



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:48 PM UTC

PDB ID : 2QUJ / pdb_00002quj
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

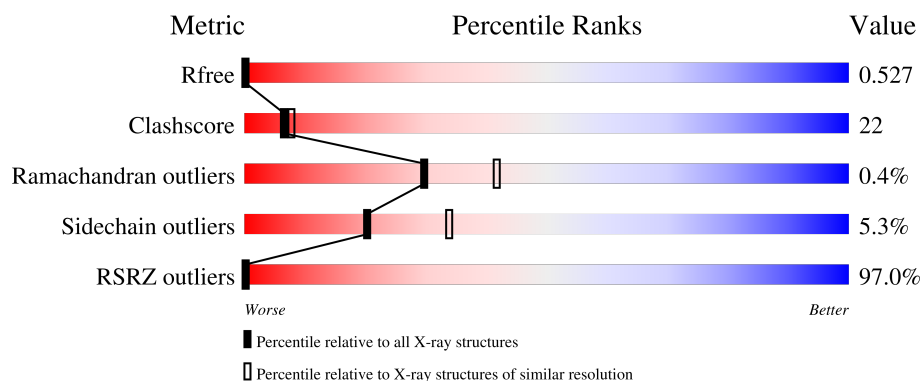
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (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 $\leq 5\%$. 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	477	79% 73% 6% 19%
1	B	477	77% 12% 62% 5% 21%

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	X
2	CL	A	805	-	-	X	-
2	CL	A	807	-	-	X	-
2	CL	A	809	-	-	-	X
2	CL	B	801	-	-	-	X
2	CL	B	806	-	-	-	X
2	CL	B	808	-	-	X	-
3	TYM	A	810	-	-	-	X
4	GOL	A	813	-	X	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

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
1	A	388	Total	C	N	O	S	0	0	0
			3106	1988	533	570	15			
1	B	378	Total	C	N	O	S	0	0	0
			3033	1947	511	560	15			

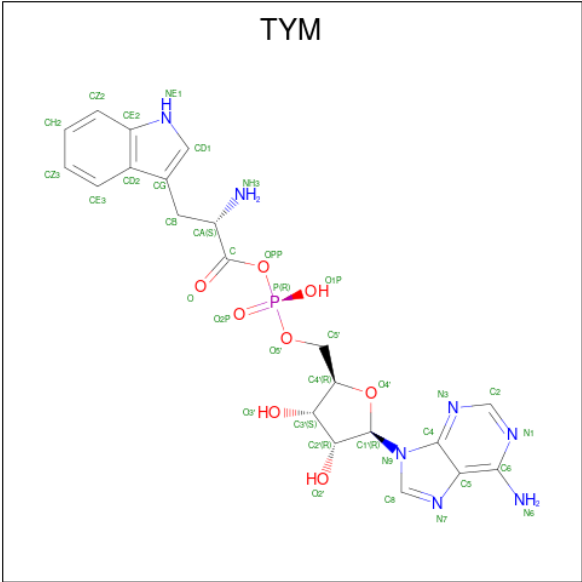
There are 12 discrepancies between the modelled and reference sequences:

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 (CCD ID: CL) (formula: Cl).

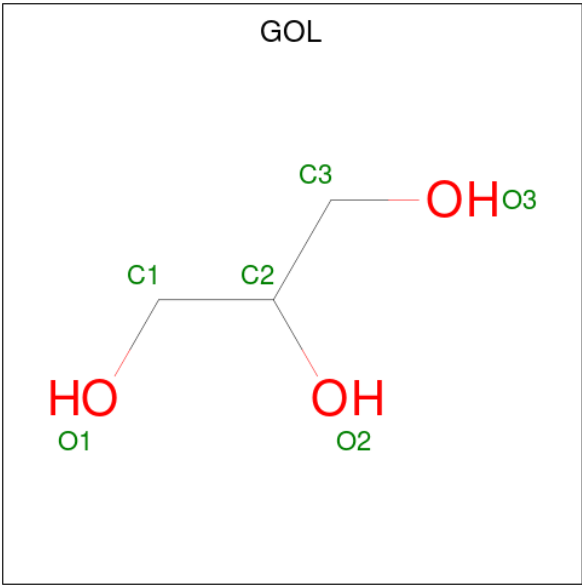
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Cl	0	0
			5	5		
2	B	4	Total	Cl	0	0
			4	4		

- Molecule 3 is TRYPTOPHANYL-5'AMP (CCD ID: TYM) (formula: C₂₁H₂₄N₇O₈P).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



