

Full wwPDB X-ray Structure Validation Report (i)

Mar 15, 2022 - 06:07 PM EDT

PDB ID	:	6AMI
Title	:	Engineered tryptophan synthase b-subunit from Pyrococcus furiosus,
		PfTrpB4D11 with Trp non-covalently bound
Authors	:	Buller, A.R.
Deposited on	:	2017-08-09
Resolution	:	1.97 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 (i) symbol.

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

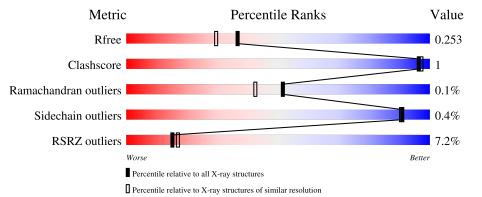
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.97 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	А	396	94%	
1	В	396	9%	•••
1	С	396	<u>6%</u> 93%	•••
1	D	396	9%	•••



6AMI

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11819 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.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	А	383	Total	С	Ν	0	Р	\mathbf{S}	0	0	0
	A	000	2867	1831	489	534	1	12	0	0	0
1	В	387	Total	С	Ν	0	Р	S	0	2	0
	I D	301	2941	1873	511	544	1	12	0	2	0
1	С	385	Total	С	Ν	0	Р	S	0	0	0
			2870	1830	490	537	1	12			0
1	1 D 384	384	Total	С	Ν	0	Р	S	0	0	0
		384	2857	1825	489	530	1	12	0	0	0

• Molecule 1 is a protein called Tryptophan synthase beta chain 1.

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	17	GLY	GLU	engineered mutation	UNP Q8U093
А	68	VAL	ILE	engineered mutation	UNP Q8U093
А	274	SER	PHE	engineered mutation	UNP Q8U093
А	292	SER	THR	engineered mutation	UNP Q8U093
А	321	ALA	THR	engineered mutation	UNP Q8U093
А	389	LEU	-	expression tag	UNP Q8U093
А	390	GLU	-	expression tag	UNP Q8U093
А	391	HIS	-	expression tag	UNP Q8U093
А	392	HIS	-	expression tag	UNP Q8U093
А	393	HIS	-	expression tag	UNP Q8U093
А	394	HIS	-	expression tag	UNP Q8U093
А	395	HIS	-	expression tag	UNP Q8U093
А	396	HIS	-	expression tag	UNP Q8U093
В	17	GLY	GLU	engineered mutation	UNP Q8U093
В	68	VAL	ILE	engineered mutation	UNP Q8U093
В	274	SER	PHE	engineered mutation	UNP Q8U093
В	292	SER	THR	engineered mutation	UNP Q8U093
В	321	ALA	THR	engineered mutation	UNP Q8U093
В	389	LEU	-	expression tag	UNP Q8U093
В	390	GLU	-	expression tag	UNP Q8U093
В	391	HIS	-	expression tag	UNP Q8U093



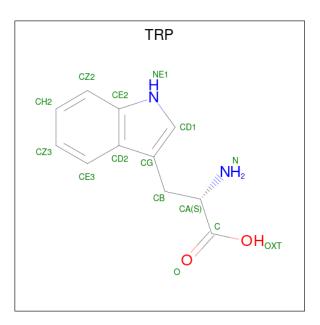
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Chain	Residue	Modelled	Actual	Comment	Reference
В	392	HIS	-	expression tag	UNP Q8U093
В	393	HIS	-	expression tag	UNP Q8U093
В	394	HIS	-	expression tag	UNP Q8U093
В	395	HIS	-	expression tag	UNP Q8U093
В	396	HIS	-	expression tag	UNP Q8U093
С	17	GLY	GLU	engineered mutation	UNP Q8U093
С	68	VAL	ILE	engineered mutation	UNP Q8U093
С	274	SER	PHE	engineered mutation	UNP Q8U093
С	292	SER	THR	engineered mutation	UNP Q8U093
С	321	ALA	THR	engineered mutation	UNP Q8U093
С	389	LEU	-	expression tag	UNP Q8U093
С	390	GLU	-	expression tag	UNP Q8U093
С	391	HIS	-	expression tag	UNP Q8U093
С	392	HIS	-	expression tag	UNP Q8U093
С	393	HIS	-	expression tag	UNP Q8U093
С	394	HIS	-	expression tag	UNP Q8U093
С	395	HIS	-	expression tag	UNP Q8U093
С	396	HIS	-	expression tag	UNP Q8U093
D	17	GLY	GLU	engineered mutation	UNP Q8U093
D	68	VAL	ILE	engineered mutation	UNP Q8U093
D	274	SER	PHE	engineered mutation	UNP Q8U093
D	292	SER	THR	engineered mutation	UNP Q8U093
D	321	ALA	THR	engineered mutation	UNP Q8U093
D	389	LEU	-	expression tag	UNP Q8U093
D	390	GLU	-	expression tag	UNP Q8U093
D	391	HIS	-	expression tag	UNP Q8U093
D	392	HIS	-	expression tag	UNP Q8U093
D	393	HIS	-	expression tag	UNP Q8U093
D	394	HIS	-	expression tag	UNP Q8U093
D	395	HIS	-	expression tag	UNP Q8U093
D	396	HIS	-	expression tag	UNP Q8U093

