



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2023 – 01:53 PM EST

PDB ID : 2QUJ
Title : Crystal structures of human tryptophanyl-tRNA synthetase in complex with TrpAMP
Authors : Shen, N.; Ding, J.P.
Deposited on : 2007-08-05
Resolution : 2.42 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 ⓘ 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 ⓘ](#)) 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 : 2.36
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

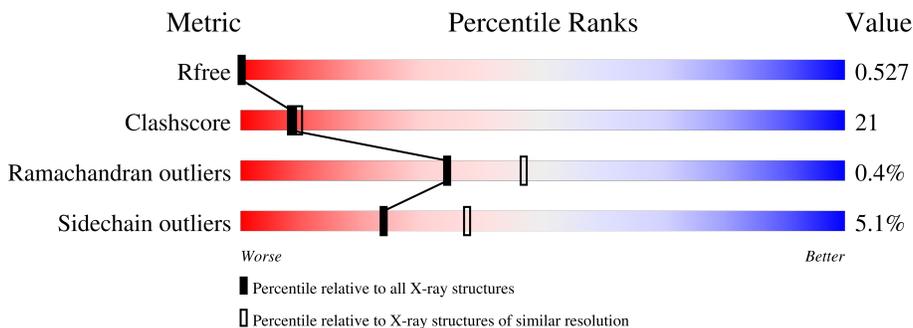
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	477	
1	B	477	

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
2	CL	A	802	-	-	X	-
2	CL	A	804	-	-	X	-
2	CL	A	805	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	807	-	-	X	-
2	CL	B	808	-	-	X	-
4	GOL	A	813	-	X	X	-
4	GOL	A	814	-	X	X	-
4	GOL	B	812	-	X	X	-
4	GOL	B	815	-	X	X	-
5	TRP	B	817	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6422 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3106	1988	533	570	15	0	0	0
1	B	378	3033	1947	511	560	15	0	0	0

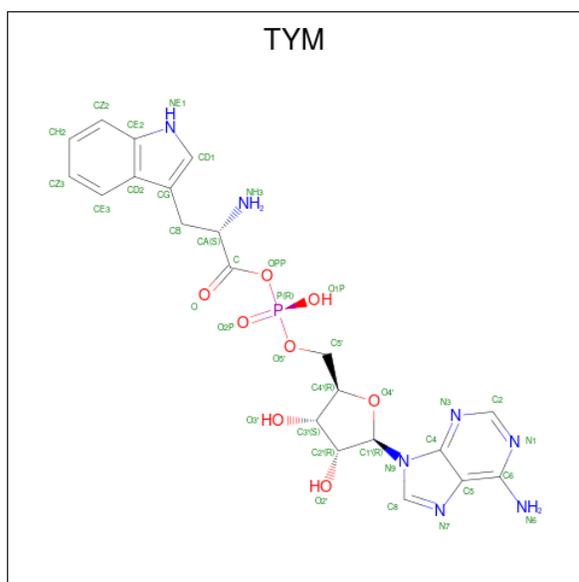
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	472	HIS	-	expression tag	UNP P23381
A	473	HIS	-	expression tag	UNP P23381
A	474	HIS	-	expression tag	UNP P23381
A	475	HIS	-	expression tag	UNP P23381
A	476	HIS	-	expression tag	UNP P23381
A	477	HIS	-	expression tag	UNP P23381
B	472	HIS	-	expression tag	UNP P23381
B	473	HIS	-	expression tag	UNP P23381
B	474	HIS	-	expression tag	UNP P23381
B	475	HIS	-	expression tag	UNP P23381
B	476	HIS	-	expression tag	UNP P23381
B	477	HIS	-	expression tag	UNP P23381

