



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 01:28 AM EDT

PDB ID : 7ROF
Title : Engineered tryptophan synthase b-subunit from *Pyrococcus furiosus*, PfTrpB2B9-H275E with L-Trp non-covalently bound
Authors : Higgins, P.M.; Buller, A.R.
Deposited on : 2021-07-30
Resolution : 2.39 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 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

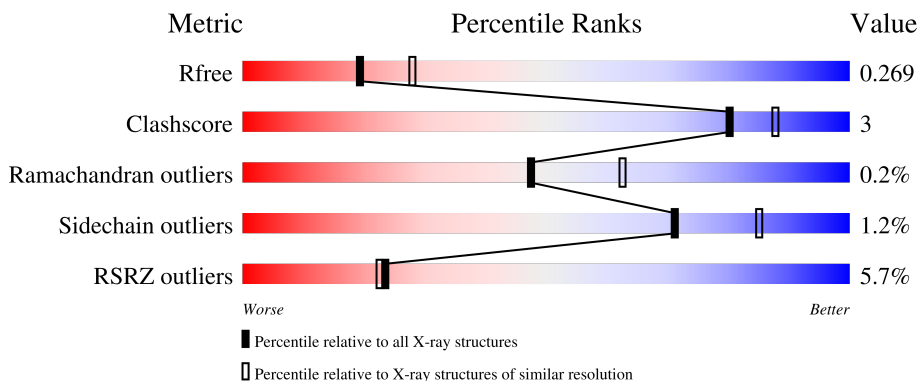
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	396	
1	B	396	
1	C	396	
1	D	396	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11153 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 Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	385	2851	1819	493	527	1	11	0	1	0
1	B	385	2749	1764	470	502	1	12	0	1	0
1	C	381	2718	1745	467	494	1	11	0	1	0
1	D	385	2792	1785	479	516	1	11	0	1	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	ILE	conflict	UNP Q8U093
A	17	GLY	GLU	conflict	UNP Q8U093
A	68	VAL	ILE	conflict	UNP Q8U093
A	95	LEU	PHE	conflict	UNP Q8U093
A	274	SER	PHE	conflict	UNP Q8U093
A	275	GLU	HIS	engineered mutation	UNP Q8U093
A	292	SER	THR	conflict	UNP Q8U093
A	321	ALA	THR	conflict	UNP Q8U093
A	384	ALA	VAL	conflict	UNP Q8U093
A	389	LEU	-	expression tag	UNP Q8U093
A	390	GLU	-	expression tag	UNP Q8U093
A	391	HIS	-	expression tag	UNP Q8U093
A	392	HIS	-	expression tag	UNP Q8U093
A	393	HIS	-	expression tag	UNP Q8U093
A	394	HIS	-	expression tag	UNP Q8U093
A	395	HIS	-	expression tag	UNP Q8U093
A	396	HIS	-	expression tag	UNP Q8U093
B	16	VAL	ILE	conflict	UNP Q8U093
B	17	GLY	GLU	conflict	UNP Q8U093
B	68	VAL	ILE	conflict	UNP Q8U093
B	95	LEU	PHE	conflict	UNP Q8U093