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• Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	Δ	1	Total	С	Ν	0	0	0
2	Л	1	15	11	2	2	0	0
2	В	1	Total	С	Ν	Ο	0	0
	D	1	15	11	2	2	0	0
2	С	1	Total	С	Ν	Ο	0	0
			15	11	2	2	0	0
2	Л	1	Total	С	Ν	Ο	0	0
	D	I	15	11	2	2	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Na 1 1	0	0
3	В	1	Total Na 1 1	0	0
3	С	2	Total Na 2 2	0	0
3	D	1	Total Na 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	56	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 56 & 56 \end{array}$	0	0



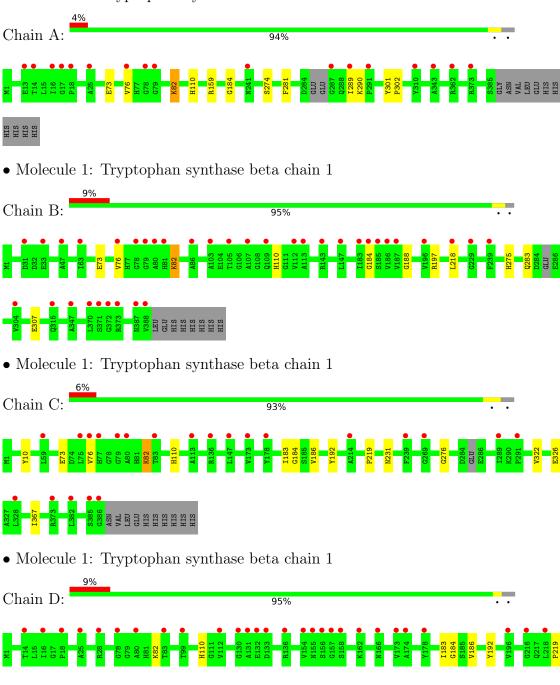
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	71	Total O 71 71	0	1
4	С	51	$\begin{array}{cc} \text{Total} & \text{O} \\ 51 & 51 \end{array}$	0	0
4	D	41	Total O 41 41	0	0



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: Tryptophan synthase beta chain 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	84.68Å 109.92Å 160.27Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 - 1.97	Depositor
Resolution (A)	39.51 - 1.97	EDS
% Data completeness	99.2 (40.00-1.97)	Depositor
(in resolution range)	99.2(39.51-1.97)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.55 (at 1.97 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
D D	0.215 , 0.251	Depositor
R, R_{free}	0.219 , 0.253	DCC
R_{free} test set	5311 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	37.1	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 33.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11819	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 7.38% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: LLP, NA

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		
	Unam	RMSZ $ \# Z > 5$		RMSZ	# Z > 5	
1	А	0.39	0/2901	0.58	0/3933	
1	В	0.38	0/2978	0.61	0/4030	
1	С	0.38	0/2904	0.59	0/3941	
1	D	0.38	0/2891	0.58	0/3922	
All	All	0.38	0/11674	0.59	0/15826	

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 (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	А	2867	0	2791	6	0
1	В	2941	0	2894	5	0
1	С	2870	0	2766	7	0
1	D	2857	0	2764	4	0
2	А	15	0	9	1	0
2	В	15	0	9	1	0
2	С	15	0	9	1	0
2	D	15	0	9	0	0
3	А	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	1	0	0	0	0
3	С	2	0	0	0	0
3	D	1	0	0	0	0
4	А	56	0	0	0	0
4	В	71	0	0	0	0
4	С	51	0	0	0	0
4	D	41	0	0	0	0
All	All	11819	0	11251	22	0