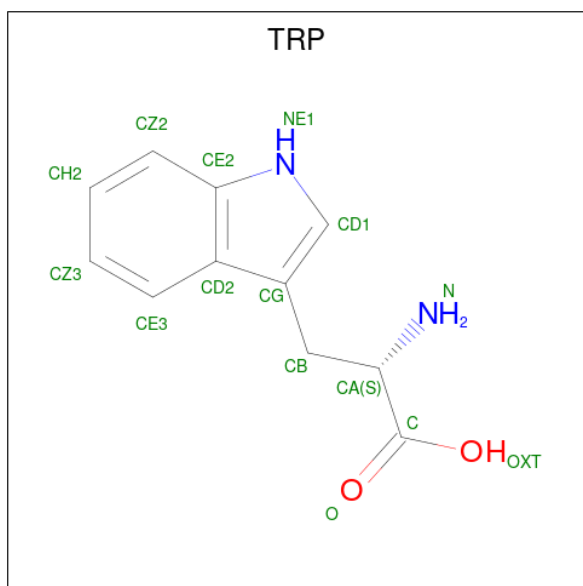
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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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 (CCD ID: 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		

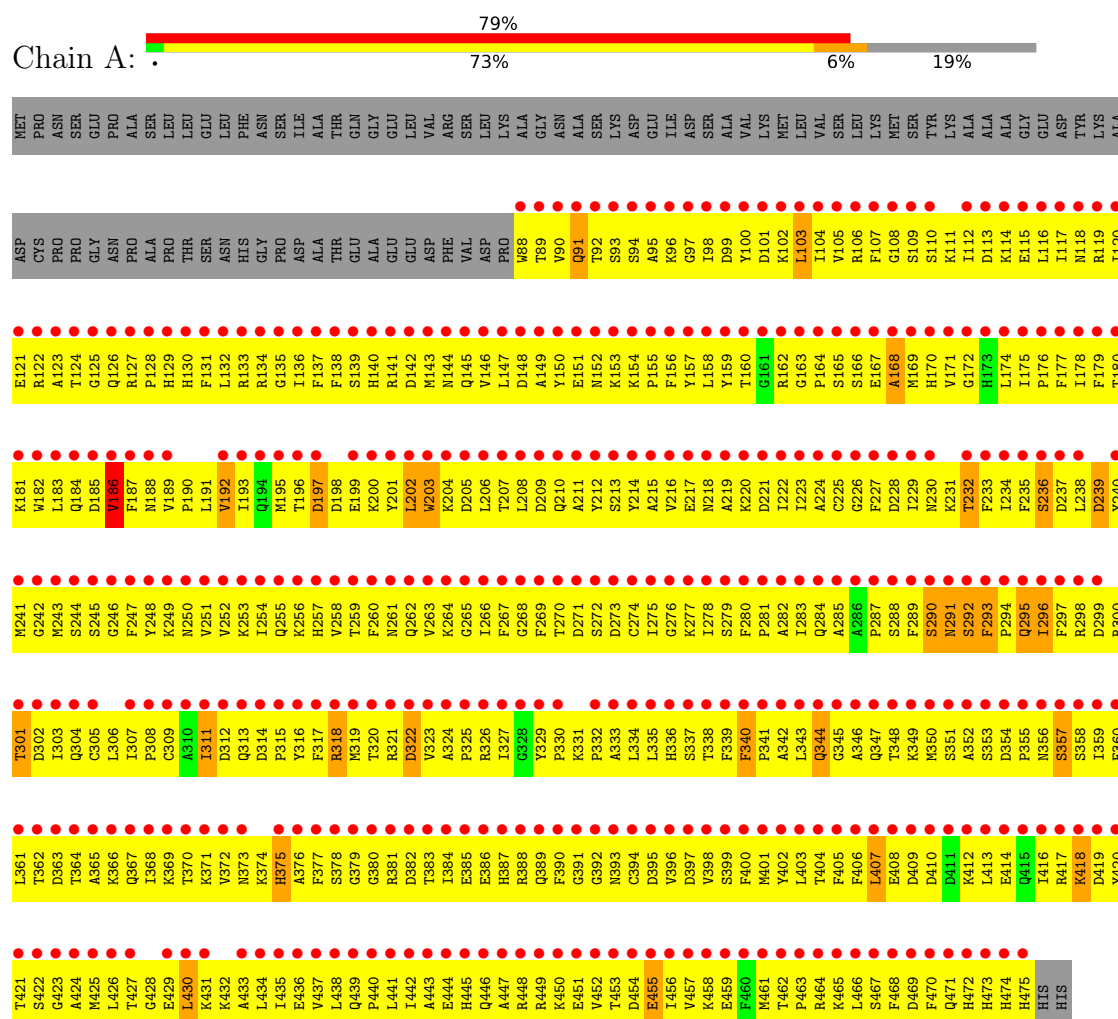
- Molecule 6 is water.