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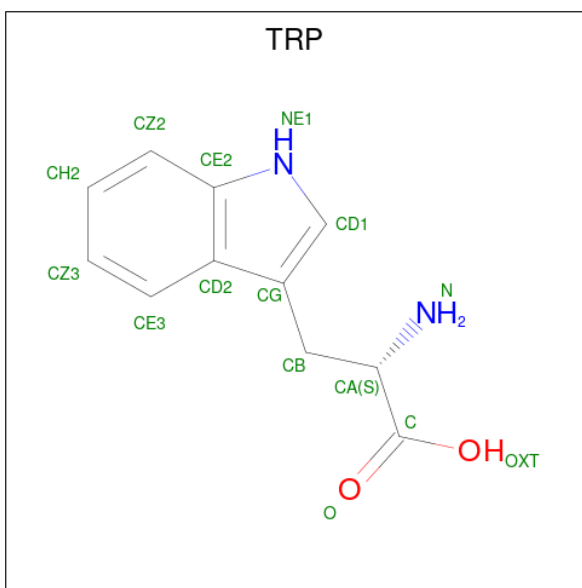
Chain	Residue	Modelled	Actual	Comment	Reference
B	274	SER	PHE	conflict	UNP Q8U093
B	275	GLU	HIS	engineered mutation	UNP Q8U093
B	292	SER	THR	conflict	UNP Q8U093
B	321	ALA	THR	conflict	UNP Q8U093
B	384	ALA	VAL	conflict	UNP Q8U093
B	389	LEU	-	expression tag	UNP Q8U093
B	390	GLU	-	expression tag	UNP Q8U093
B	391	HIS	-	expression tag	UNP Q8U093
B	392	HIS	-	expression tag	UNP Q8U093
B	393	HIS	-	expression tag	UNP Q8U093
B	394	HIS	-	expression tag	UNP Q8U093
B	395	HIS	-	expression tag	UNP Q8U093
B	396	HIS	-	expression tag	UNP Q8U093
C	16	VAL	ILE	conflict	UNP Q8U093
C	17	GLY	GLU	conflict	UNP Q8U093
C	68	VAL	ILE	conflict	UNP Q8U093
C	95	LEU	PHE	conflict	UNP Q8U093
C	274	SER	PHE	conflict	UNP Q8U093
C	275	GLU	HIS	engineered mutation	UNP Q8U093
C	292	SER	THR	conflict	UNP Q8U093
C	321	ALA	THR	conflict	UNP Q8U093
C	384	ALA	VAL	conflict	UNP Q8U093
C	389	LEU	-	expression tag	UNP Q8U093
C	390	GLU	-	expression tag	UNP Q8U093
C	391	HIS	-	expression tag	UNP Q8U093
C	392	HIS	-	expression tag	UNP Q8U093
C	393	HIS	-	expression tag	UNP Q8U093
C	394	HIS	-	expression tag	UNP Q8U093
C	395	HIS	-	expression tag	UNP Q8U093
C	396	HIS	-	expression tag	UNP Q8U093
D	16	VAL	ILE	conflict	UNP Q8U093
D	17	GLY	GLU	conflict	UNP Q8U093
D	68	VAL	ILE	conflict	UNP Q8U093
D	95	LEU	PHE	conflict	UNP Q8U093
D	274	SER	PHE	conflict	UNP Q8U093
D	275	GLU	HIS	engineered mutation	UNP Q8U093
D	292	SER	THR	conflict	UNP Q8U093
D	321	ALA	THR	conflict	UNP Q8U093
D	384	ALA	VAL	conflict	UNP Q8U093
D	389	LEU	-	expression tag	UNP Q8U093
D	390	GLU	-	expression tag	UNP Q8U093
D	391	HIS	-	expression tag	UNP Q8U093

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	11	2	2	0	0
2	D	1	15	11	2	2	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0

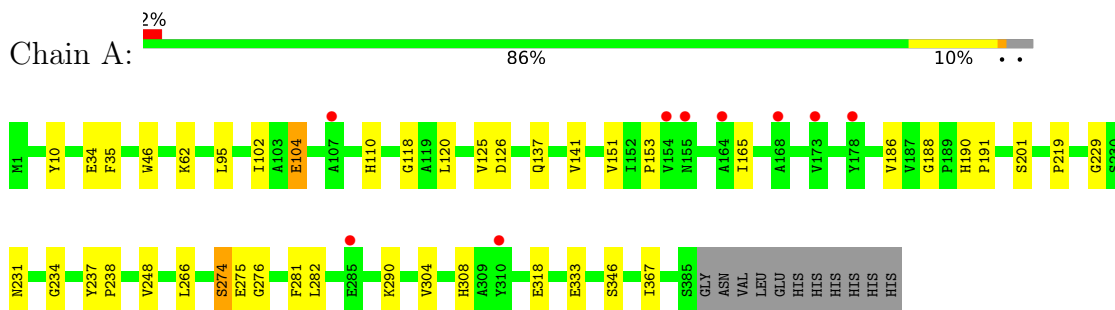
- Molecule 4 is water.

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

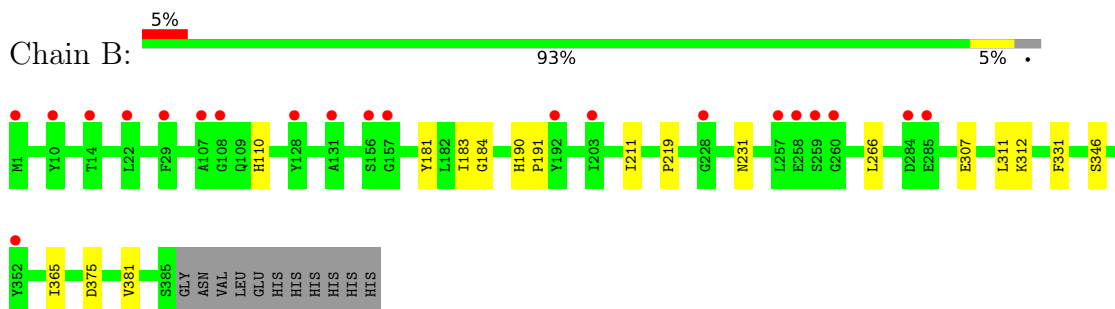
3 Residue-property plots [i](#)

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.

