



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2020 – 12:10 PM JST

PDB ID : 7CBG
Title : Crystal structure of threonyl-tRNA synthetase (ThrRS) from *Salmonella enterica* in complex with an inhibitor
Authors : Guo, J.; Chen, B.; Zhou, H.
Deposited on : 2020-06-12
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.14.6
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) : 2.14.6

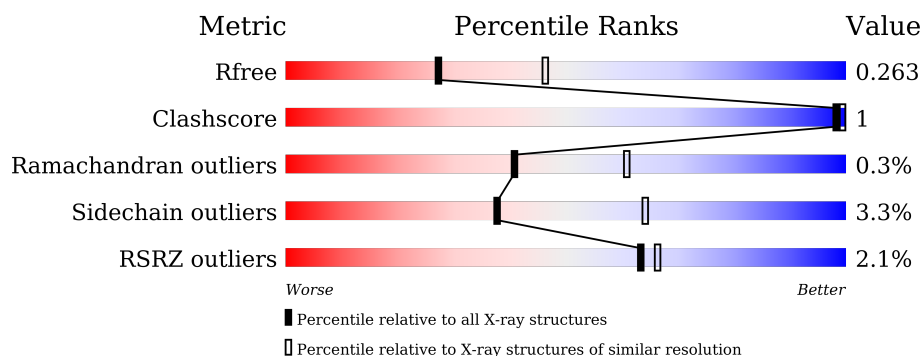
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	411	<div> <div>%</div> <div> <div></div> <div>93%</div> <div></div> </div> </div>
1	B	411	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div></div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6923 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.

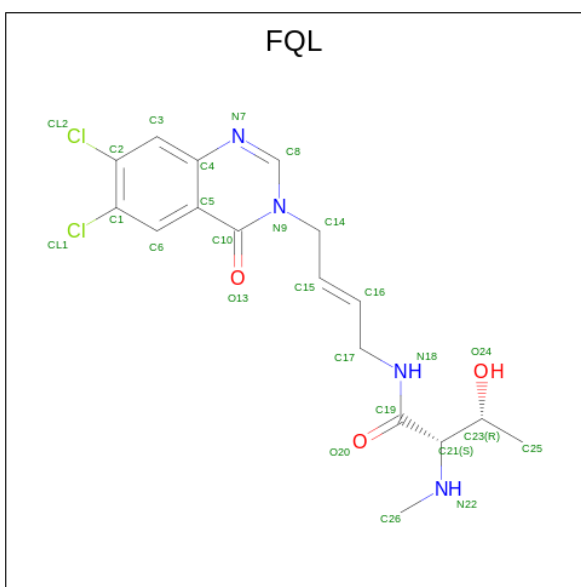
- Molecule 1 is a protein called Threonine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3246	2050	573	600	23			
1	B	400	Total	C	N	O	S	0	0	0
			3237	2045	574	595	23			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	MET	-	expression tag	UNP V7II86
A	241	GLY	-	expression tag	UNP V7II86
A	643	LEU	-	expression tag	UNP V7II86
A	644	GLU	-	expression tag	UNP V7II86
A	645	HIS	-	expression tag	UNP V7II86
A	646	HIS	-	expression tag	UNP V7II86
A	647	HIS	-	expression tag	UNP V7II86
A	648	HIS	-	expression tag	UNP V7II86
A	649	HIS	-	expression tag	UNP V7II86
A	650	HIS	-	expression tag	UNP V7II86
B	240	MET	-	expression tag	UNP V7II86
B	241	GLY	-	expression tag	UNP V7II86
B	643	LEU	-	expression tag	UNP V7II86
B	644	GLU	-	expression tag	UNP V7II86
B	645	HIS	-	expression tag	UNP V7II86
B	646	HIS	-	expression tag	UNP V7II86
B	647	HIS	-	expression tag	UNP V7II86
B	648	HIS	-	expression tag	UNP V7II86
B	649	HIS	-	expression tag	UNP V7II86
B	650	HIS	-	expression tag	UNP V7II86