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

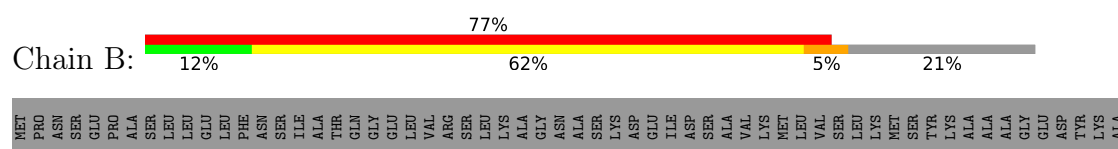
3 Residue-property plots

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: Tryptophanyl-tRNA synthetase



• Molecule 1: Tryptophanyl-tRNA synthetase



T421	L361	T301	M241	E121	ASP
S422	T362	D302	G242	K182	CYS
G423	D363	I303	N243	L183	PRO
A424	T364	Q304	S244	Q184	PRO
M425	A365	C305	S245	D185	GLY
L426	T366	L306	G246	V186	ASN
T427	T367	L307	F247	F187	PRO
G428	T368	P308	F248	N188	ALA
E429	T369	C309	K249	V189	PRO
L430	T370	A310	N250	H130	THR
K431	T371	I311	V251	L191	SER
K432	T372	D312	V252	V192	ASN
A433	N373	K313	K253	L132	HIS
L434	K374	D314	L254	R134	GLY
I435	H375	P315	Q255	G135	PRO
A436	A376	F316	K256	I136	ASP
V437	T377	V317	H257	F137	ALA
L438	T378	R318	V258	F138	THR
Q439	G379	M319	T259	D198	GLU
P440	G380	T320	F260	E199	ALA
L441	R381	N321	N261	K200	GLU
A443	D382	D322	Q262	Y201	GLU
A444	T383	V323	V263	L202	GLU
H445	T384	A324	K264	M143	ASP
H446	E385	P325	G265	K204	PHE
Q447	E386	R326	L266	D205	VAL
A448	T387	I327	F267	V146	ASP
R449	R388	G328	G268	L147	TRP
R450	Q389	V329	F269	D148	THR
K450	F390	F330	T270	A149	VAL
E451	G391	K331	D271	Q210	GLN
V452	G392	P332	S272	A211	THR
T453	N393	L333	D273	Y212	THR
D454	C394	L334	C274	K153	THR
E455	D395	L335	L275	Y214	THR
L456	V396	H336	G276	A215	THR
V457	T397	S337	K277	V216	THR
K458	V398	T338	L278	E217	THR
E459	S399	F339	S279	N218	THR
F460	F400	F340	M280	A219	THR
M461	M401	P341	P281	K220	THR
T462	Y402	A342	L282	D221	THR
P463	L403	L343	L283	L222	THR
R464	T404	Q344	Q284	I223	THR
K465	F405	G345	A285	P164	THR
L466	F406	A346	A286	C225	THR
S467	L407	Q347	P287	S165	THR
F468	E408	T348	S288	G226	THR
D469	D409	T349	F289	F227	THR
F470	D410	N350	S290	D228	THR
Q471	D411	S351	N291	M169	THR
HIS	K412	A352	S292	N230	THR
HIS	L413	S353	F293	K231	THR
HIS	E414	D354	P294	T232	THR
HIS	Q415	P355	Q295	F233	THR
HIS	L416	N356	L296	L234	THR
HIS	R417	F357	F297	F175	THR
HIS	K418	S358	R298	P176	THR
	D419	T359	D299	F177	THR
	Y420	F360	S300	I178	THR
				K181	THR
				L182	THR
				L183	THR
				Q184	THR
				D185	THR
				V186	THR
				F187	THR
				N188	THR
				V189	THR
				H130	THR
				F131	THR
				L132	THR
				R133	THR
				G134	THR
				M195	THR
				T196	THR
				D197	THR
				D198	THR
				E199	THR
				K200	THR
				Y201	THR
				L202	THR
				M143	THR
				K204	THR
				D205	THR
				V146	THR
				L147	THR
				D148	THR
				A149	THR
				Q210	THR
				A211	THR
				Y212	THR