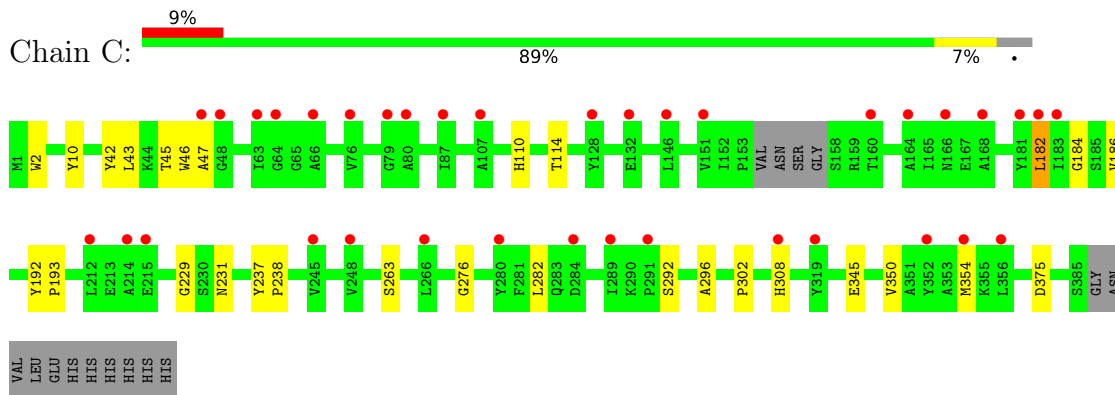
- Molecule 1: Tryptophan synthase beta chain 1



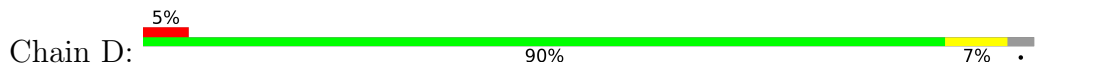
- Molecule 1: Tryptophan synthase beta chain 1

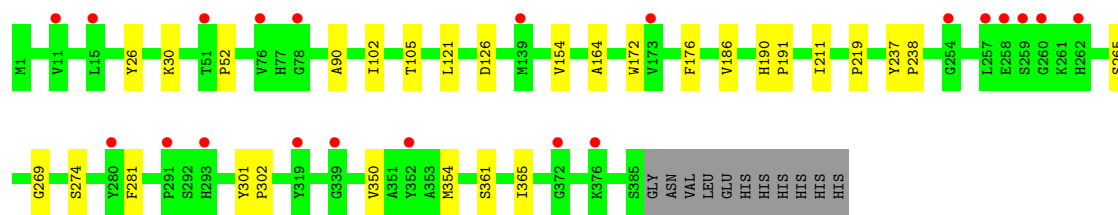


- Molecule 1: Tryptophan synthase beta chain 1



- Molecule 1: Tryptophan synthase beta chain 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.40Å 82.66Å 322.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.39 46.65 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.70-2.39) 99.3 (46.65-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.227 , 0.271 0.228 , 0.269	Depositor DCC
R_{free} test set	3098 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtrriage
Anisotropy	0.402	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.3	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	0.94	EDS
Total number of atoms	11153	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.86% 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: NA, LLP

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	0.68	1/2887 (0.0%)	0.73	0/3922
1	B	0.67	0/2785	0.72	0/3800
1	C	0.68	0/2753	0.71	0/3757
1	D	0.67	0/2828	0.71	0/3853
All	All	0.67	1/11253 (0.0%)	0.72	0/15332

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	GLU	CD-OE2	5.70	1.31	1.25

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	A	2851	0	2755	20	0
1	B	2749	0	2585	9	0
1	C	2718	0	2548	14	0
1	D	2792	0	2643	16	0
2	A	15	0	9	1	0
2	D	15	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
All	All	11153	0	10549	58	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 3.