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

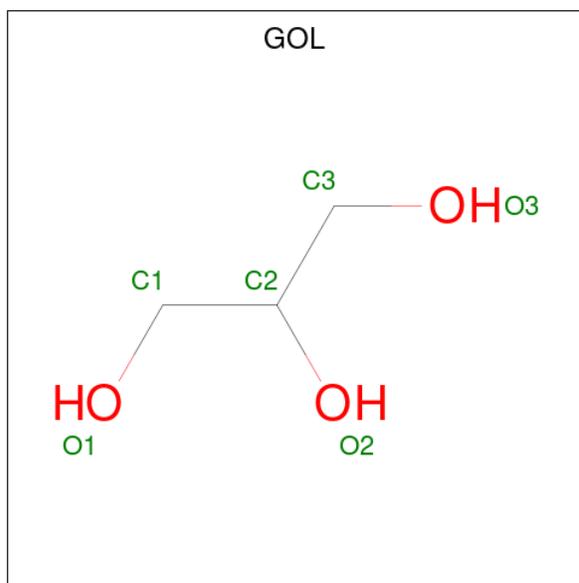
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Cl	0	0
			5	5		
2	B	4	Total	Cl	0	0
			4	4		

- Molecule 3 is TRYPTOPHANYL-5'AMP (three-letter code: TYM) (formula: C₂₁H₂₄N₇O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	37	21	7	8	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



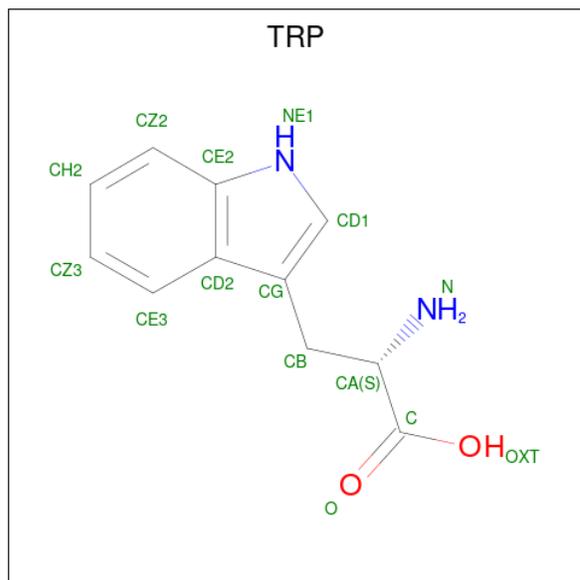
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	98	Total	O	0	0
			98	98		
6	B	100	Total	O	0	0
			100	100		

R449	I193
K450	Q194
E451	M196
V452	T196
T453	D197
D454	D198
E455	E199
L456	K200
V457	Y201
K458	L202
E459	W203
F460	
M461	L206
T462	T207
P463	L208
R464	D209
K465	L210
L466	Q211
S467	A211
F468	Y212
D469	S213
F470	Y214
Q471	A215
HIS	E217
HIS	N218
HIS	A219
HIS	K220
HIS	D221
HIS	I222
	I223
	A224
	C225
	G226
	F227
	D228
	I229
	N230
	K231
	T232
	F233
	I234
	F235
	S236
	D237
	L238
	D239
	Y240
	M241
	G242
	M243
	S244
	S245
	G246
	F247
	Y248
	K249
	N250
	V251
	Q252
	K253
	I254
	Q255
	K256
	H257
	V258
	T259
	F260
	M261
	Q262
	K263
	K264
	G265
	L266
	F267
	G268
	F269
	D270
	D271
	D272
	D273
	C274
	I275
	G276
	K277
	L278
	S279
	F280
	P281
	A282
	I283
	I284
	A285
	Q286
	P287
	S288
	F289
	S290
	N291
	S292
	F293
	P294
	Q295
	I296
	F297
	R298
	D299
	R300
	T301
	D302
	I303
	Q304
	C305
	L306
	I307
	P308
	C309
	A310
	I311
	D312
	Q313
	D314
	P315
	Y316
	F317
	R318
	M319
	T320
	R321
	D322
	V323
	A324
	P325
	R326
	I327
	G328
	Y329
	P332
	T333
	L334
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	H336
	S337
	T338
	F339
	F340
	P341
	A342
	L343
	Q344
	G345
	A346
	Q347
	T348
	K349
	D354
	P355
	N356
	S357
	S358
	I359
	F360
	L361
	T362
	D363
	T364
	A365
	K366
	Q367
	I368
	K369
	T370
	K371
	V372
	N373
	K374
	H375
	A376
	F377
	S378
	D382
	T383
	E386
	H387
	R388
	Q389
	F390
	N393
	V396
	D397
	V398
	S399
	F400
	M401
	Y402
	L403
	T404
	F405
	F406
	L407
	K412
	L413
	E414
	R417
	K418
	D419
	Y420
	G423
	A424
	M425
	L426
	T427
	G428
	E429
	L430
	K431
	K432
	A433
	L434
	I435
	E436
	V437
	L438
	Q439
	P440
	L441
	I442
	A443
	E444
	H445
	Q446
	A447
	R448