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 50.00 – 2.42	Depositor EDS
% Data completeness (in resolution range)	87.9 (50.00-2.42) 88.1 (50.00-2.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.238 0.516 , 0.527	Depositor DCC
R_{free} test set	2190 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.79 , 744.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.37	EDS
Total number of atoms	6422	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TYM, CL, GOL

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	0.41	0/3184	0.95	12/4296 (0.3%)
1	B	0.43	0/3107	0.95	12/4195 (0.3%)
All	All	0.42	0/6291	0.95	24/8491 (0.3%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	ARG	N-CA-C	-10.36	100.06	111.36
1	A	318	ARG	N-CA-C	-9.89	100.58	111.36
1	A	357	SER	N-CA-C	-8.59	102.55	113.72
1	B	292	SER	N-CA-C	-7.12	104.39	113.23
1	A	340	PHE	N-CA-C	-6.51	101.45	109.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3106	0	3024	150	5477
1	B	3033	0	2971	124	3728
2	A	5	0	0	0	12
2	B	4	0	0	2	5

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	267	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 22.

The worst 5 of 267 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:350:MET:HE2	1:A:358:SER:HA	1.45	0.95

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%)	36	49
1	B	376/477 (79%)	362 (96%)	12 (3%)	2 (0%)	24	35
All	All	762/954 (80%)	732 (96%)	27 (4%)	3 (0%)	30	42

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 ⓘ

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%)	20	33
1	B	329/416 (79%)	312 (95%)	17 (5%)	21	34
All	All	664/832 (80%)	629 (95%)	35 (5%)	20	34

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	304	GLN
1	B	311	ILE
1	B	430	LEU
1	A	311	ILE
1	A	301	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	HIS
1	B	446	GLN
1	B	257	HIS

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Mol	Chain	Res	Type
1	B	347	GLN
1	B	170	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	40,41,41	1.78	7 (17%)	58,61,61	1.59	9 (15%)
4	GOL	B	812	-	5,5,5	4.56	5 (100%)	5,5,5	5.86	3 (60%)
4	GOL	A	813	-	5,5,5	4.60	5 (100%)	5,5,5	5.87	3 (60%)
4	GOL	A	814	-	5,5,5	4.69	5 (100%)	5,5,5	5.85	3 (60%)
4	GOL	B	815	-	5,5,5	4.57	5 (100%)	5,5,5	5.83	3 (60%)
5	TRP	B	817	-	15,16,16	1.53	5 (33%)	18,22,22	1.04	2 (11%)

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	-	-	1/21/39/39	0/5/5/5
4	GOL	B	812	-	-	2/4/4/4	-
4	GOL	A	813	-	-	3/4/4/4	-
4	GOL	A	814	-	-	3/4/4/4	-
4	GOL	B	815	-	-	2/4/4/4	-
5	TRP	B	817	-	-	0/8/8/8	0/2/2/2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	814	GOL	C3-C2	-8.06	1.21	1.51
4	B	812	GOL	C3-C2	-7.77	1.22	1.51
4	B	815	GOL	C3-C2	-7.75	1.22	1.51
4	A	813	GOL	C3-C2	-7.71	1.22	1.51
3	A	810	TYM	P-OPP	6.83	1.73	1.60

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	813	GOL	O3-C3-C2	10.10	155.86	110.38
4	B	812	GOL	O3-C3-C2	10.07	155.69	110.38
4	A	814	GOL	O3-C3-C2	10.06	155.67	110.38
4	B	815	GOL	O3-C3-C2	9.95	155.19	110.38
4	B	812	GOL	O2-C2-C3	7.68	140.99	109.18