All (58) 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:62:LYS:NZ	1:A:333:GLU:OE2	2.31	0.64
1:B:110:HIS:CE1	1:B:184:GLY:HA2	2.35	0.62
1:D:172:TRP:O	1:D:176:PHE:HB3	2.01	0.61
1:D:274:SER:HB3	1:D:281:PHE:CE2	2.40	0.57
1:D:102:ILE:HA	1:D:126:ASP:O	2.08	0.54
1:A:151:VAL:O	1:A:153:PRO:HD3	2.11	0.51
1:C:114:THR:HG23	1:C:182:LEU:HD13	1.93	0.51
1:C:350:VAL:O	1:C:354:MET:HG3	2.11	0.50
1:A:110:HIS:HB2	2:A:401:TRP:HA	1.94	0.49
1:B:266:LEU:O	1:B:312:LYS:HE3	2.13	0.48
1:D:211:ILE:HD11	1:D:365:ILE:HG21	1.96	0.47
1:D:301:TYR:CD1	1:D:302:PRO:HD2	2.48	0.47
1:D:90:ALA:HB1	1:D:121:LEU:HD12	1.97	0.47
1:B:190:HIS:CG	1:B:191:PRO:HA	2.50	0.46
1:C:296:ALA:HB1	1:C:345:GLU:HG3	1.97	0.46
1:A:118:GLY:HA3	1:A:125:VAL:HG21	1.98	0.46
1:A:237:TYR:HB3	1:A:238:PRO:HD3	1.97	0.46
1:D:237:TYR:HB3	1:D:238:PRO:HD3	1.98	0.46
1:A:35:PHE:HD1	1:A:95:LEU:HD12	1.81	0.46
1:A:219:PRO:HG3	1:A:367:ILE:HD12	1.99	0.45
1:A:104:GLU:HG2	1:A:165:ILE:HG12	1.97	0.45
1:C:42:TYR:O	1:C:46:TRP:HB3	2.16	0.45
1:B:190:HIS:ND1	1:B:191:PRO:HA	2.30	0.45
1:A:282:LEU:HB3	1:A:290:LYS:HE2	1.98	0.45
1:C:192:TYR:HB2	1:C:193:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:SER:OG	1:C:292:SER:HB2	2.16	0.45
1:D:211:ILE:HG21	1:D:219:PRO:HD3	1.98	0.45
1:C:229:GLY:HA3	1:C:308:HIS:CD2	2.51	0.45
1:A:10:TYR:O	1:A:276:GLY:HA2	2.17	0.44
1:C:110:HIS:CE1	1:C:184:GLY:HA2	2.53	0.44
1:B:331:PHE:CZ	1:B:381:VAL:HG21	2.52	0.44
1:A:201:SER:HA	1:A:234:GLY:O	2.18	0.44
1:A:266:LEU:HG	1:A:304:VAL:HG11	2.00	0.44
1:D:102:ILE:HD11	1:D:172:TRP:HB2	1.99	0.44
1:A:137:GLN:O	1:A:141:VAL:HG23	2.19	0.43
1:C:237:TYR:HB3	1:C:238:PRO:HD3	2.00	0.43
1:D:154:VAL:HG21	1:D:164:ALA:HA	1.99	0.43
1:B:211:ILE:HD11	1:B:365:ILE:HG21	2.00	0.43
1:D:350:VAL:O	1:D:354:MET:HG3	2.17	0.43
1:C:45:THR:HA	1:D:52:PRO:HB2	2.01	0.43
1:D:190:HIS:CG	1:D:191:PRO:HA	2.54	0.43
1:A:102:ILE:HA	1:A:126:ASP:O	2.19	0.42
1:A:229:GLY:HA3	1:A:308:HIS:CD2	2.55	0.42
1:C:43:LEU:O	1:C:47:ALA:HB3	2.20	0.42
1:B:307:GLU:O	1:B:311:LEU:HG	2.19	0.42
1:C:10:TYR:O	1:C:276:GLY:HA2	2.20	0.42
1:A:188:GLY:HA2	1:A:275:GLU:O	2.20	0.41
1:B:211:ILE:HG21	1:B:219:PRO:HD3	2.02	0.41
1:D:26:TYR:O	1:D:30:LYS:HB3	2.20	0.41
1:A:190:HIS:ND1	1:A:191:PRO:HA	2.36	0.41
1:A:248:VAL:HA	1:A:318:GLU:O	2.21	0.41
1:A:274:SER:HB3	1:A:281:PHE:CE1	2.56	0.40
1:A:46:TRP:CD1	1:A:120:LEU:HD13	2.57	0.40
1:C:282:LEU:HD12	1:C:302:PRO:HA	2.04	0.40
1:B:181:TYR:CE2	1:B:183:ILE:HD11	2.56	0.40
1:C:2:TRP:HH2	1:C:10:TYR:HH	1.66	0.40
1:D:190:HIS:ND1	1:D:191:PRO:HA	2.36	0.40
1:D:265:SER:O	1:D:269:GLY:HA3	2.22	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	Percentiles	
1	A	383/396 (97%)	370 (97%)	12 (3%)	1 (0%)	41	55
1	B	383/396 (97%)	370 (97%)	13 (3%)	0	100	100
1	C	377/396 (95%)	360 (96%)	16 (4%)	1 (0%)	41	55
1	D	383/396 (97%)	371 (97%)	11 (3%)	1 (0%)	41	55
All	All	1526/1584 (96%)	1471 (96%)	52 (3%)	3 (0%)	47	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	186	VAL
1	A	186	VAL
1	D	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	Percentiles	
1	A	270/312 (86%)	266 (98%)	4 (2%)	65	80
1	B	245/312 (78%)	242 (99%)	3 (1%)	71	85
1	C	240/312 (77%)	237 (99%)	3 (1%)	69	84
1	D	255/312 (82%)	253 (99%)	2 (1%)	81	91
All	All	1010/1248 (81%)	998 (99%)	12 (1%)	71	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	GLU
1	A	231	ASN
1	A	274	SER
1	A	346	SER
1	B	231	ASN
1	B	346	SER
1	B	375	ASP
1	C	182	LEU
1	C	231	ASN
1	C	375	ASP
1	D	105	THR
1	D	361	SER