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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 (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:73:GLU:O	1:B:76:VAL:HG12	1.97	0.64
1:B:197:ARG:HD3	1:B:307:GLU:OE1	2.04	0.57
1:A:110:HIS:CE1	1:A:184:GLY:HA2	2.41	0.55
1:C:73:GLU:O	1:C:76:VAL:HG12	2.11	0.49
1:A:73:GLU:O	1:A:76:VAL:HG12	2.13	0.49
1:B:110:HIS:CE1	1:B:184:GLY:HA2	2.49	0.48
1:A:82:LLP:HE3	2:A:401:TRP:HB2	1.94	0.48
1:C:110:HIS:CE1	1:C:184:GLY:HA2	2.51	0.46
1:A:274:SER:HB3	1:A:281:PHE:CZ	2.52	0.44
1:D:110:HIS:CE1	1:D:184:GLY:HA2	2.52	0.44
1:C:82:LLP:HE3	2:C:401:TRP:HB2	2.01	0.43
1:B:188:GLY:HA2	1:B:275:HIS:O	2.19	0.42
1:D:219:PRO:HG3	1:D:367:ILE:HD12	2.01	0.42
1:A:274:SER:HB2	1:A:289:ILE:HD11	2.01	0.42
1:D:183:ILE:HD12	1:D:192:TYR:CG	2.55	0.42
1:A:301:TYR:CD1	1:A:302:PRO:HD2	2.56	0.41
1:C:10:TYR:O	1:C:276:GLY:HA2	2.21	0.41
1:C:183:ILE:HD12	1:C:192:TYR:CD2	2.55	0.41
1:B:82:LLP:HE3	2:B:401:TRP:HB2	2.02	0.41
1:C:219:PRO:HG3	1:C:367:ILE:HD12	2.02	0.41
1:D:183:ILE:HD12	1:D:192:TYR:CD2	2.56	0.40
1:C:322:VAL:HG13	1:C:326:GLU:HB2	2.03	0.40

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	Perce	entiles
1	А	378/396~(96%)	372~(98%)	6(2%)	0	100	100
1	В	384/396~(97%)	376~(98%)	8 (2%)	0	100	100
1	С	380/396~(96%)	371 (98%)	8 (2%)	1 (0%)	41	29
1	D	379/396~(96%)	369~(97%)	9~(2%)	1 (0%)	41	29
All	All	1521/1584~(96%)	1488 (98%)	31~(2%)	2~(0%)	51	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	186	VAL
1	С	186	VAL

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	Perc	entiles
1	А	279/313~(89%)	277~(99%)	2(1%)	84	83
1	В	290/313~(93%)	288 (99%)	2 (1%)	84	83
1	С	276/313~(88%)	275 (100%)	1 (0%)	91	90
1	D	274/313~(88%)	274 (100%)	0	100	100
All	All	1119/1252~(89%)	1114 (100%)	5 (0%)	91	90

All (5) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	159	ARG
1	А	290	LYS
1	В	218	LEU
1	В	283	GLN
1	С	231	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	40	ASN
1	D	166	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	l Type Chain Res		Dec	Link	Bond lengths			Bond angles		
10101	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	LLP	В	82	1	23,24,25	2.47	5 (21%)	25,32,34	1.43	5 (20%)
1	LLP	А	82	1	23,24,25	2.54	5 (21%)	25,32,34	1.45	3 (12%)
1	LLP	D	82	1	23,24,25	2.67	5 (21%)	25,32,34	1.28	3 (12%)
1	LLP	С	82	1	$23,\!24,\!25$	2.54	5 (21%)	25,32,34	1.36	3 (12%)