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

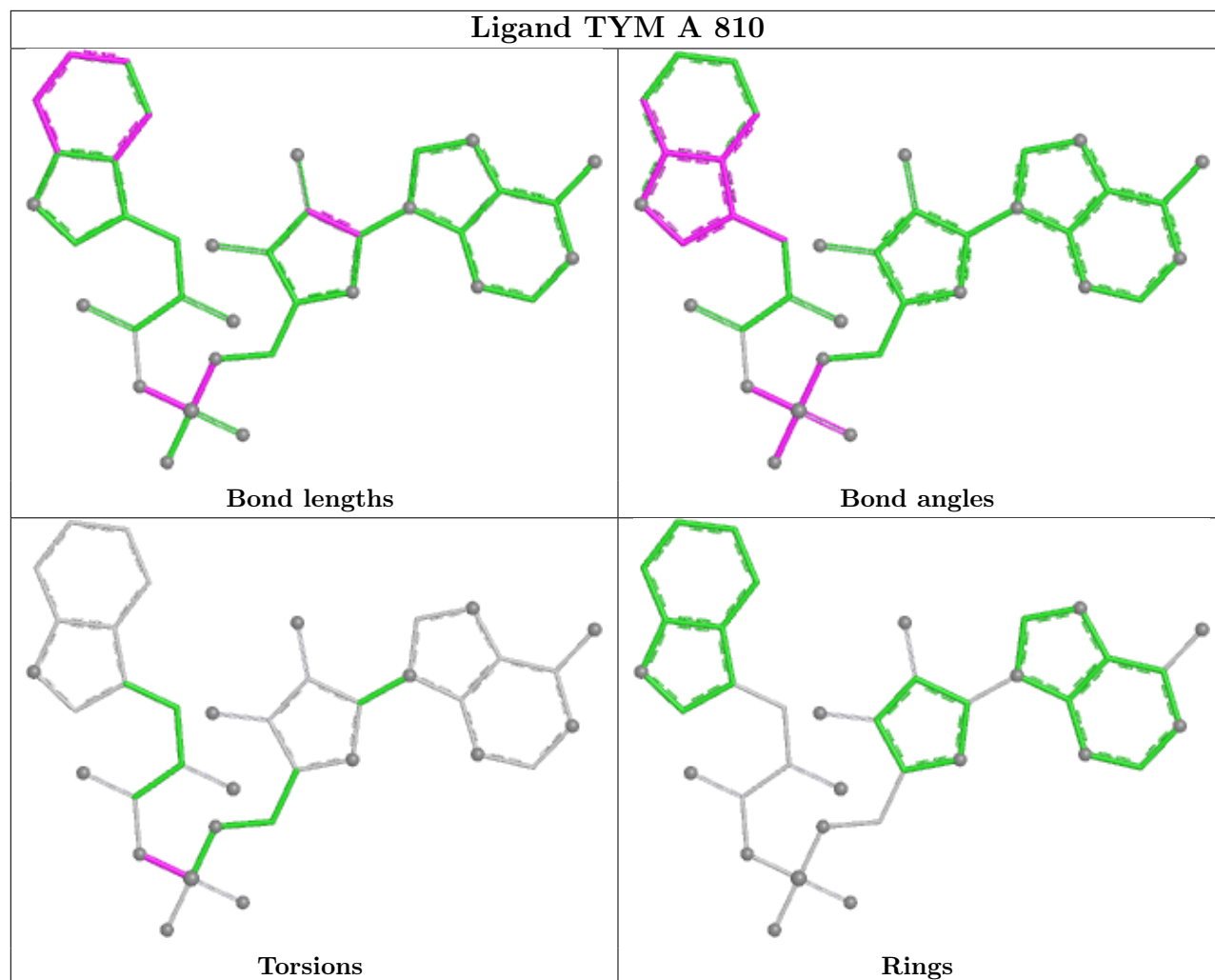
Mol	Chain	Res	Type	Atoms
4	A	813	GOL	O1-C1-C2-C3
4	A	813	GOL	C1-C2-C3-O3
4	A	814	GOL	O1-C1-C2-C3
4	A	814	GOL	C1-C2-C3-O3
4	B	812	GOL	C1-C2-C3-O3

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	812	GOL	0	33
4	A	813	GOL	0	4
4	A	814	GOL	2	28
4	B	815	GOL	1	3
5	B	817	TRP	0	25

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](#)

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	388/477 (81%)	5.14	376 (96%) 0 0	30, 47, 75, 107	0
1	B	378/477 (79%)	5.65	367 (97%) 0 0	28, 43, 69, 105	0
All	All	766/954 (80%)	5.39	743 (96%) 0 0	28, 45, 72, 107	0

The worst 5 of 743 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	GLY	17.8
1	B	348	THR	15.7
1	B	97	GLY	15.3
1	A	411	ASP	15.1
1	B	122	ARG	14.8

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](#)