- Molecule 2 is (2S,3R)-N-[(E)-4-[6,7-bis(chloranyl)-4-oxidanylidene-quinazolin-3-yl]but-2-enyl]-2-(methylamino)-3-oxidanyl-butanamide (three-letter code: FQL) (formula: C₁₇H₂₀Cl₂N₄O₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 26	C 17	Cl 2	N 4	O 3	0	0
2	B	1	Total 26	C 17	Cl 2	N 4	O 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	222	Total O 222 222	0	0
4	B	164	Total O 164 164	0	0

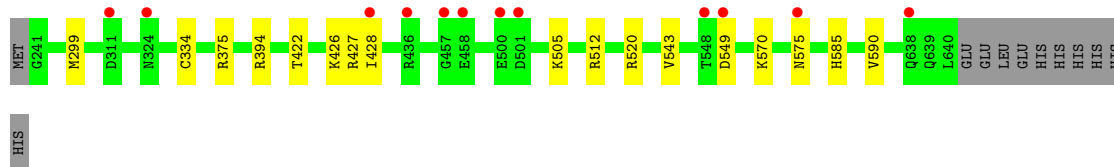
3 Residue-property plots [i](#)

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: Threonine-tRNA ligase



- Molecule 1: Threonine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.79Å 101.80Å 105.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 22.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.50) 99.3 (22.17-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.53 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.215 , 0.261 0.218 , 0.263	Depositor DCC
R_{free} test set	1606 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6923	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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, FQL

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	0.36	0/3317	0.58	0/4475
1	B	0.36	0/3308	0.58	0/4462
All	All	0.36	0/6625	0.58	0/8937

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3246	0	3149	5	0
1	B	3237	0	3152	2	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	222	0	0	0	0
4	B	164	0	0	0	0
All	All	6923	0	6301	7	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 1.

All (7) 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:548:THR:H	1:A:551:GLN:HE22	1.53	0.57
1:A:331:PRO:O	1:A:363:ARG:NH1	2.41	0.54
1:B:543:VAL:HG11	1:B:585:HIS:CE1	2.50	0.46
1:A:338:VAL:HG11	1:A:493:LEU:HB2	1.99	0.45
1:A:543:VAL:HG23	1:A:590:VAL:HG11	2.02	0.42
1:B:543:VAL:HG23	1:B:590:VAL:HG11	2.02	0.42
1:A:551:GLN:HB2	1:A:551:GLN:HE21	1.72	0.41

There are no symmetry-related clashes.

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	
1	A	399/411 (97%)	394 (99%)	5 (1%)	0	100	100
1	B	398/411 (97%)	393 (99%)	3 (1%)	2 (0%)	29	48
All	All	797/822 (97%)	787 (99%)	8 (1%)	2 (0%)	41	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	427	ARG
1	B	426	LYS

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	
1	A	346/363 (95%)	335 (97%)	11 (3%)	39	65
1	B	345/363 (95%)	333 (96%)	12 (4%)	36	62
All	All	691/726 (95%)	668 (97%)	23 (3%)	38	64

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
1	A	286	LYS
1	A	299	MET
1	A	319	THR
1	A	332	MET
1	A	334	CYS
1	A	363	ARG
1	A	505	LYS
1	A	512	ARG
1	A	551	GLN
1	A	619	LEU
1	B	299	MET
1	B	334	CYS
1	B	375	ARG
1	B	394	ARG
1	B	422	THR
1	B	428	ILE
1	B	505	LYS
1	B	512	ARG
1	B	520	ARG
1	B	549	ASP
1	B	570	LYS
1	B	575	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	ASN
1	A	342	ASN
1	A	551	GLN
1	B	257	GLN

