



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:52 am BST

PDB ID : 6AM8
Title : Engineered tryptophan synthase b-subunit from *Pyrococcus furiosus*, PfTrpB2B9 with Trp bound as E(Aex2)
Authors : Buller, A.R.; van Roye, P.
Deposited on : 2017-08-09
Resolution : 1.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

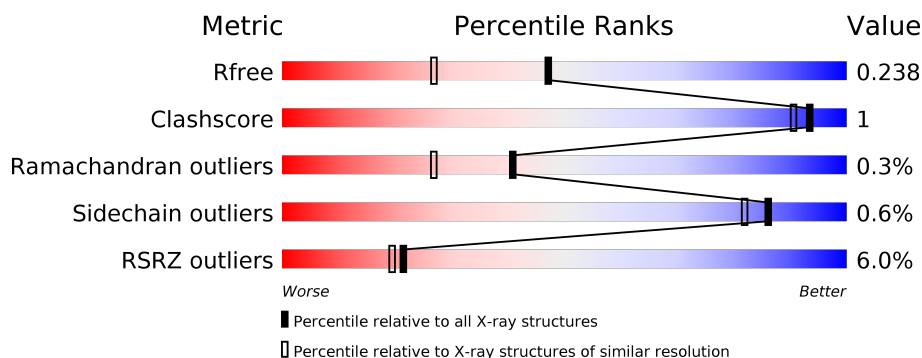
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	<div> <div>5%</div> <div>93%</div> <div>5%</div> <div>5%</div> </div>
1	D	396	<div> <div>8%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
2	B	396	<div> <div>4%</div> <div>96%</div> <div>5%</div> <div>5%</div> </div>
2	C	396	<div> <div>7%</div> <div>95%</div> <div>5%</div> <div>5%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12210 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
1	A	384	Total	C	N	O	P	S	0	3	0
			2911	1855	504	539	1	12			
1	D	377	Total	C	N	O	P	S	0	18	0
			2924	1867	501	542	1	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	ILE	engineered mutation	UNP Q8U093
A	17	GLY	GLU	engineered mutation	UNP Q8U093
A	68	VAL	ILE	engineered mutation	UNP Q8U093
A	95	LEU	PHE	engineered mutation	UNP Q8U093
A	274	SER	PHE	engineered mutation	UNP Q8U093
A	292	SER	THR	engineered mutation	UNP Q8U093
A	321	ALA	THR	engineered mutation	UNP Q8U093
A	384	ALA	VAL	engineered mutation	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
D	16	VAL	ILE	engineered mutation	UNP Q8U093
D	17	GLY	GLU	engineered mutation	UNP Q8U093
D	68	VAL	ILE	engineered mutation	UNP Q8U093
D	95	LEU	PHE	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	384	ALA	VAL	engineered mutation	UNP Q8U093
D	389	LEU	-	expression tag	UNP Q8U093

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is a protein called Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	0	4	0
			2931	1872	505	542	12			
2	C	387	Total	C	N	O	S	0	5	0
			2928	1872	502	542	12			

There are 32 discrepancies between the modelled and reference sequences:

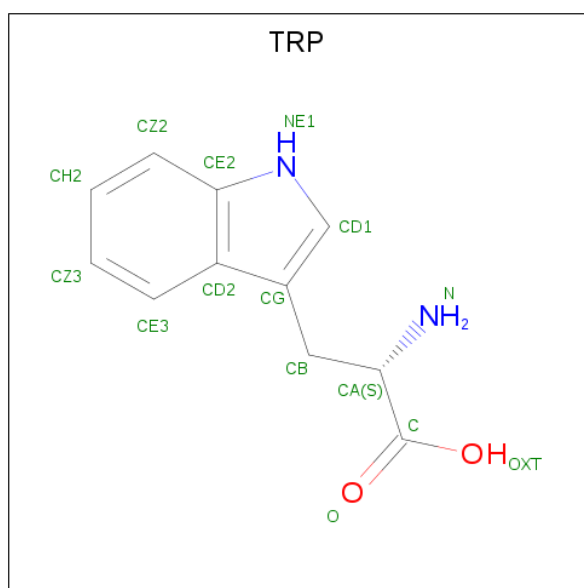
Chain	Residue	Modelled	Actual	Comment	Reference
B	16	VAL	ILE	engineered mutation	UNP Q8U093
B	17	GLY	GLU	engineered mutation	UNP Q8U093
B	68	VAL	ILE	engineered mutation	UNP Q8U093
B	95	LEU	PHE	engineered mutation	UNP Q8U093
B	274	SER	PHE	engineered mutation	UNP Q8U093
B	292	SER	THR	engineered mutation	UNP Q8U093
B	321	ALA	THR	engineered mutation	UNP Q8U093
B	384	ALA	VAL	engineered mutation	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	engineered mutation	UNP Q8U093
C	17	GLY	GLU	engineered mutation	UNP Q8U093
C	68	VAL	ILE	engineered mutation	UNP Q8U093
C	95	LEU	PHE	engineered mutation	UNP Q8U093
C	274	SER	PHE	engineered mutation	UNP Q8U093
C	292	SER	THR	engineered mutation	UNP Q8U093
C	321	ALA	THR	engineered mutation	UNP Q8U093

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Chain	Residue	Modelled	Actual	Comment	Reference
C	384	ALA	VAL	engineered mutation	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

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by author).



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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

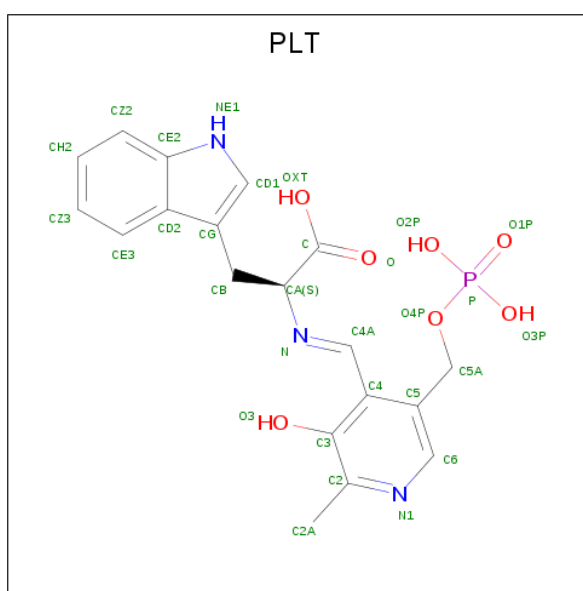
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

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

- Molecule 5 is [3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YL METHYL]-L-TRYPTOPHANE (three-letter code: PLT) (formula: C₁₉H₂₀N₃O₇P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			30	19	3	7	1		
5	C	1	Total	C	N	O	P	0	0
			30	19	3	7	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	90	Total	O	0	0
			90	90		
6	B	119	Total	O	0	0
			119	119		
6	C	99	Total	O	0	0
			99	99		