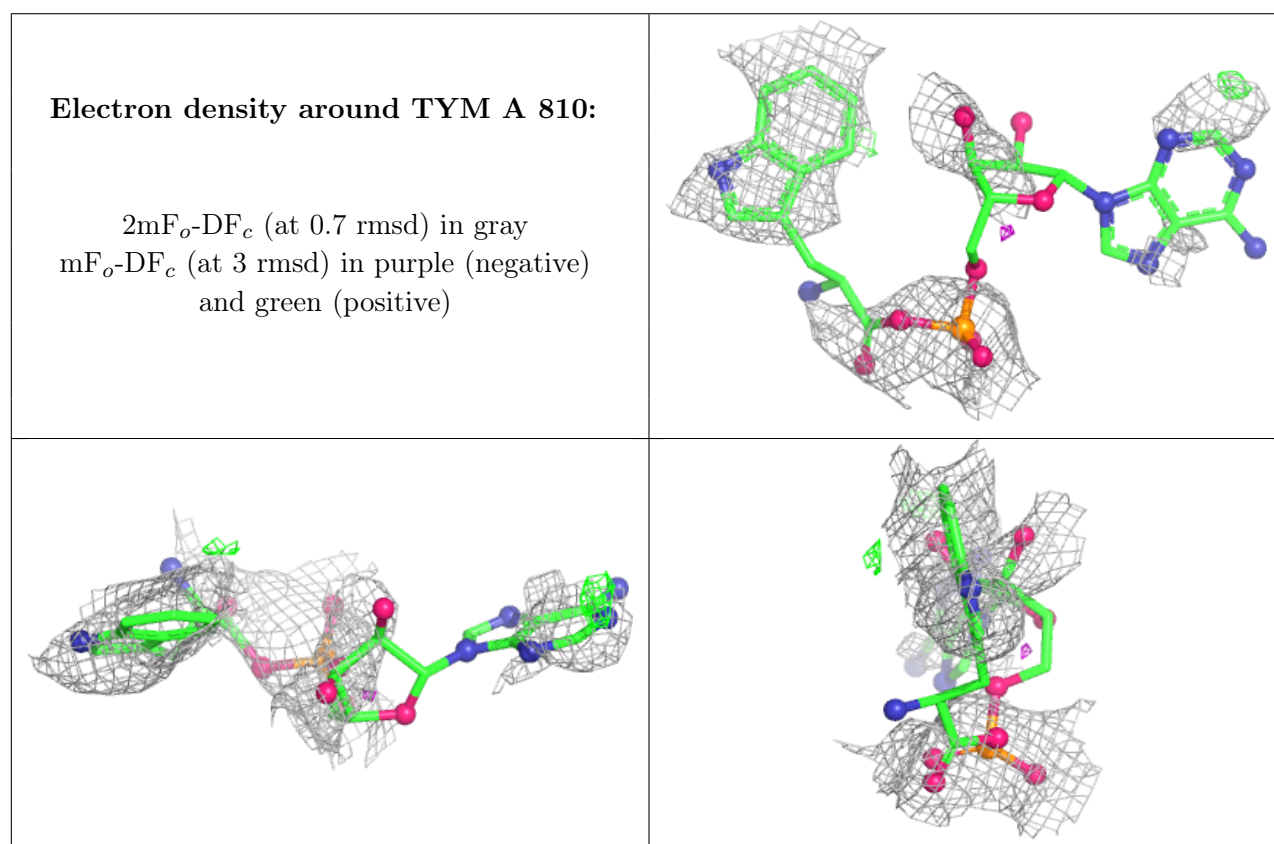
There are no oligosaccharides in this entry.

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
2	CL	B	801	1/1	-0.03	0.67	84,84,84,84	0
3	TYM	A	810	37/37	0.48	0.52	39,86,94,95	0
2	CL	B	806	1/1	0.50	0.86	66,66,66,66	0
4	GOL	A	813	6/6	0.56	0.56	61,62,63,63	0
2	CL	A	804	1/1	0.74	0.42	88,88,88,88	0
4	GOL	B	815	6/6	0.75	0.39	73,79,79,81	0
5	TRP	B	817	15/15	0.75	0.30	33,36,42,42	0
2	CL	A	807	1/1	0.77	0.24	73,73,73,73	0
2	CL	A	809	1/1	0.78	0.46	70,70,70,70	0
2	CL	A	802	1/1	0.82	0.46	89,89,89,89	0
4	GOL	A	814	6/6	0.82	0.21	72,73,73,75	0
4	GOL	B	812	6/6	0.83	0.21	62,62,62,62	0
2	CL	B	808	1/1	0.83	0.40	83,83,83,83	0
2	CL	A	805	1/1	0.83	0.34	78,78,78,78	0
2	CL	B	803	1/1	0.89	0.34	82,82,82,82	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.