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Mol	Chain	Res	Type
1	B	268	ASN
1	B	291	GLN
1	B	312	ASN
1	B	342	ASN
1	B	484	GLN
1	B	575	ASN
1	B	585	HIS
1	B	629	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 4 ligands modelled in this entry, 2 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$
2	FQL	A	701	3	26,27,27	0.91	1 (3%)	27,37,37	0.68	1 (3%)
2	FQL	B	701	3	26,27,27	0.91	1 (3%)	27,37,37	0.69	1 (3%)

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
2	FQL	A	701	3	-	7/18/18/18	0/2/2/2
2	FQL	B	701	3	-	3/18/18/18	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FQL	C10-C5	3.37	1.47	1.41
2	A	701	FQL	C10-C5	3.31	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FQL	C5-C10-N9	-3.25	113.93	116.15
2	A	701	FQL	C5-C10-N9	-3.24	113.94	116.15

There are no chirality outliers.

All (10) torsion outliers are listed below:

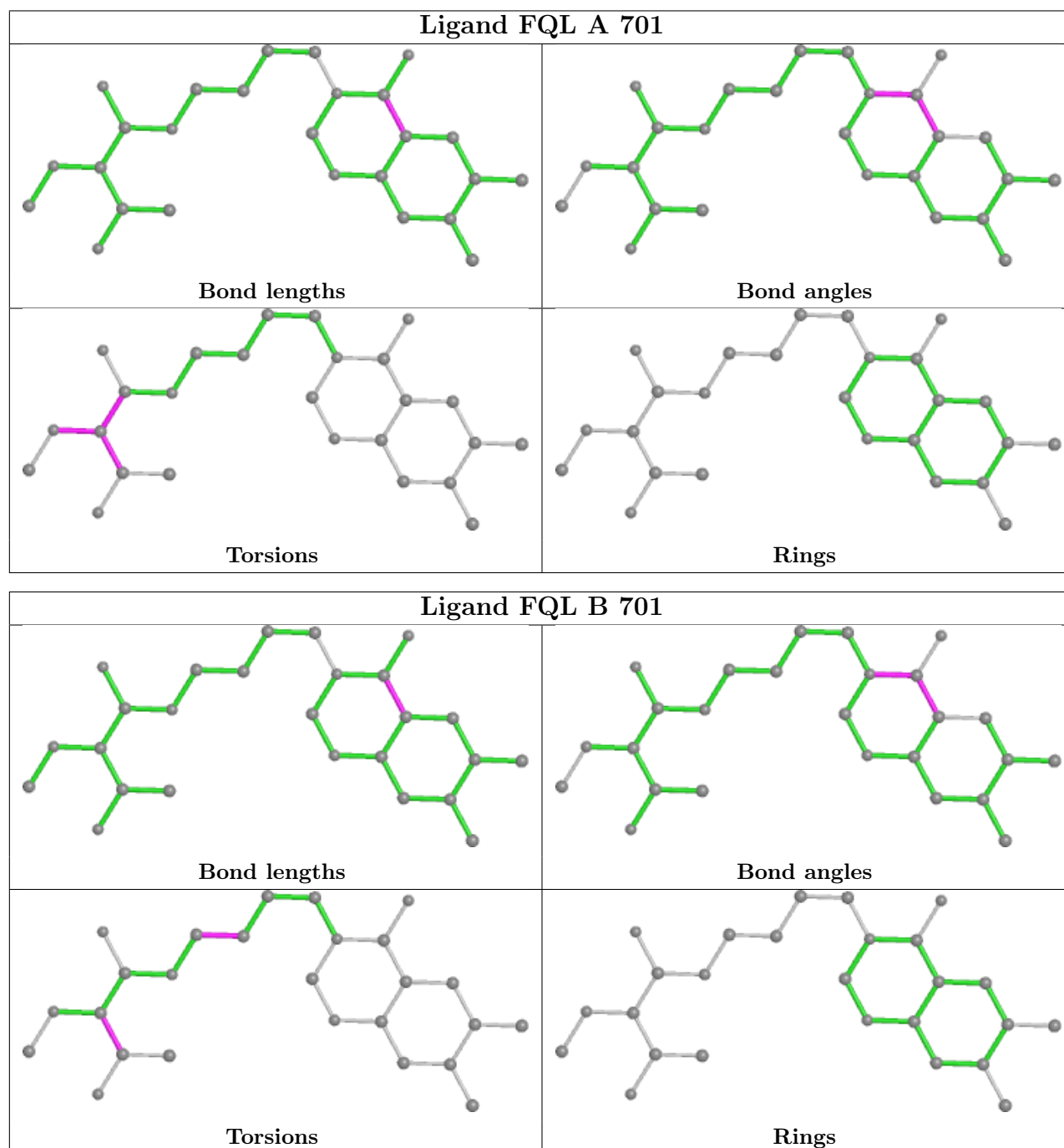
Mol	Chain	Res	Type	Atoms
2	A	701	FQL	C19-C21-N22-C26
2	A	701	FQL	N22-C21-C23-O24
2	B	701	FQL	N22-C21-C23-O24
2	A	701	FQL	C23-C21-N22-C26
2	A	701	FQL	C19-C21-C23-O24
2	B	701	FQL	C15-C16-C17-N18
2	B	701	FQL	N22-C21-C23-C25
2	A	701	FQL	O20-C19-C21-N22
2	A	701	FQL	N22-C21-C23-C25
2	A	701	FQL	N18-C19-C21-N22