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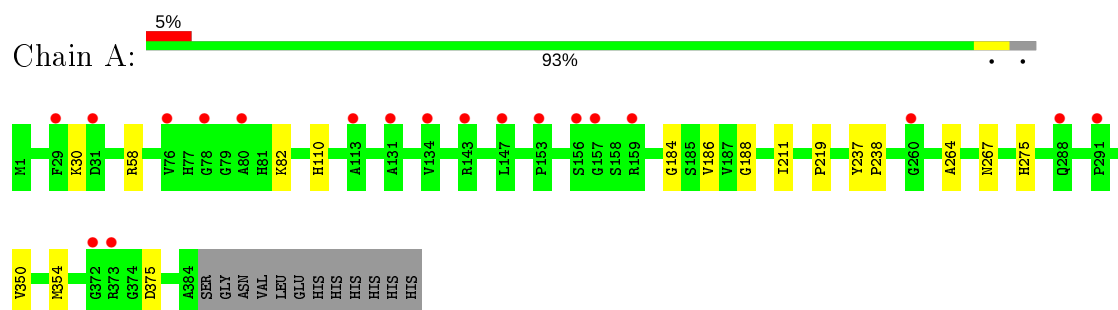
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	99	Total	O	0	1
			99	99		

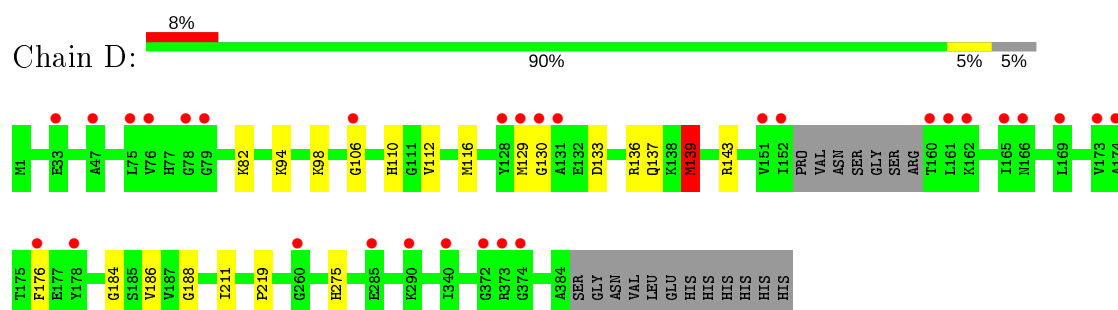
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

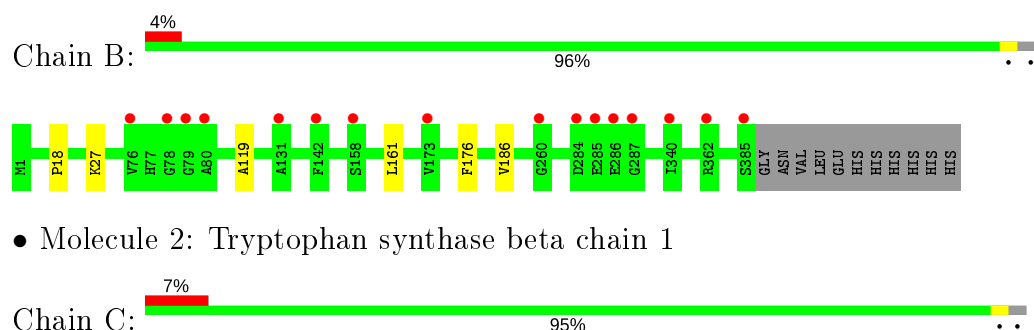
• Molecule 1: Tryptophan synthase beta chain 1



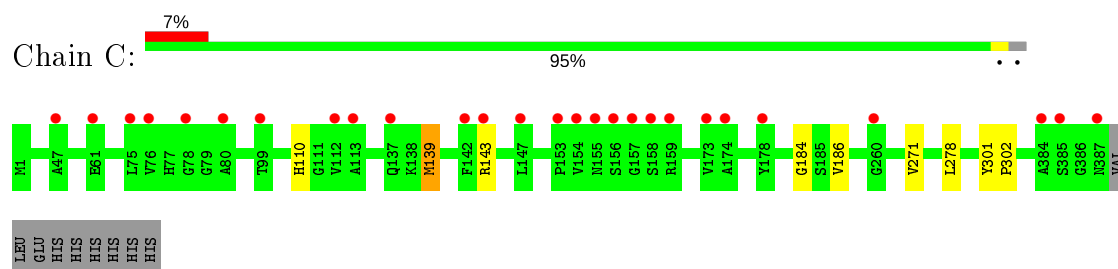
• Molecule 1: Tryptophan synthase beta chain 1



• Molecule 2: Tryptophan synthase beta chain 1



• Molecule 2: 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	82.23Å 106.04Å 158.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.83 38.85 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.00-1.83) 98.6 (38.85-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.202 , 0.231 0.208 , 0.238	Depositor DCC
R_{free} test set	6031 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12210	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.45% 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, PLT, 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	0.31	0/2951	0.52	0/3996
1	D	2.08	2/2964 (0.1%)	0.52	0/4018
2	B	0.31	0/2997	0.53	0/4055
2	C	0.31	0/2994	0.52	0/4051
All	All	1.07	2/11906 (0.0%)	0.52	0/16120

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	139[A]	MET	CB-CG	79.25	4.04	1.51
1	D	139[B]	MET	CB-CG	79.25	4.04	1.51

