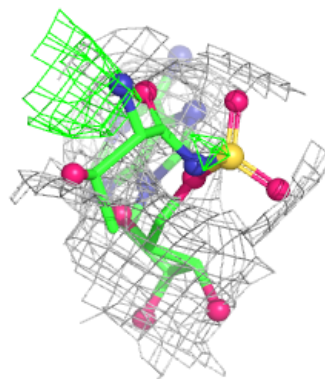
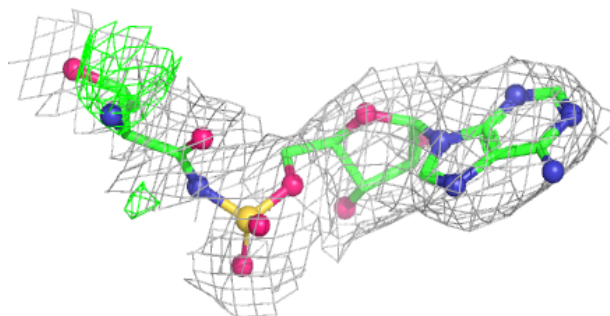
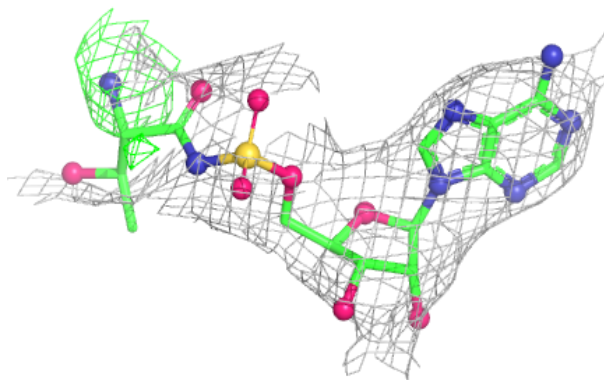
**Electron density around TSB C 4002:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

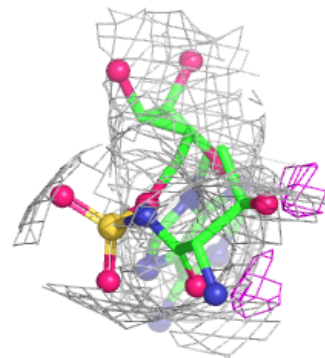
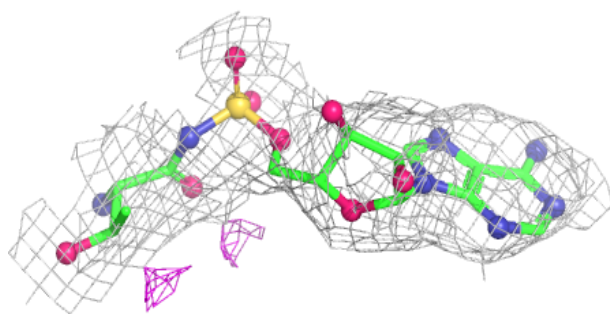
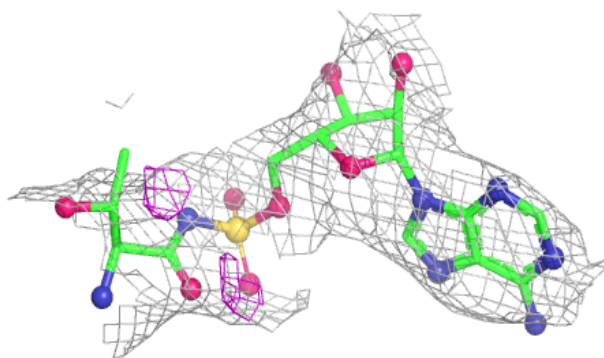


Electron density around TSB H 9002:

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

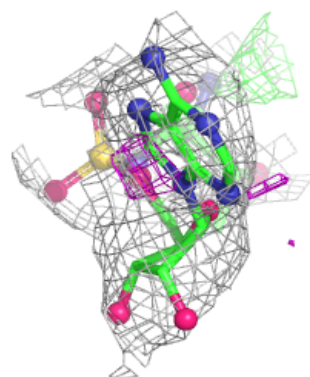
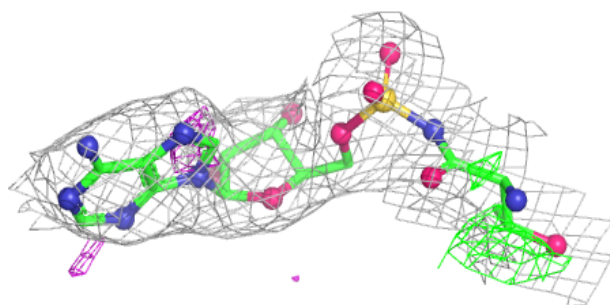
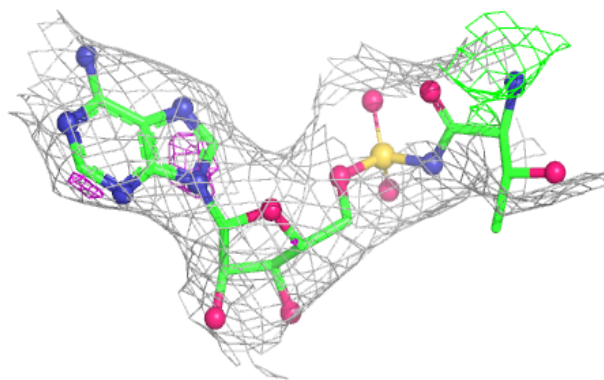
**Electron density around TSB A 2002:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

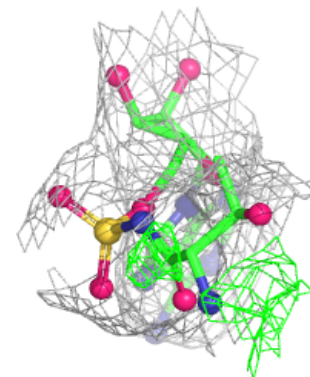
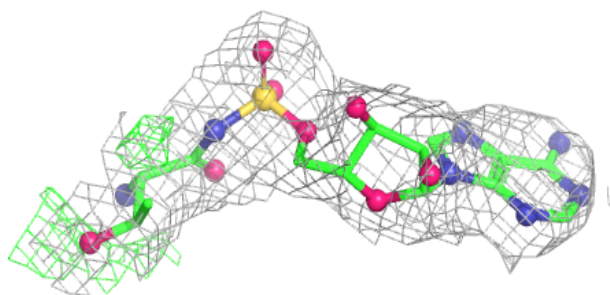
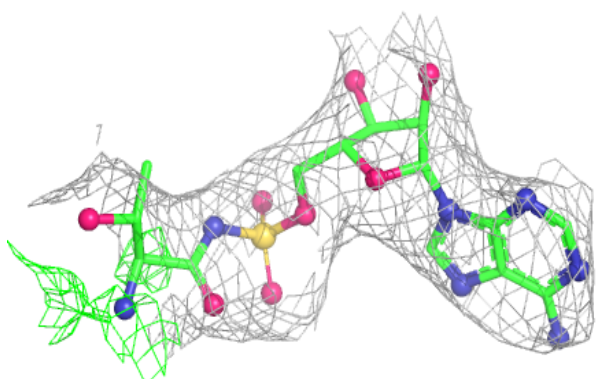


Electron density around TSB G 8002:

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

**Electron density around TSB B 3002:**

$2mF_o-DF_c$ (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.