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	80.00Å 80.00Å 383.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.42 49.90 – 2.42	Depositor EDS
% Data completeness (in resolution range)	87.9 (50.00-2.42) 88.1 (49.90-2.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.42Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.238 0.515 , 0.527	Depositor DCC
R_{free} test set	2190 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtrriage
Anisotropy	0.507	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.52	EDS
Total number of atoms	6422	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: CL, GOL, TYM

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	0.37	0/3184	0.60	0/4296
1	B	0.39	0/3107	0.61	0/4195
All	All	0.38	0/6291	0.61	0/8491

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	3106	0	3024	145	5477
1	B	3033	0	2971	120	3728
2	A	5	0	0	0	12
2	B	4	0	0	2	5
3	A	37	0	23	5	7
4	A	12	0	8	2	32
4	B	12	0	8	1	36
5	B	15	0	9	0	25
6	A	98	0	0	1	283
6	B	100	0	0	1	123
All	All	6422	0	6043	258	7242

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 21.

The worst 5 of 258 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:344:GLN:HE22	1:A:357:SER:HA	1.12	1.08
1:B:95:ALA:HA	1:B:347:GLN:HE21	1.19	1.06
1:B:207:THR:HG22	1:B:210:GLN:H	1.18	1.05
1:A:250:ASN:HD21	1:A:291:ASN:ND2	1.57	1.01
1:A:250:ASN:HD21	1:A:291:ASN:HD21	1.18	0.88

The worst 5 of 7242 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)
1:B:102:LYS:C	1:B:401:MET:C[3_675]	0.07	2.13
1:A:112:ILE:CG1	1:A:275:ILE:N[8_664]	0.10	2.10
1:A:117:ILE:C	1:B:262:GLN:CA[8_664]	0.13	2.07
1:A:157:TYR:C	1:B:239:ASP:N[5_454]	0.14	2.06
1:A:123:ALA:N	1:B:177:PHE:CZ[5_454]	0.19	2.01

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	
1	A	386/477 (81%)	370 (96%)	15 (4%)	1 (0%)	41	54
1	B	376/477 (79%)	362 (96%)	12 (3%)	2 (0%)	29	40
All	All	762/954 (80%)	732 (96%)	27 (4%)	3 (0%)	34	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	B	299	ASP
1	B	467	SER

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	
1	A	335/416 (80%)	317 (95%)	18 (5%)	22	34
1	B	329/416 (79%)	313 (95%)	16 (5%)	25	39
All	All	664/832 (80%)	630 (95%)	34 (5%)	24	37

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	322	ASP
1	B	349	LYS
1	B	430	LEU
1	A	322	ASP
1	A	311	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	ASN
1	B	170	HIS
1	B	347	GLN
1	B	140	HIS
1	B	257	HIS

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 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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
3	TYM	A	810	-	36,41,41	1.75	7 (19%)	39,61,61	1.43	5 (12%)
4	GOL	B	815	-	5,5,5	4.32	5 (100%)	5,5,5	5.49	3 (60%)
4	GOL	B	812	-	5,5,5	4.31	5 (100%)	5,5,5	5.53	3 (60%)
5	TRP	B	817	-	14,16,16	1.22	1 (7%)	16,22,22	0.98	1 (6%)
4	GOL	A	814	-	5,5,5	4.43	5 (100%)	5,5,5	5.52	3 (60%)
4	GOL	A	813	-	5,5,5	4.35	5 (100%)	5,5,5	5.54	3 (60%)

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
3	TYM	A	810	-	-	1/16/39/39	0/5/5/5
4	GOL	B	815	-	-	2/4/4/4	-
4	GOL	B	812	-	-	2/4/4/4	-
5	TRP	B	817	-	-	0/7/8/8	0/2/2/2
4	GOL	A	814	-	-	3/4/4/4	-
4	GOL	A	813	-	-	3/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	814	GOL	C3-C2	-7.46	1.21	1.51
4	B	812	GOL	C3-C2	-7.19	1.22	1.51
4	B	815	GOL	C3-C2	-7.17	1.22	1.51
4	A	813	GOL	C3-C2	-7.13	1.22	1.51
3	A	810	TYM	P-OPP	6.26	1.73	1.60