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	2911	0	2858	10	0
1	D	2924	0	2805	18	0
2	B	2931	0	2912	2	0
2	C	2928	0	2898	4	0
3	A	15	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	9	0	0
3	D	15	0	9	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	30	0	16	0	0
5	C	30	0	16	0	0
6	A	90	0	0	0	0
6	B	119	0	0	0	0
6	C	99	0	0	0	0
6	D	99	0	0	0	0
All	All	12210	0	11532	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (33) 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:D:129[B]:MET:HG2	1:D:130[B]:GLY:H	1.53	0.71
1:D:112:VAL:HG12	1:D:116:MET:HE3	1.75	0.69
1:D:129[B]:MET:HG2	1:D:130[B]:GLY:N	2.11	0.65
1:D:129[B]:MET:CG	1:D:130[B]:GLY:H	2.14	0.61
1:A:82:LLP:H4'1	3:A:401:TRP:CB	2.31	0.59
1:D:112:VAL:HG12	1:D:116:MET:CE	2.32	0.59
1:D:82:LLP:H4'1	3:D:401:TRP:CB	2.34	0.58
1:A:58:ARG:NH1	2:B:119:ALA:O	2.37	0.58
1:D:130[A]:GLY:O	1:D:133[A]:ASP:N	2.36	0.56
1:D:106:GLY:O	1:D:133[B]:ASP:CB	2.55	0.54
2:C:139[A]:MET:SD	2:C:143[A]:ARG:HD2	2.48	0.53
1:D:129[B]:MET:CG	1:D:130[B]:GLY:N	2.72	0.53
1:D:82:LLP:H4'1	3:D:401:TRP:HB2	1.93	0.51
1:A:82:LLP:H4'1	3:A:401:TRP:HB2	1.92	0.50
1:A:350:VAL:O	1:A:354:MET:HG3	2.12	0.49
1:A:211:ILE:HG21	1:A:219:PRO:HD3	1.95	0.49
1:D:211:ILE:HG21	1:D:219:PRO:HD3	1.96	0.48
1:D:82:LLP:H4'1	3:D:401:TRP:HB3	1.97	0.47
2:B:18:PRO:HG3	2:B:176:PHE:CD1	2.50	0.47
2:C:301:TYR:CD1	2:C:302:PRO:HD2	2.50	0.46
2:C:110:HIS:CE1	2:C:184:GLY:HA2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ALA:HB1	1:A:267:ASN:HB2	1.97	0.46
1:A:82:LLP:C4'	3:A:401:TRP:HB2	2.46	0.46
1:D:82:LLP:C4'	3:D:401:TRP:HB2	2.47	0.45
2:C:271:VAL:CG1	2:C:278:LEU:HD11	2.47	0.45
1:D:136[B]:ARG:C	1:D:137[B]:GLN:HG2	2.37	0.45
1:A:110:HIS:CE1	1:A:184:GLY:HA2	2.53	0.43
1:D:110:HIS:CE1	1:D:184:GLY:HA2	2.53	0.43
1:D:188:GLY:HA2	1:D:275:HIS:O	2.18	0.43
1:D:139[B]:MET:O	1:D:143[B]:ARG:HG3	2.19	0.42
1:D:98:LYS:NZ	1:D:176:PHE:O	2.39	0.42
1:A:188:GLY:HA2	1:A:275:HIS:O	2.19	0.42
1:A:237:TYR:HB3	1:A:238:PRO:HD3	2.04	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	384/396 (97%)	375 (98%)	8 (2%)	1 (0%)	41	27
1	D	390/396 (98%)	381 (98%)	8 (2%)	1 (0%)	41	27
2	B	387/396 (98%)	380 (98%)	6 (2%)	1 (0%)	41	27
2	C	389/396 (98%)	381 (98%)	7 (2%)	1 (0%)	41	27
All	All	1550/1584 (98%)	1517 (98%)	29 (2%)	4 (0%)	41	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	186	VAL
2	B	186	VAL
1	A	186	VAL

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Mol	Chain	Res	Type
2	C	186	VAL

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	284/312 (91%)	282 (99%)	2 (1%)	84	78
1	D	275/312 (88%)	272 (99%)	3 (1%)	73	64
2	B	294/313 (94%)	292 (99%)	2 (1%)	84	78
2	C	291/313 (93%)	290 (100%)	1 (0%)	92	90
All	All	1144/1250 (92%)	1136 (99%)	8 (1%)	86	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	375	ASP
2	B	27	LYS
2	B	161	LEU
2	C	139[A]	MET
1	D	94	LYS
1	D	139[A]	MET
1	D	139[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	D	82	1	23,24,25	2.68	5 (21%)	25,32,34	1.49	4 (16%)
1	LLP	A	82	1	23,24,25	2.59	5 (21%)	25,32,34	1.68	7 (28%)

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	D	82	1	-	4/16/17/19	0/1/1/1
1	LLP	A	82	1	-	4/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	82	LLP	C3-C2	7.62	1.48	1.40
1	A	82	LLP	C3-C2	6.94	1.47	1.40
1	A	82	LLP	C4'-NZ	6.05	1.47	1.27
1	D	82	LLP	C4'-NZ	5.94	1.47	1.27
1	D	82	LLP	C4-C5	5.93	1.49	1.42
1	A	82	LLP	C4-C5	5.91	1.49	1.42
1	D	82	LLP	C4-C3	4.90	1.48	1.40
1	A	82	LLP	C4-C3	4.75	1.48	1.40
1	D	82	LLP	C4-C4'	2.50	1.51	1.46
1	A	82	LLP	C4-C4'	2.36	1.51	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	LLP	C4-C4'-NZ	-3.27	109.28	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	LLP	C4-C4'-NZ	-3.00	110.53	124.31
1	A	82	LLP	C4-C3-C2	-2.89	118.40	120.19
1	A	82	LLP	OP4-C5'-C5	2.86	114.80	109.35
1	D	82	LLP	C4-C3-C2	-2.82	118.44	120.19
1	A	82	LLP	CD-CE-NZ	2.61	117.33	110.93
1	A	82	LLP	C5-C4-C4'	2.36	125.43	121.56
1	A	82	LLP	C6-N1-C2	2.22	123.28	119.17
1	D	82	LLP	C6-N1-C2	2.12	123.09	119.17
1	D	82	LLP	C3-C4-C5	-2.12	116.63	118.26
1	A	82	LLP	O3-C3-C2	2.01	121.88	117.49

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	82	LLP	4	0
1	A	82	LLP	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	TRP	D	401	-	12,16,16	0.88	0	12,22,22	0.87	0
5	PLT	B	402	-	28,32,32	2.31	3 (10%)	34,46,46	1.71	5 (14%)
3	TRP	B	401	-	12,16,16	0.75	0	12,22,22	0.90	0
5	PLT	C	401	-	28,32,32	2.39	3 (10%)	34,46,46	1.62	6 (17%)
3	TRP	A	401	-	12,16,16	0.92	0	12,22,22	0.91	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
3	TRP	D	401	-	-	0/3/8/8	0/2/2/2
5	PLT	B	402	-	-	5/14/19/19	0/3/3/3
3	TRP	B	401	-	-	0/3/8/8	0/2/2/2
5	PLT	C	401	-	-	5/14/19/19	0/3/3/3
3	TRP	A	401	-	-	0/3/8/8	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	401	PLT	C3-C2	8.31	1.49	1.40
5	B	402	PLT	C3-C2	7.91	1.48	1.40
5	C	401	PLT	C4-C5	6.03	1.49	1.42
5	B	402	PLT	C4-C3	5.84	1.49	1.40
5	B	402	PLT	C4-C5	5.68	1.49	1.42
5	C	401	PLT	C4-C3	5.60	1.49	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	PLT	CA-N-C4A	5.81	125.28	117.40
5	C	401	PLT	CA-N-C4A	5.05	124.25	117.40
5	B	402	PLT	C4-C3-C2	-4.24	117.57	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	PLT	C4-C3-C2	-4.12	117.64	120.19
5	C	401	PLT	C3-C4-C5	-2.79	116.12	118.26
5	B	402	PLT	CG-CB-CA	-2.64	108.00	113.33
5	B	402	PLT	C6-N1-C2	2.44	123.68	119.17
5	C	401	PLT	C6-N1-C2	2.26	123.36	119.17
5	C	401	PLT	CE3-CD2-CE2	2.21	121.11	118.17
5	B	402	PLT	CE3-CD2-CE2	2.19	121.07	118.17
5	C	401	PLT	CG-CB-CA	-2.08	109.12	113.33