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

Mol	Chain	Res	Type
1	A	155	ASN
1	C	217	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](#)

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LLP	C	82	1	23,24,25	0.48	0	25,32,34	0.59	0
1	LLP	A	82	1	23,24,25	0.55	0	25,32,34	0.55	0
1	LLP	D	82	1	23,24,25	0.47	0	25,32,34	0.52	0
1	LLP	B	82	1	23,24,25	0.47	0	25,32,34	0.50	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
1	LLP	C	82	1	-	5/16/17/19	0/1/1/1
1	LLP	A	82	1	-	6/16/17/19	0/1/1/1
1	LLP	D	82	1	-	9/16/17/19	0/1/1/1
1	LLP	B	82	1	-	7/16/17/19	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	82	LLP	C4-C4'-NZ-CE
1	B	82	LLP	C5-C4-C4'-NZ
1	B	82	LLP	C4-C4'-NZ-CE
1	B	82	LLP	C5'-OP4-P-OP2
1	B	82	LLP	C5'-OP4-P-OP3
1	C	82	LLP	C4-C4'-NZ-CE
1	D	82	LLP	C4-C4'-NZ-CE
1	D	82	LLP	C5'-OP4-P-OP2
1	B	82	LLP	C3-C4-C4'-NZ
1	D	82	LLP	CA-CB-CG-CD
1	B	82	LLP	C5'-OP4-P-OP1
1	D	82	LLP	C5'-OP4-P-OP1
1	D	82	LLP	C3-C4-C4'-NZ
1	A	82	LLP	CE-CD-CG-CB
1	D	82	LLP	C5'-OP4-P-OP3
1	B	82	LLP	CD-CE-NZ-C4'
1	D	82	LLP	CD-CE-NZ-C4'
1	C	82	LLP	CE-CD-CG-CB
1	A	82	LLP	CG-CD-CE-NZ
1	D	82	LLP	CG-CD-CE-NZ
1	A	82	LLP	C3-C4-C4'-NZ
1	C	82	LLP	C3-C4-C4'-NZ
1	C	82	LLP	CG-CD-CE-NZ
1	A	82	LLP	C5'-OP4-P-OP3
1	C	82	LLP	C5'-OP4-P-OP3

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Mol	Chain	Res	Type	Atoms
1	A	82	LLP	C5'-OP4-P-OP1
1	D	82	LLP	C5-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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	TRP	D	401	-	14,16,16	0.82	1 (7%)	16,22,22	1.07	2 (12%)
2	TRP	A	401	-	14,16,16	0.85	1 (7%)	16,22,22	1.00	1 (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
2	TRP	D	401	-	-	5/7/8/8	0/2/2/2
2	TRP	A	401	-	-	5/7/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	TRP	OXT-C	-2.33	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	TRP	OXT-C	-2.21	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	TRP	OXT-C-O	-2.50	118.41	124.09
2	A	401	TRP	OXT-C-O	-2.27	118.94	124.09
2	D	401	TRP	CH2-CZ2-CE2	-2.03	117.17	120.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	TRP	O-C-CA-N
2	D	401	TRP	O-C-CA-N
2	D	401	TRP	CA-CB-CG-CD1
2	A	401	TRP	OXT-C-CA-N
2	D	401	TRP	OXT-C-CA-N
2	D	401	TRP	O-C-CA-CB
2	D	401	TRP	OXT-C-CA-CB
2	A	401	TRP	O-C-CA-CB
2	A	401	TRP	OXT-C-CA-CB
2	A	401	TRP	CA-CB-CG-CD1