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	401/411 (97%)	-0.09	5 (1%) 79 80	14, 21, 33, 43	0
1	B	400/411 (97%)	0.03	12 (3%) 50 53	13, 24, 40, 45	0
All	All	801/822 (97%)	-0.03	17 (2%) 63 66	13, 22, 39, 45	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	GLY	4.1
1	B	457	GLY	3.9
1	B	575	ASN	3.7
1	A	311	ASP	3.0
1	B	638	GLN	2.7
1	A	241	GLY	2.7
1	B	548	THR	2.7
1	B	458	GLU	2.6
1	B	428	ILE	2.3
1	A	502	ASN	2.3
1	B	324	ASN	2.3
1	B	501	ASP	2.3
1	B	500	GLU	2.1
1	B	311	ASP	2.1
1	B	549	ASP	2.0
1	B	436	ARG	2.0
1	A	297	PHE	2.0

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](#)

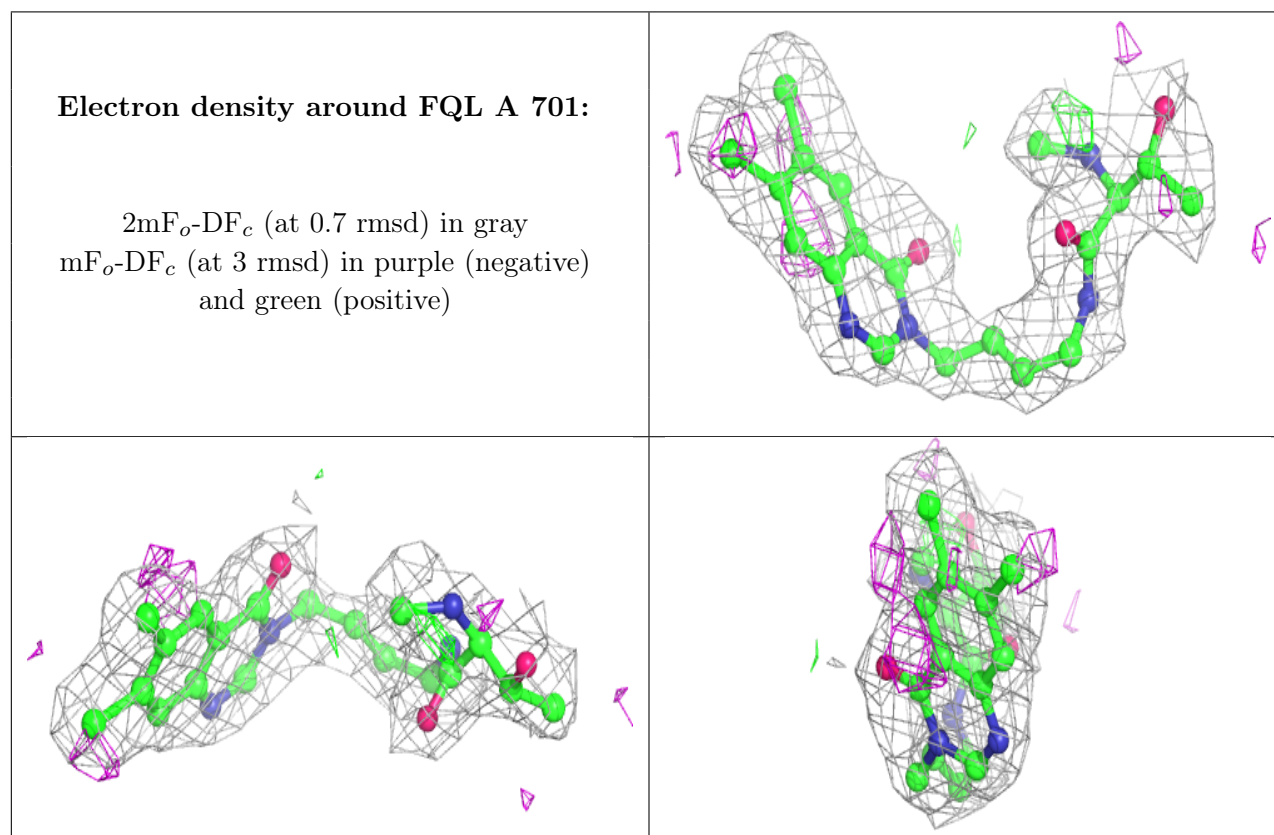
There are no monosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

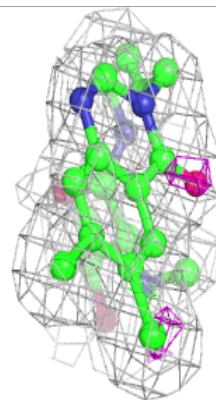
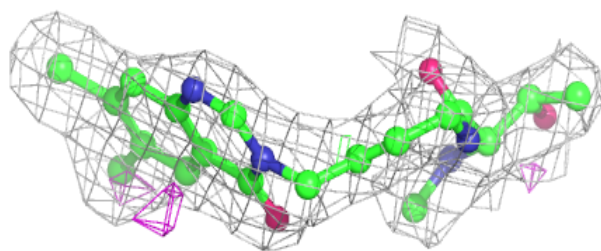
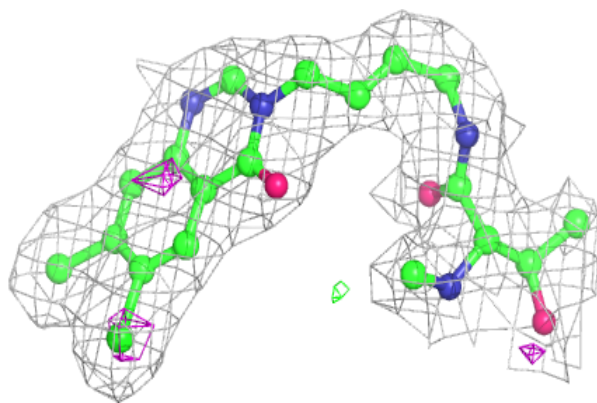
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FQL	A	701	26/26	0.92	0.15	20,23,24,25	0
2	FQL	B	701	26/26	0.93	0.13	21,24,26,26	0
3	ZN	A	702	1/1	0.99	0.02	12,12,12,12	0
3	ZN	B	702	1/1	1.00	0.02	18,18,18,18	0

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 FQL B 701:

$2mF_o-DF_c$ (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.