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	402	PLT	C-CA-N-C4A
5	B	402	PLT	CB-CA-N-C4A
5	B	402	PLT	N-CA-CB-CG
5	B	402	PLT	C-CA-CB-CG
5	C	401	PLT	C-CA-N-C4A
5	C	401	PLT	CB-CA-N-C4A
5	C	401	PLT	N-CA-CB-CG
5	C	401	PLT	C-CA-CB-CG
5	B	402	PLT	CA-CB-CG-CD1
5	C	401	PLT	CA-CB-CG-CD1

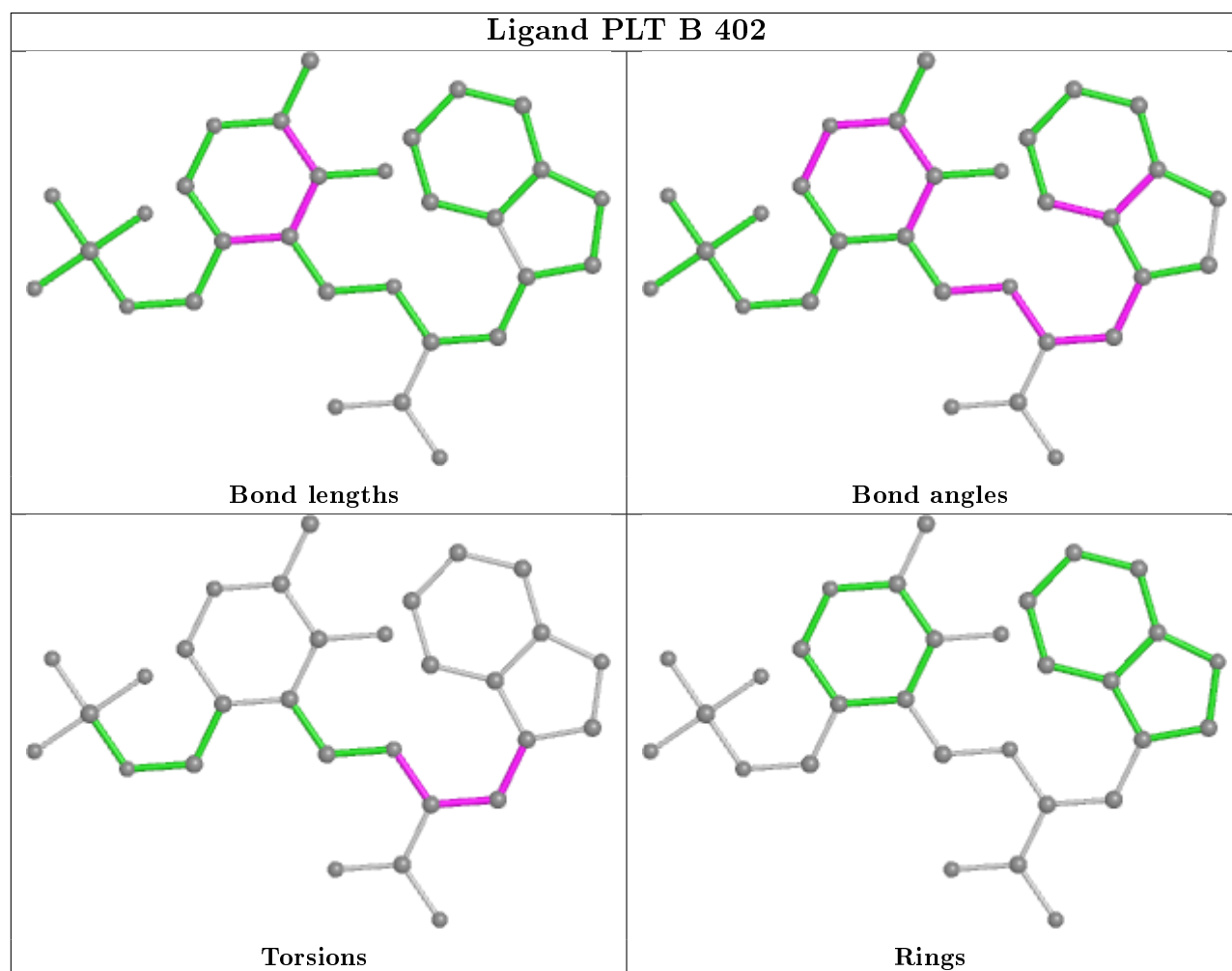
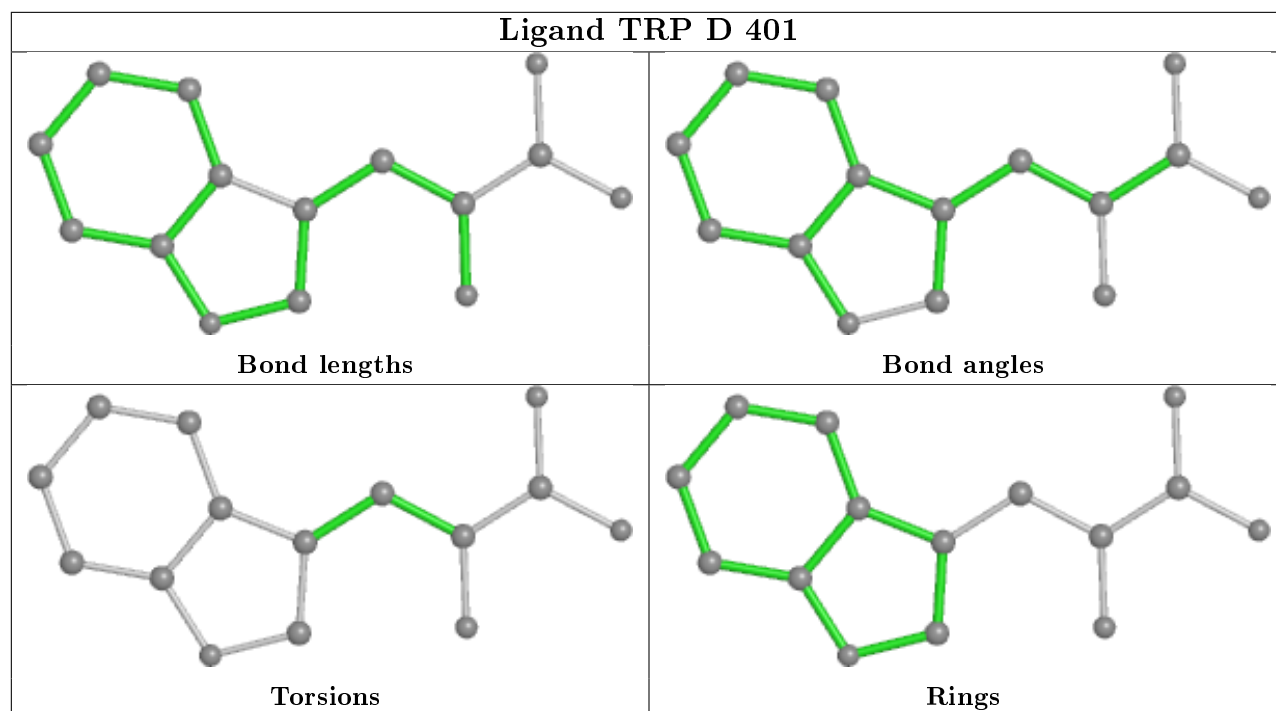
There are no ring outliers.