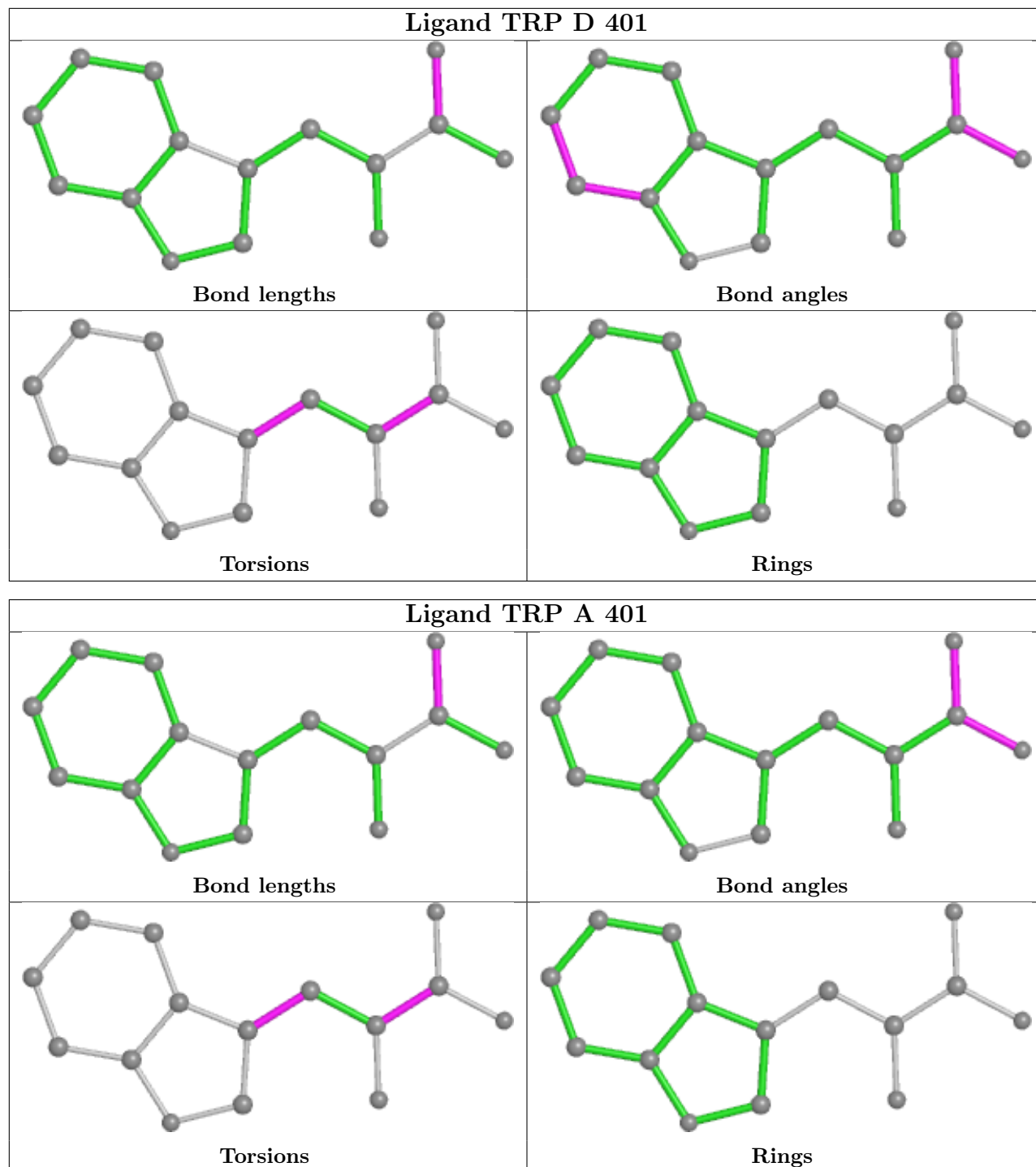
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	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 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

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	A	384/396 (96%)	0.13	9 (2%) 60 58	41, 61, 92, 116	0
1	B	384/396 (96%)	0.35	21 (5%) 25 24	49, 87, 122, 136	0
1	C	380/396 (95%)	0.53	36 (9%) 8 7	61, 91, 129, 145	0
1	D	384/396 (96%)	0.32	21 (5%) 25 24	56, 82, 118, 145	0
All	All	1532/1584 (96%)	0.33	87 (5%) 23 22	41, 81, 121, 145	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	164	ALA	8.9
1	C	151	VAL	8.0
1	A	168	ALA	6.0
1	A	164	ALA	5.6
1	D	258	GLU	5.3
1	B	108	GLY	4.0
1	C	160	THR	4.0
1	B	107	ALA	3.9
1	C	352	TYR	3.9
1	C	215	GLU	3.8
1	A	178	TYR	3.8
1	C	166	ASN	3.7
1	D	260	GLY	3.7
1	C	128	TYR	3.7
1	A	155	ASN	3.6
1	B	257	LEU	3.6
1	D	259	SER	3.6
1	C	245	VAL	3.5
1	D	293	HIS	3.5
1	B	259	SER	3.5
1	B	352	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	260	GLY	3.4
1	D	257	LEU	3.3
1	D	262	HIS	3.2
1	C	291	PRO	3.2
1	B	128	TYR	3.2
1	C	64	GLY	3.1
1	C	214	ALA	3.1
1	C	248	VAL	3.0
1	C	280	TYR	3.0
1	C	266	LEU	3.0
1	A	154	VAL	3.0
1	C	168	ALA	3.0
1	B	228	GLY	2.9
1	C	284	ASP	2.9
1	B	131	ALA	2.9
1	D	78	GLY	2.9
1	C	183	ILE	2.8
1	C	181	TYR	2.8
1	C	47	ALA	2.7
1	D	254	GLY	2.7
1	A	107	ALA	2.7
1	B	157	GLY	2.7
1	D	15	LEU	2.6
1	B	10	TYR	2.6
1	B	29	PHE	2.6
1	D	280	TYR	2.5
1	B	284	ASP	2.5
1	D	51	THR	2.5
1	C	107	ALA	2.4
1	C	182	LEU	2.4
1	D	11	VAL	2.4
1	B	22	LEU	2.4
1	B	285	GLU	2.4
1	C	132	GLU	2.3
1	C	87	ILE	2.3
1	B	14	THR	2.3
1	C	146	LEU	2.3
1	D	76	VAL	2.3
1	C	48	GLY	2.3
1	C	289	ILE	2.3
1	B	192	TYR	2.3
1	B	156	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	354	MET	2.2
1	A	310	TYR	2.2
1	C	319	TYR	2.2
1	D	291	PRO	2.2
1	C	356	LEU	2.2
1	D	352	TYR	2.2
1	A	173	VAL	2.2
1	C	80	ALA	2.2
1	B	258	GLU	2.2
1	B	1	MET	2.2
1	C	66	ALA	2.1
1	C	79	GLY	2.1
1	D	372	GLY	2.1
1	C	308	HIS	2.1
1	D	376	LYS	2.1
1	C	63	ILE	2.1
1	D	173	VAL	2.1
1	D	319	TYR	2.1
1	D	139	MET	2.1
1	C	212	LEU	2.0
1	D	339	GLY	2.0
1	C	76	VAL	2.0
1	A	285	GLU	2.0
1	B	203	ILE	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, 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(Å ²)	Q<0.9
1	LLP	A	82	24/25	0.93	0.19	50,60,65,67	0
1	LLP	B	82	24/25	0.93	0.17	58,77,80,82	0
1	LLP	C	82	24/25	0.95	0.21	67,77,80,81	0
1	LLP	D	82	24/25	0.95	0.18	63,73,76,76	0