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
1	LLP	В	82	1	-	4/16/17/19	0/1/1/1
1	LLP	А	82	1	-	3/16/17/19	0/1/1/1
1	LLP	D	82	1	-	2/16/17/19	0/1/1/1
1	LLP	С	82	1	-	3/16/17/19	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	82	LLP	C3-C2	7.48	1.48	1.40
1	А	82	LLP	C3-C2	7.12	1.48	1.40
1	С	82	LLP	C3-C2	6.81	1.47	1.40
1	В	82	LLP	C3-C2	6.70	1.47	1.40
1	D	82	LLP	C4-C3	5.98	1.49	1.40
1	С	82	LLP	C4-C3	5.64	1.49	1.40
1	А	82	LLP	C4'-NZ	5.38	1.45	1.27
1	D	82	LLP	C4'-NZ	5.37	1.45	1.27
1	С	82	LLP	C4'-NZ	5.35	1.45	1.27
1	В	82	LLP	C4'-NZ	5.31	1.45	1.27
1	В	82	LLP	C4-C5	5.26	1.48	1.42
1	D	82	LLP	C4-C5	5.17	1.48	1.42
1	А	82	LLP	C4-C5	5.15	1.48	1.42
1	А	82	LLP	C4-C3	5.11	1.48	1.40
1	С	82	LLP	C4-C5	5.01	1.48	1.42
1	В	82	LLP	C4-C3	4.94	1.48	1.40
1	А	82	LLP	C4-C4'	2.81	1.52	1.46
1	D	82	LLP	C4-C4'	2.76	1.51	1.46
1	В	82	LLP	C4-C4'	2.69	1.51	1.46
1	С	82	LLP	C4-C4'	2.64	1.51	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	82	LLP	C3-C4-C5	-3.22	115.79	118.26
1	А	82	LLP	C4-C4'-NZ	-2.96	110.73	124.31
1	С	82	LLP	C4-C4'-NZ	-2.80	111.46	124.31
1	В	82	LLP	C3-C4-C5	-2.78	116.13	118.26
1	С	82	LLP	C3-C4-C5	-2.66	116.22	118.26
1	D	82	LLP	C4-C4'-NZ	-2.63	112.24	124.31
1	В	82	LLP	C4-C4'-NZ	-2.62	112.30	124.31
1	В	82	LLP	C6-N1-C2	2.43	123.67	119.17
1	D	82	LLP	C3-C4-C5	-2.42	116.41	118.26
1	С	82	LLP	C6-N1-C2	2.29	123.42	119.17



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	D	82	LLP	C6-N1-C2	2.21	123.27	119.17
1	В	82	LLP	O3-C3-C2	2.08	122.02	117.49
1	А	82	LLP	C2'-C2-N1	2.01	121.59	117.67
1	В	82	LLP	C2'-C2-N1	2.00	121.58	117.67

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There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	В	82	LLP	O-C-CA-CB
1	С	82	LLP	O-C-CA-CB
1	В	82	LLP	C4-C4'-NZ-CE
1	С	82	LLP	C4-C4'-NZ-CE
1	D	82	LLP	C4-C4'-NZ-CE
1	А	82	LLP	C4-C4'-NZ-CE
1	С	82	LLP	CD-CE-NZ-C4'
1	D	82	LLP	CD-CE-NZ-C4'
1	А	82	LLP	CD-CE-NZ-C4'
1	А	82	LLP	C3-C4-C4'-NZ
1	В	82	LLP	CD-CE-NZ-C4'
1	В	82	LLP	C3-C4-C4'-NZ

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	82	LLP	1	0
1	А	82	LLP	1	0
1	С	82	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	Turne	Chain	Res	Link	Bond lengths			Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	TRP	В	401	-	12,16,16	0.77	0	12,22,22	0.84	0
2	TRP	А	401	-	12,16,16	0.84	0	12,22,22	0.84	0
2	TRP	D	401	-	12,16,16	0.78	0	12,22,22	0.82	0
2	TRP	С	401	-	12,16,16	0.78	0	12,22,22	0.83	0

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	TRP	В	401	-	-	0/3/8/8	0/2/2/2
2	TRP	А	401	-	-	0/3/8/8	0/2/2/2
2	TRP	D	401	-	-	0/3/8/8	0/2/2/2
2	TRP	С	401	-	-	0/3/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