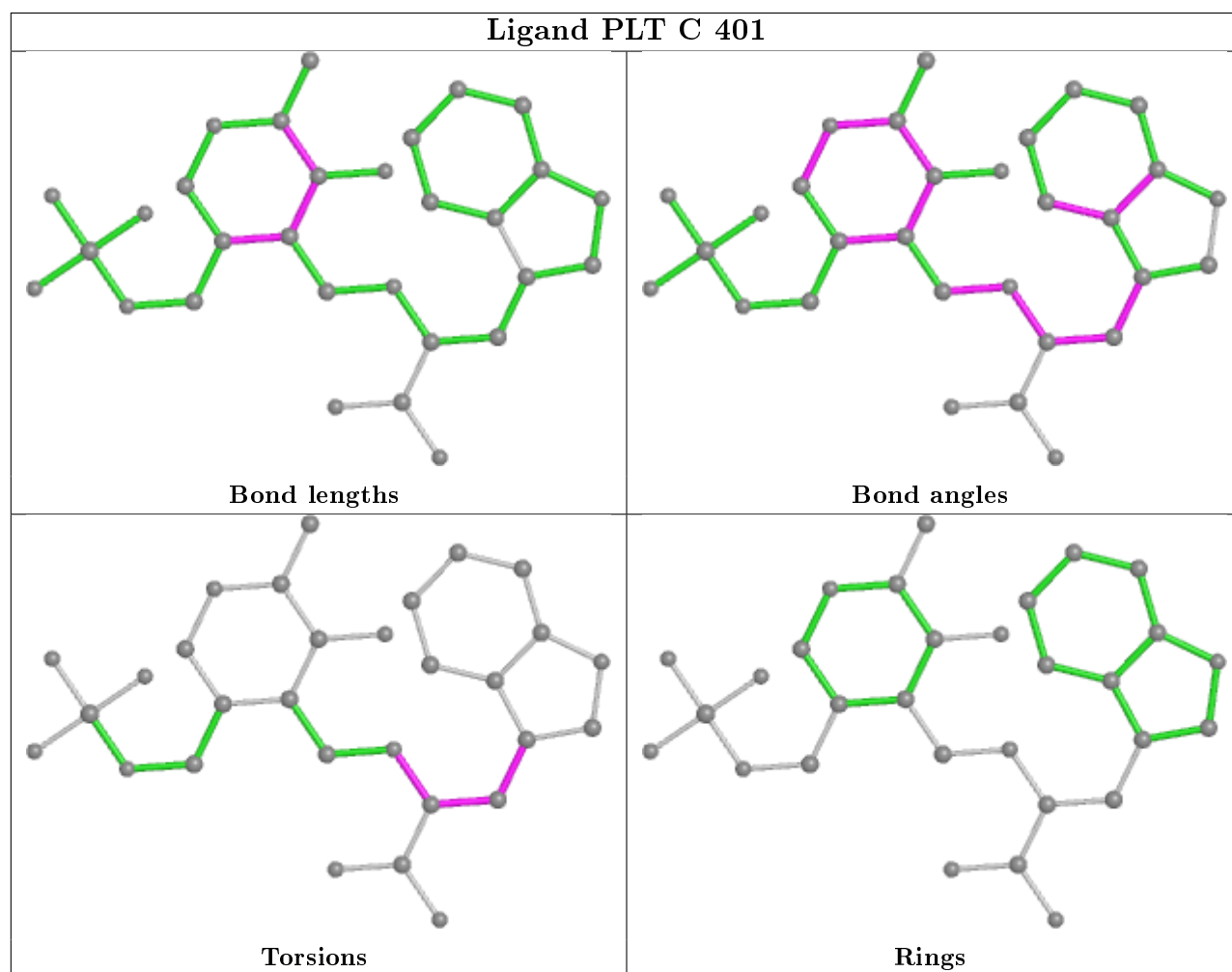
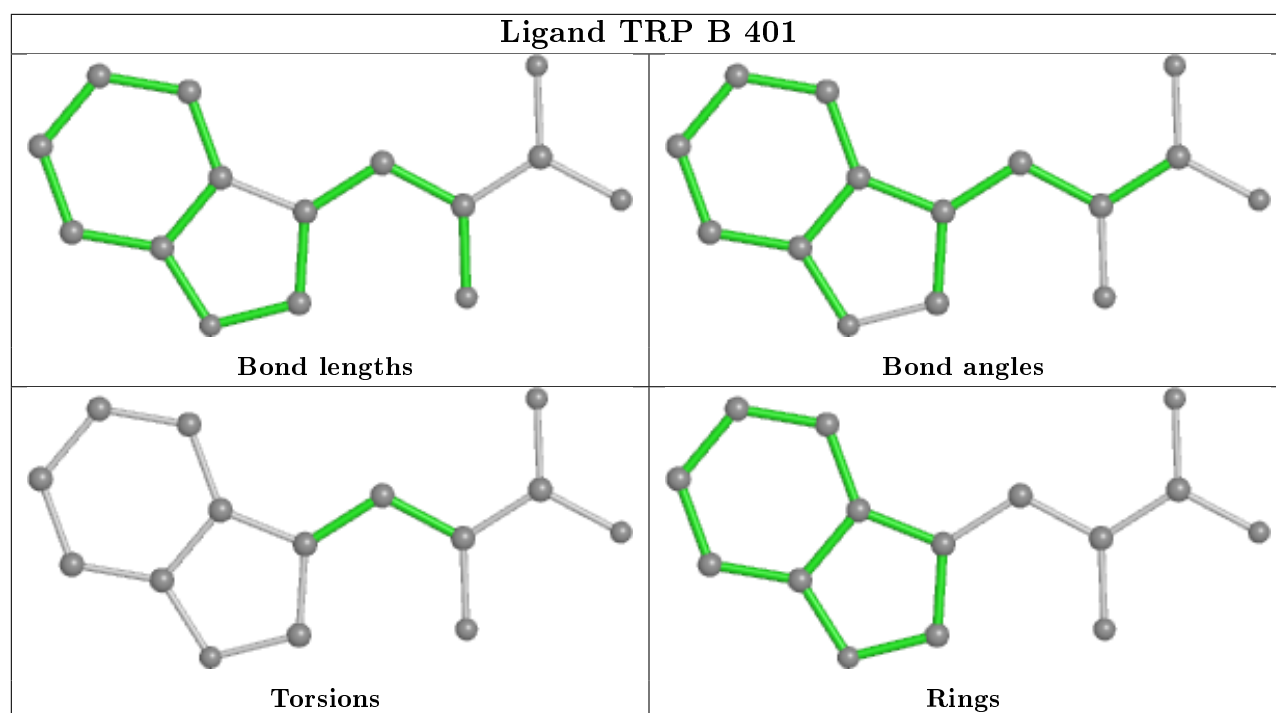
2 monomers are involved in 7 short contacts:

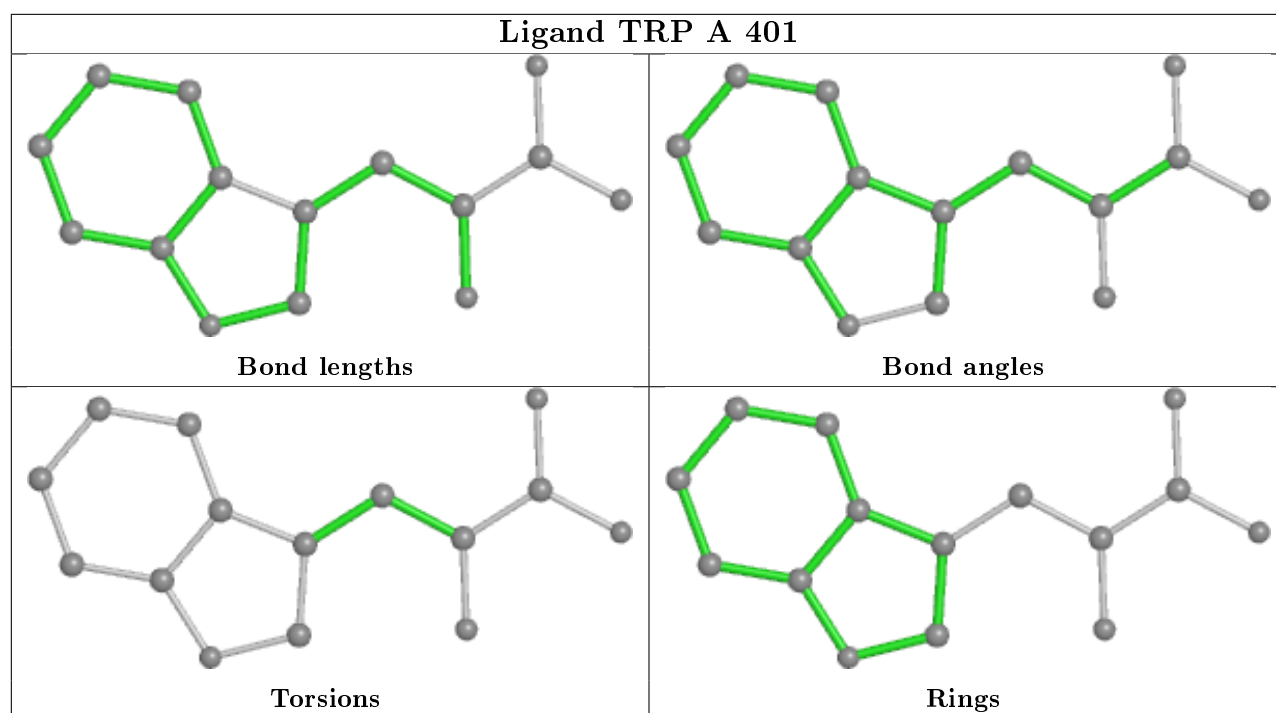
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	TRP	4	0
3	A	401	TRP	3	0

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 [i](#)

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	383/396 (96%)	0.33	19 (4%) 28 26	25, 38, 72, 102	0
1	D	376/396 (94%)	0.38	30 (7%) 12 11	26, 41, 68, 99	1 (0%)
2	B	385/396 (97%)	0.16	16 (4%) 36 33	26, 37, 54, 72	0
2	C	387/396 (97%)	0.28	27 (6%) 16 14	24, 38, 58, 88	1 (0%)
All	All	1531/1584 (96%)	0.29	92 (6%) 21 19	24, 38, 65, 102	2 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	GLY	7.9
1	D	174	ALA	5.8
2	C	158	SER	5.7
1	A	143[A]	ARG	5.3
1	A	134	VAL	5.3
1	D	173	VAL	5.1
1	D	152	ILE	4.2
2	C	153	PRO	4.1
1	A	156	SER	4.0
2	C	143[A]	ARG	4.0
2	C	384	ALA	3.8
2	C	154	VAL	3.8
1	A	78	GLY	3.5
1	A	131	ALA	3.4
2	B	158	SER	3.4
2	C	80	ALA	3.4
2	B	142[A]	PHE	3.4
2	C	155	ASN	3.3
1	D	373[A]	ARG	3.3
1	D	169	LEU	3.2
2	C	78	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	260	GLY	3.1
2	B	287	GLY	3.1
2	C	174	ALA	3.0
1	A	29	PHE	3.0
1	D	78	GLY	3.0
1	D	285	GLU	3.0
2	C	76	VAL	3.0
2	C	113	ALA	2.9
1	D	75	LEU	2.9
2	C	159	ARG	2.9
1	D	165	ILE	2.8
1	D	151	VAL	2.8
2	C	385	SER	2.8
1	D	106	GLY	2.8
1	D	162	LYS	2.8
2	B	285	GLU	2.8
2	C	112	VAL	2.8
1	A	76	VAL	2.7
1	D	340	ILE	2.7
1	D	130[A]	GLY	2.7
1	A	147	LEU	2.6
1	A	31	ASP	2.6
1	A	260	GLY	2.6
2	B	173	VAL	2.6
2	B	76	VAL	2.5
2	B	80	ALA	2.5
1	A	291	PRO	2.5
1	D	128[A]	TYR	2.5
1	D	372	GLY	2.4
1	D	160	THR	2.4
1	D	79	GLY	2.4
2	B	340	ILE	2.4
2	B	362	ARG	2.4
2	C	142[A]	PHE	2.4
1	D	178	TYR	2.4
2	C	178	TYR	2.4
1	A	80	ALA	2.4
2	C	173	VAL	2.4
2	C	75	LEU	2.4
1	D	176	PHE	2.4
1	A	153	PRO	2.3
1	D	166	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	387	ASN	2.3
1	D	374	GLY	2.3
1	D	129[A]	MET	2.3
1	D	290	LYS	2.3
2	B	286	GLU	2.3
2	B	131	ALA	2.2
1	A	373[A]	ARG	2.2
1	A	288	GLN	2.2
2	C	47	ALA	2.2
2	C	156	SER	2.2
2	C	99	THR	2.2
2	B	79	GLY	2.2
2	C	61	GLU	2.2
1	D	161	LEU	2.2
1	A	372	GLY	2.2
1	D	33	GLU	2.2
2	B	385	SER	2.1
1	D	260	GLY	2.1
2	B	78	GLY	2.1
2	B	284	ASP	2.1
1	D	131[A]	ALA	2.1
2	C	157	GLY	2.1
1	D	76	VAL	2.1
2	C	147	LEU	2.1
1	A	159	ARG	2.1
2	B	260	GLY	2.0
2	C	137	GLN	2.0
1	A	113	ALA	2.0
1	D	47	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LLP	D	82	24/25	0.95	0.20	31,33,35,35	0
1	LLP	A	82	24/25	0.96	0.18	29,32,33,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