6.3 Carbohydrates [i](#)

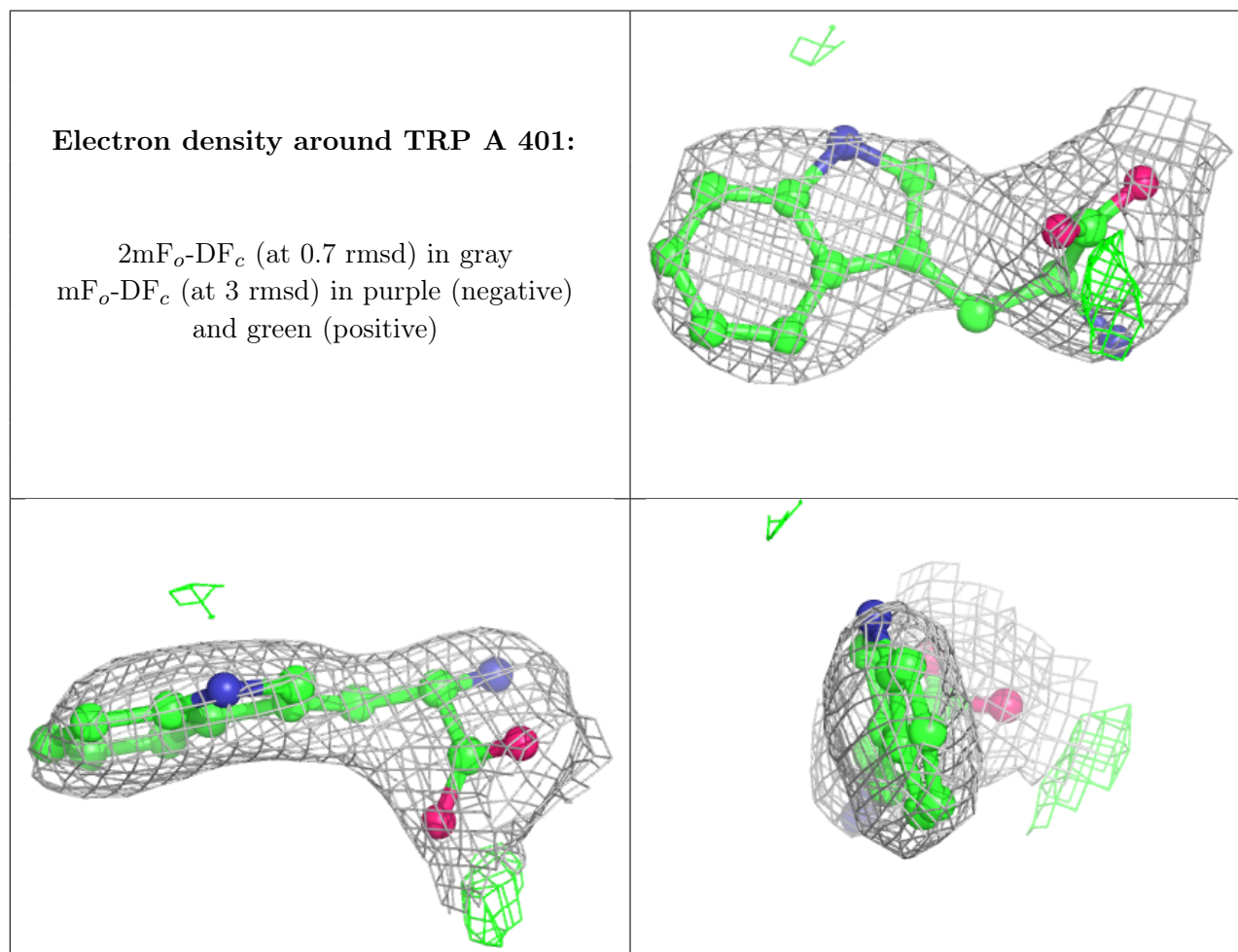
There are no monosaccharides in this entry.