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	813	GOL	O3-C3-C2	9.52	155.86	110.20
4	B	812	GOL	O3-C3-C2	9.49	155.69	110.20
4	A	814	GOL	O3-C3-C2	9.48	155.67	110.20
4	B	815	GOL	O3-C3-C2	9.38	155.19	110.20
4	B	812	GOL	O2-C2-C3	7.24	140.99	109.12

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	813	GOL	O1-C1-C2-C3
4	A	813	GOL	C1-C2-C3-O3
4	A	814	GOL	O1-C1-C2-C3
4	A	814	GOL	C1-C2-C3-O3
4	B	812	GOL	C1-C2-C3-O3

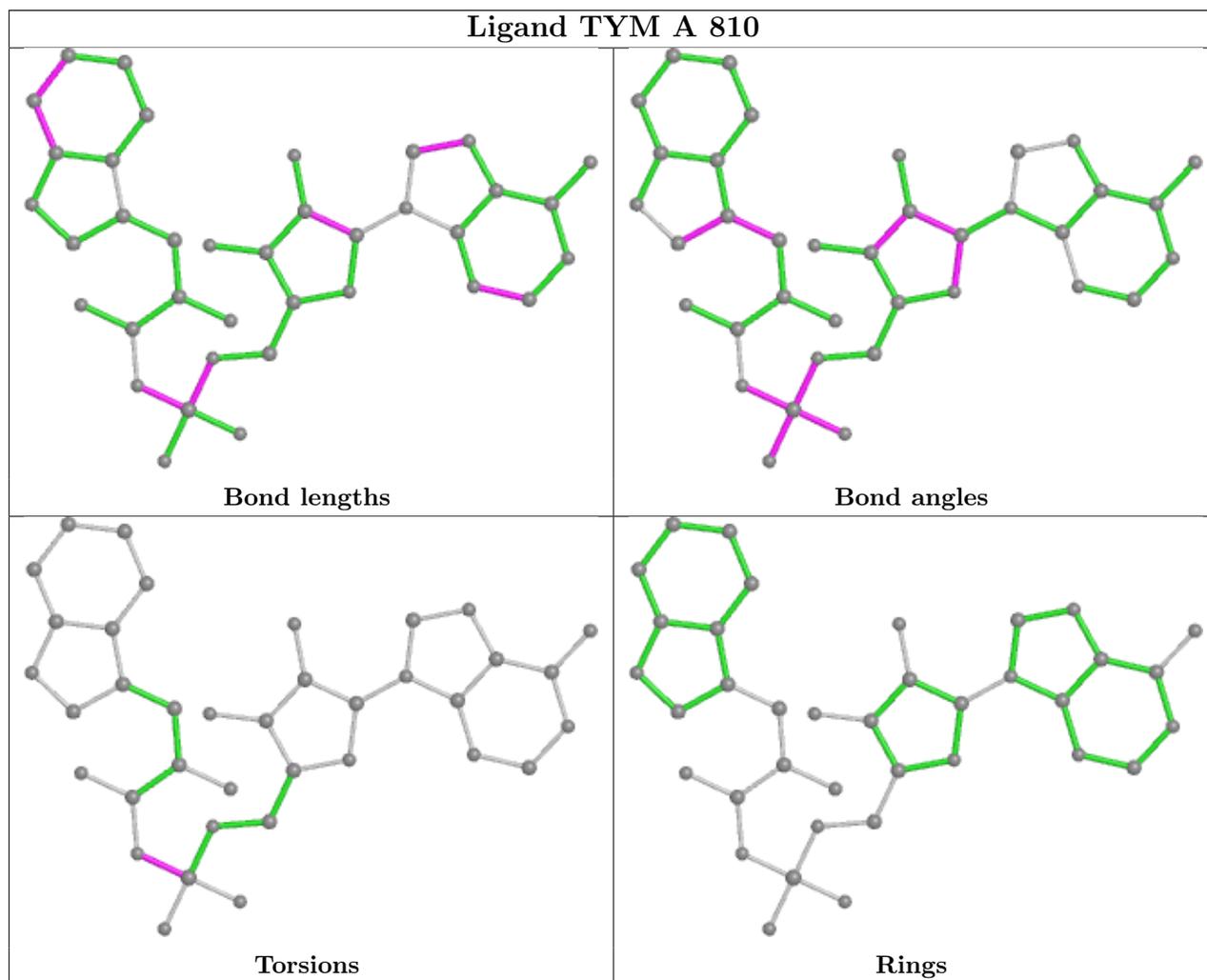
There are no ring outliers.