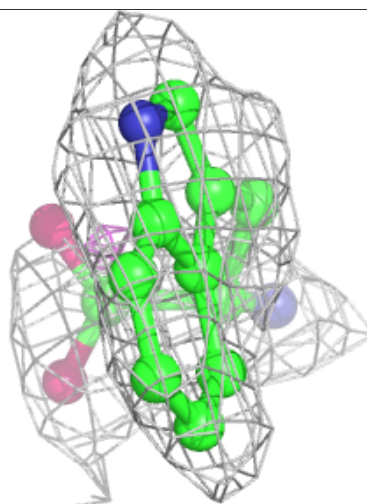
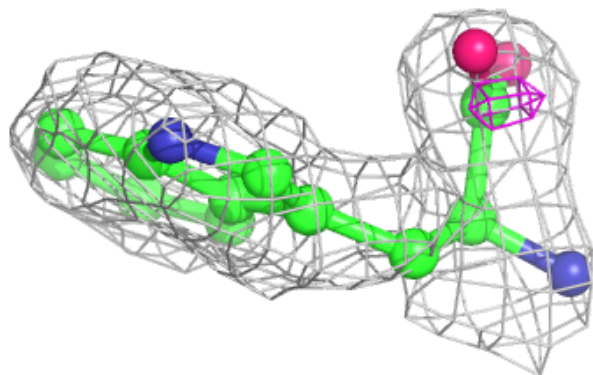
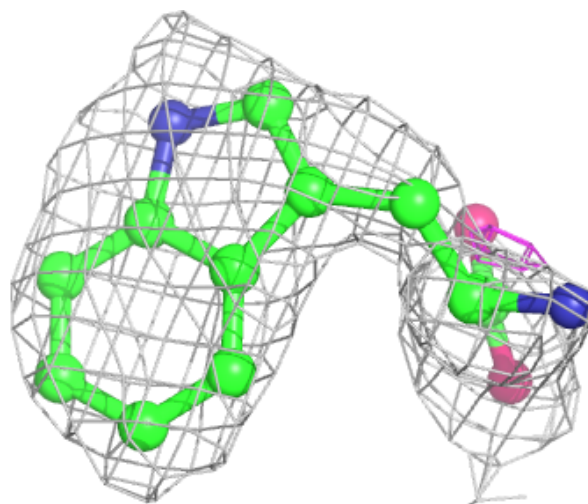
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TRP	B	401	15/15	0.80	0.23	62,64,65,67	0
4	NA	B	403	1/1	0.88	0.15	45,45,45,45	0
3	TRP	D	401	15/15	0.89	0.12	43,44,49,50	0
3	TRP	A	401	15/15	0.92	0.12	31,31,34,35	0
4	NA	C	402	1/1	0.94	0.06	31,31,31,31	0
4	NA	D	402	1/1	0.95	0.09	43,43,43,43	0
5	PLT	C	401	30/30	0.95	0.14	25,30,32,33	0
5	PLT	B	402	30/30	0.96	0.13	27,31,33,35	0
4	NA	A	402	1/1	0.97	0.09	35,35,35,35	0

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

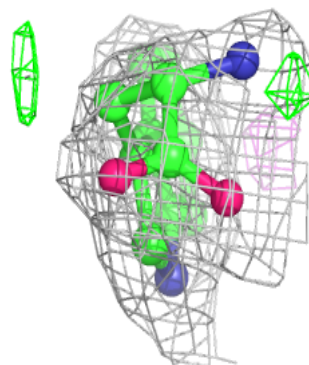
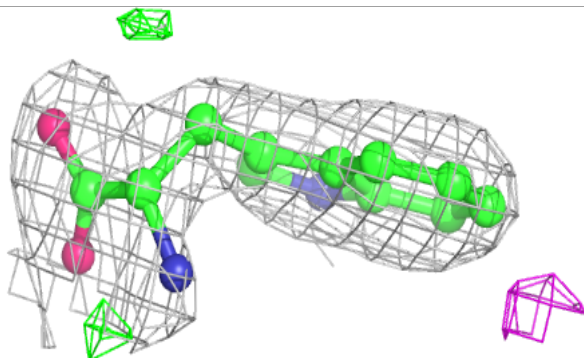
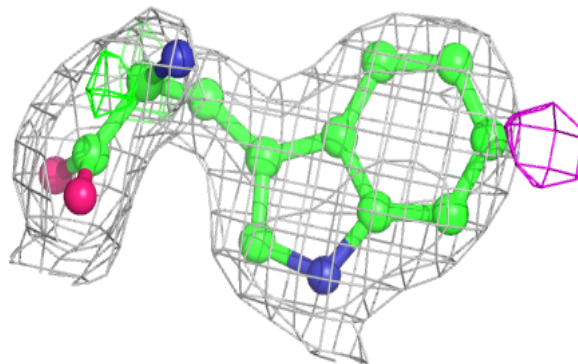
Electron density around TRP B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