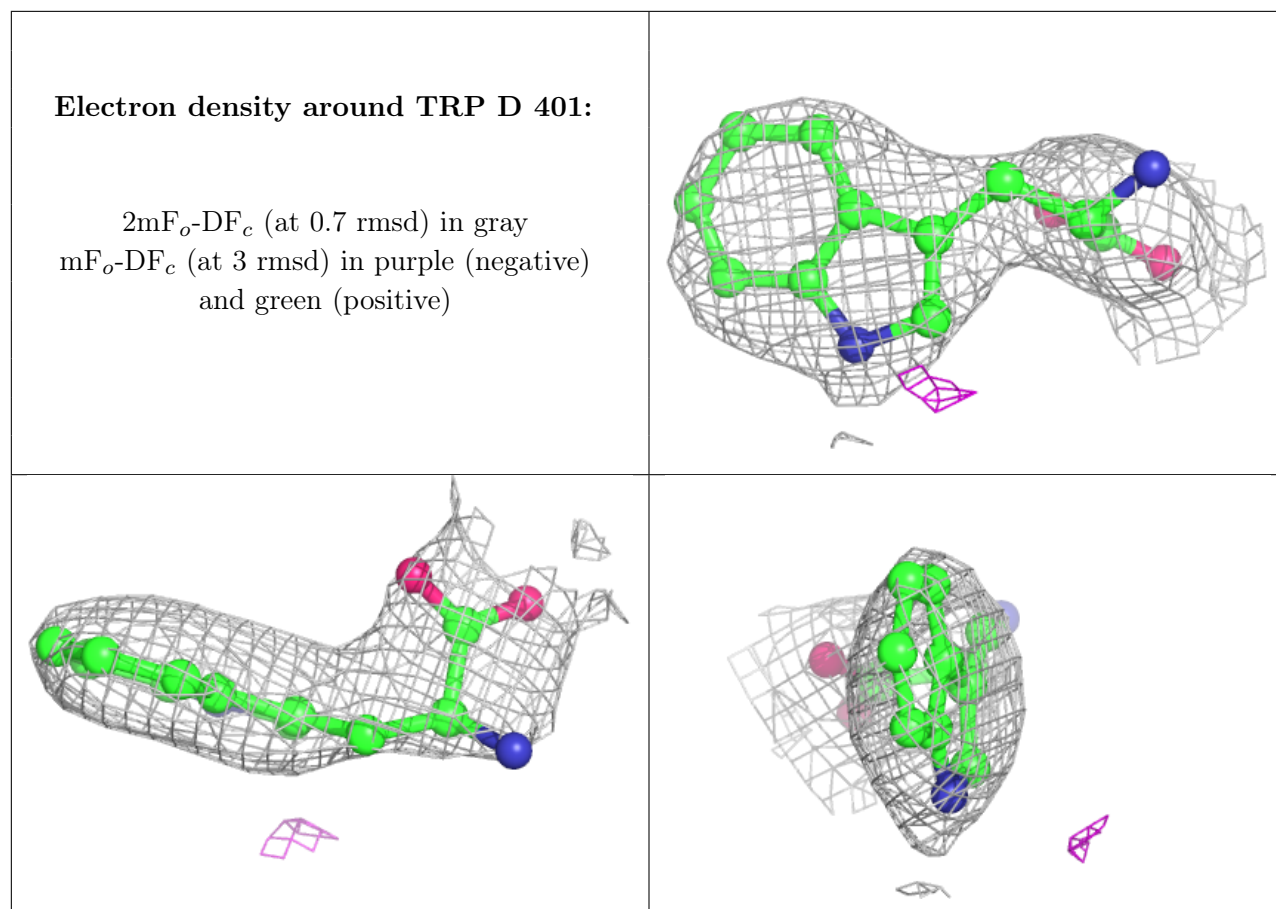
6.4 Ligands [i](#)

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, 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(Å ²)	Q<0.9
3	NA	D	402	1/1	0.86	0.21	87,87,87,87	0
2	TRP	A	401	15/15	0.90	0.16	85,88,93,94	0
3	NA	A	402	1/1	0.91	0.18	51,51,51,51	0
3	NA	B	401	1/1	0.93	0.12	85,85,85,85	0
2	TRP	D	401	15/15	0.94	0.16	105,111,116,117	0
3	NA	C	401	1/1	0.97	0.17	85,85,85,85	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.