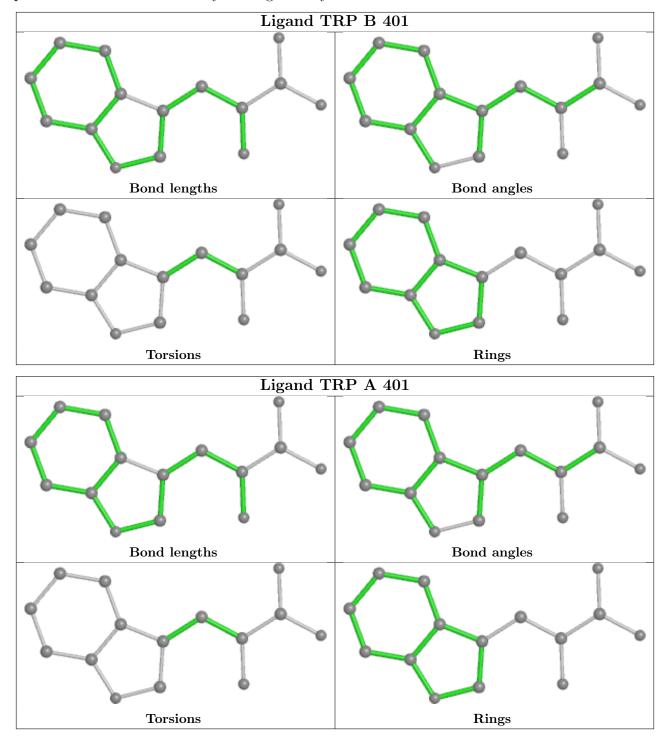
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	401	TRP	1	0
2	А	401	TRP	1	0
2	С	401	TRP	1	0

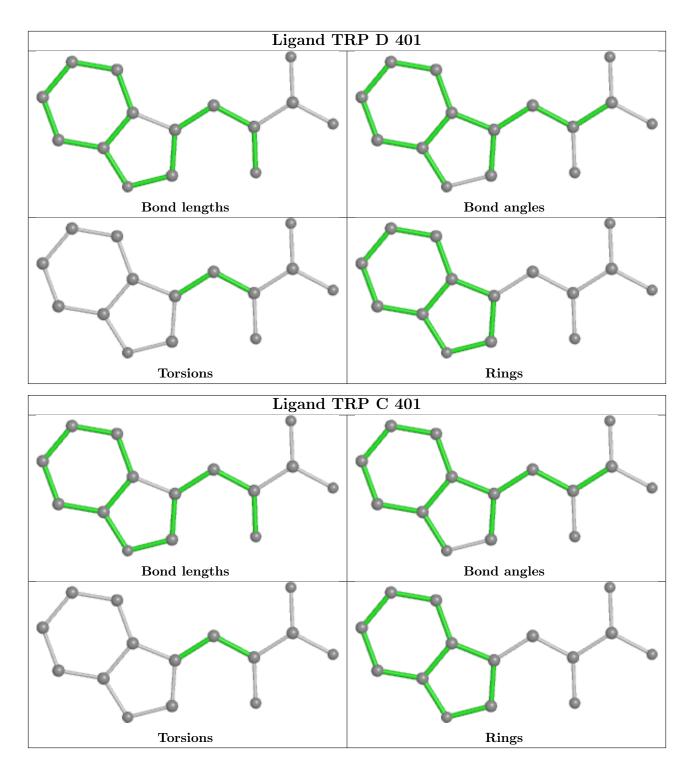
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$
1	А	382/396~(96%)	0.41	17 (4%) 33 35	32, 48, 61, 71	0
1	В	386/396~(97%)	0.62	36 (9%) 8 10	31, 41, 59, 72	0
1	С	384/396~(96%)	0.55	22 (5%) 23 25	31, 44, 63, 72	0
1	D	383/396~(96%)	0.68	35 (9%) 9 10	32, 52, 79, 114	0
All	All	1535/1584~(96%)	0.56	110 (7%) 15 17	31, 46, 67, 114	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	154	VAL	5.2
1	D	157	GLY	4.3
1	В	187	VAL	4.2
1	С	75	LEU	4.1
1	D	14	THR	4.0
1	В	372	GLY	3.9
1	С	385	SER	3.8
1	D	158	SER	3.7
1	D	173	VAL	3.7
1	С	289	ILE	3.7
1	В	109[A]	GLN	3.6
1	С	80	ALA	3.5
1	С	76	VAL	3.5
1	А	287	GLY	3.4
1	В	373	ARG	3.4
1	В	80	ALA	3.4
1	А	18	PRO	3.3
1	D	83	THR	3.2
1	D	291	PRO	3.2
1	В	79	GLY	3.2
1	А	291	PRO	3.2