6 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	810	TYM	5	7
4	B	815	GOL	1	3
4	B	812	GOL	0	33
5	B	817	TRP	0	25
4	A	814	GOL	2	28
4	A	813	GOL	0	4

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 [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

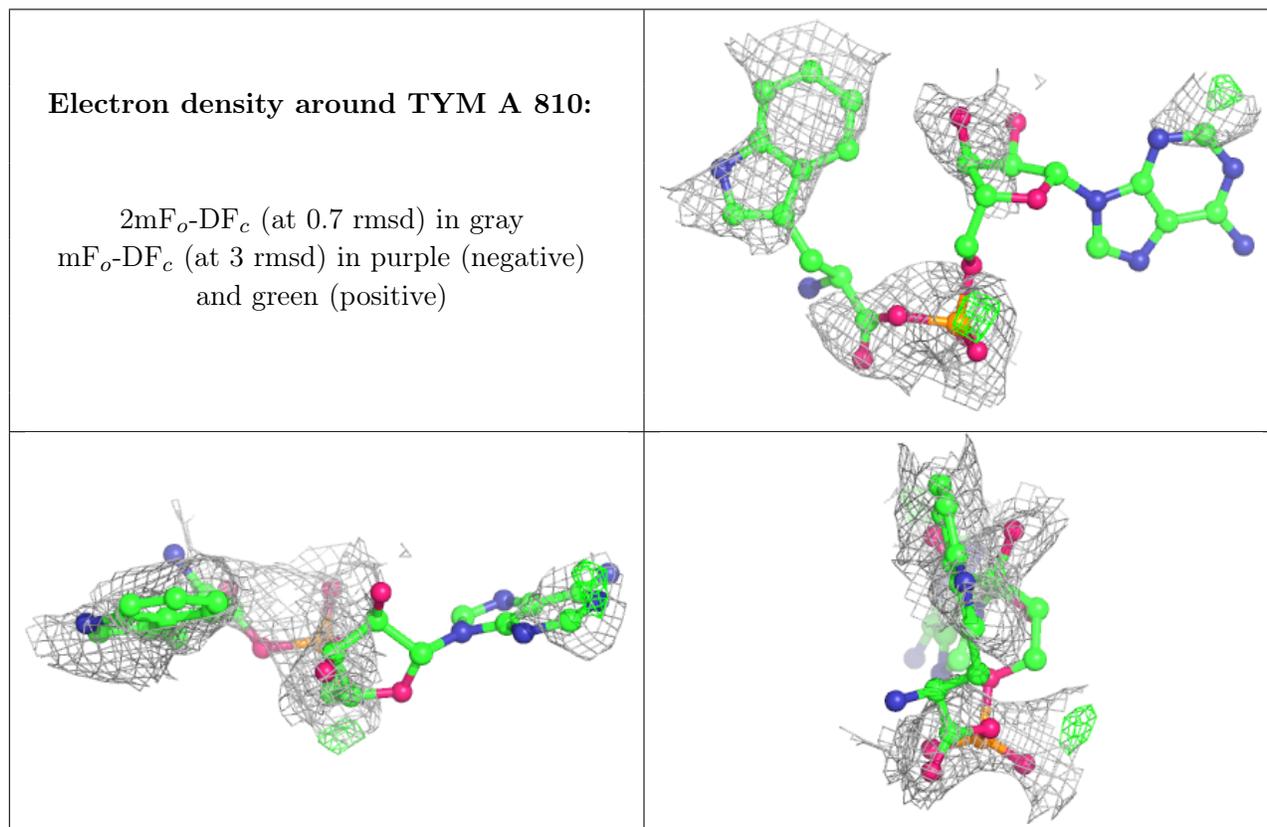
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.