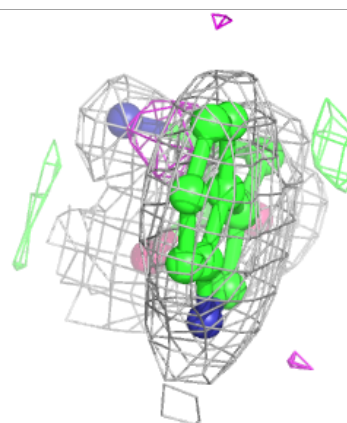
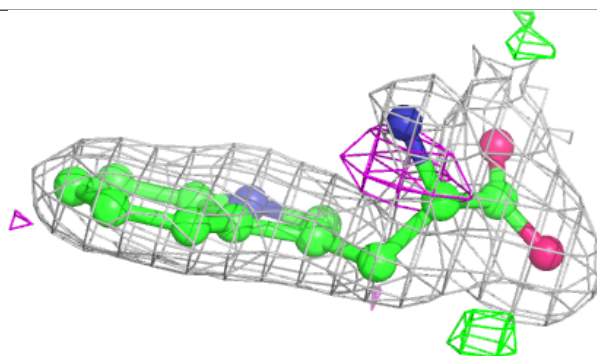
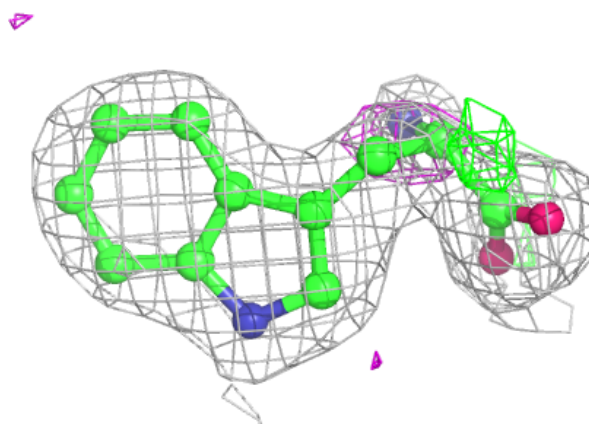


Electron density around TRP D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

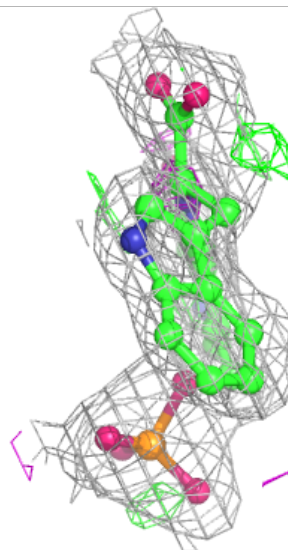
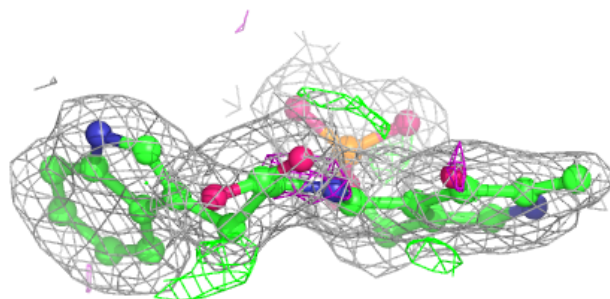
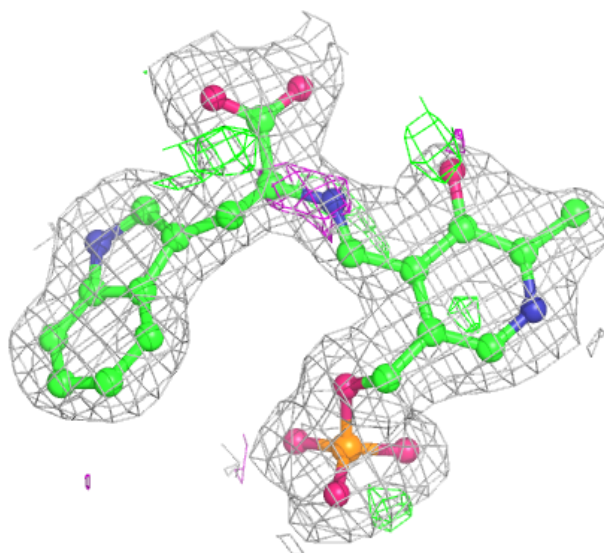
**Electron density around TRP A 401:**

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and green (positive)



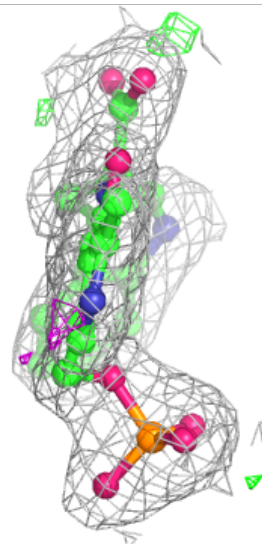
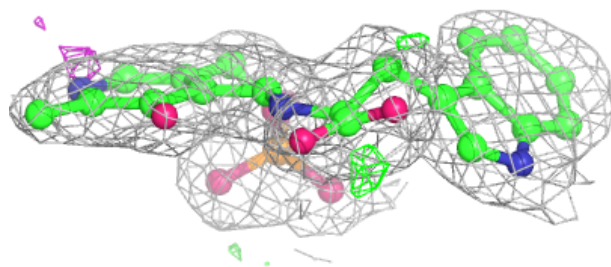
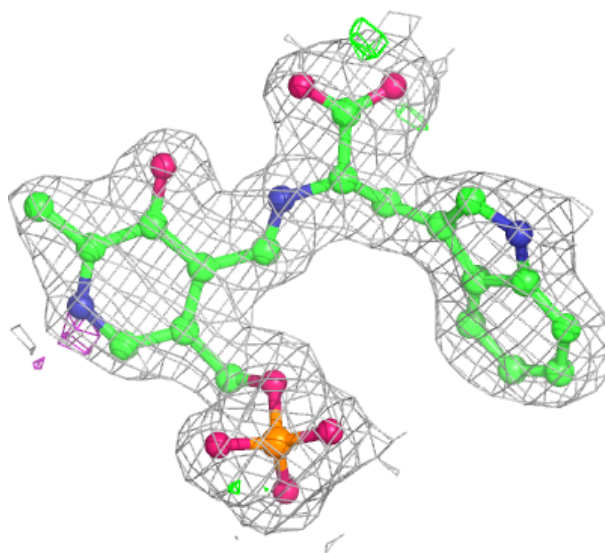
Electron density around PLT C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLT B 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.