Mol	nued fron Chain	Res	Type	RSRZ
1	D	132	GLU	3.2
1	D	287	GLY	3.2
1	А	13	GLU	3.1
1	В	76	VAL	3.1
1	D	156	SER	3.1
1	D	131	ALA	3.0
1	В	31	ASP	3.0
1	D	25	ALA	2.9
1	С	214	ALA	2.9
1	В	186	VAL	2.9
1	D	166	ASN	2.9
1	D	340	ILE	2.9
1	С	373	ARG	2.8
1	D	178	TYR	2.8
1	А	14	THR	2.7
1	В	143[A]	ARG	2.7
1	С	173	VAL	2.7
1	D	373	ARG	2.7
1	В	78	GLY	2.7
1	В	113	ALA	2.6
1	А	76	VAL	2.6
1	D	284	ASP	2.6
1	В	218	LEU	2.6
1	D	80	ALA	2.6
1	В	33	GLU	2.6
1	В	105	THR	2.6
1	С	239	PHE	2.6
1	В	185	SER	2.6
1	В	304	VAL	2.6
1	С	382	LEU	2.5
1	В	86	ALA	2.5
1	С	59	LEU	2.5
1	С	83	THR	2.5
1	В	371	SER	2.5
1	A	25	ALA	2.5
1	В	112	VAL	2.5
1	B	184	GLY	2.5
1	В	196	VAL	2.4
1	B	315	GLN	2.4
1	D	112	VAL	2.4
1	A	16	ILE	2.4
1	А	17	GLY	2.4

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Mol	nuea fron Chain	Res	Type	RSRZ
1	D	78	GLY	2.4
1	С	136	ARG	2.4
1	D	155	ASN	2.4
1	D	216	GLY	2.4
1	В	147	LEU	2.4
1	А	373	ARG	2.4
1	В	81	HIS	2.4
1	D	162	LYS	2.3
1	С	269	GLY	2.3
1	В	47	ALA	2.3
1	А	78	GLY	2.3
1	В	229	GLY	2.3
1	В	388	VAL	2.3
1	D	196	VAL	2.3
1	D	18	PRO	2.3
1	D	218	LEU	2.3
1	D	28	ARG	2.2
1	С	386	GLY	2.2
1	D	133	ASP	2.2
1	В	183	ILE	2.2
1	D	16	ILE	2.2
1	А	362	ARG	2.2
1	В	239	PHE	2.2
1	А	343	ALA	2.2
1	D	174	ALA	2.2
1	В	387	ASN	2.2
1	В	347	ALA	2.2
1	С	113	ALA	2.2
1	D	372	GLY	2.2
1	D	136	ARG	2.2
1	C C	291	PRO	2.1
1		77	HIS	2.1
1	С	79	GLY	2.1
1	А	79	GLY	2.1
1	В	103	ALA	2.1
1	D	273	VAL	2.1
1	А	289	ILE	2.1
1	В	63	ILE	2.1
1	В	107	ALA	2.1
1	С	147	LEU	2.1
1	А	241	ASN	2.1
1	А	310	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	В	370	LEU	2.1
1	D	130	GLY	2.1
1	С	178	TYR	2.0
1	С	328	LEU	2.0
1	D	99	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
1	LLP	А	82	24/25	0.96	0.19	$38,\!41,\!45,\!46$	0
1	LLP	D	82	24/25	0.97	0.18	38,42,44,45	0
1	LLP	С	82	24/25	0.98	0.18	33,35,36,37	0
1	LLP	В	82	24/25	0.98	0.24	33,34,35,35	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

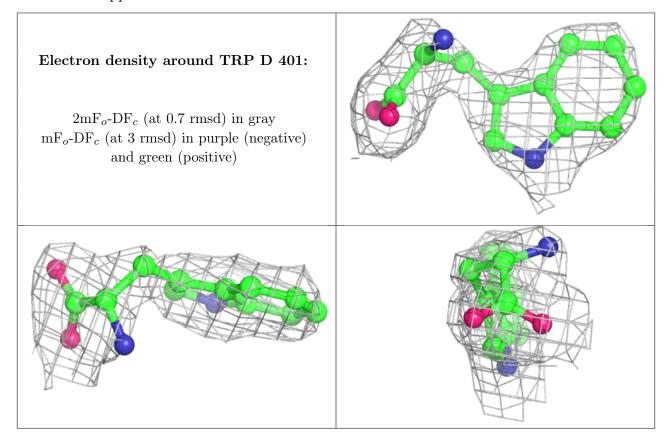
6.4 Ligands (i)

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, 95^{th} 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.

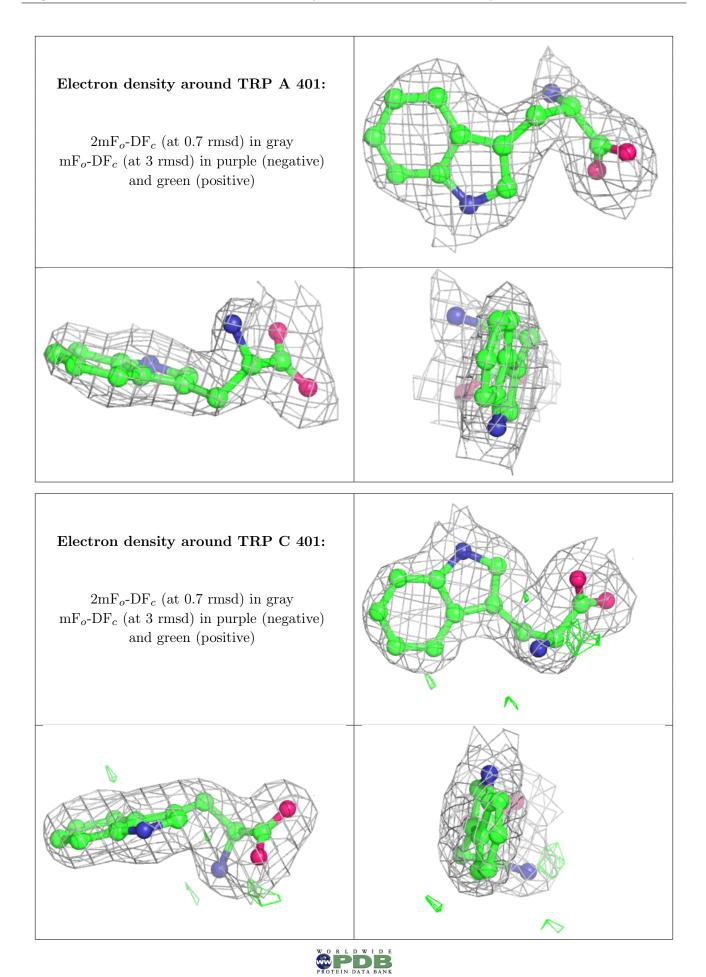
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
3	NA	D	402	1/1	0.88	0.17	48,48,48,48	0
2	TRP	D	401	15/15	0.90	0.13	49,52,53,54	0
2	TRP	А	401	15/15	0.90	0.14	41,42,43,44	0
3	NA	С	403	1/1	0.91	0.09	34,34,34,34	0
2	TRP	С	401	15/15	0.92	0.14	32,35,36,36	0
3	NA	А	402	1/1	0.93	0.10	$45,\!45,\!45,\!45$	0
2	TRP	В	401	15/15	0.95	0.17	28,29,30,30	0
3	NA	С	402	1/1	0.96	0.07	33,33,33,33	0
3	NA	В	402	1/1	0.98	0.15	36,36,36,36	0

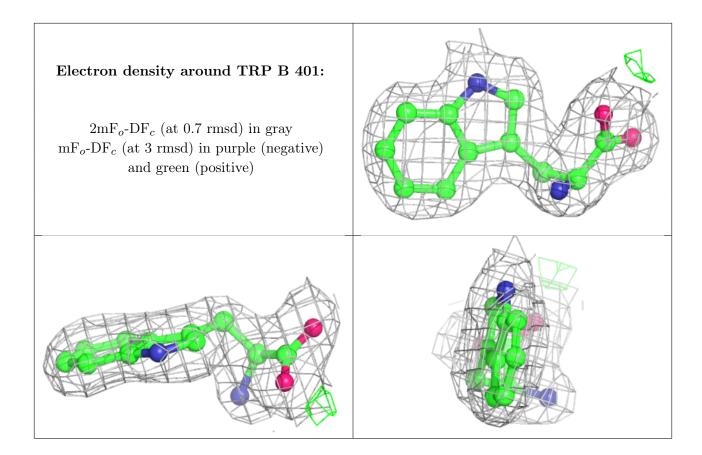


The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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









6.5 Other polymers (i)

There are no such residues in this entry.

