



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:01 PM UTC

PDB ID : 8DSR / pdb\_00008dsr  
Title : Structure of Plasmepsin X (PM10, PMX) from Plasmodium falciparum 3D7  
in complex with UCB7362  
Authors : Abendroth, J.; Lorimer, D.D.  
Deposited on : 2022-07-22  
Resolution : 2.85 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](mailto: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)  
Xtrriage (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

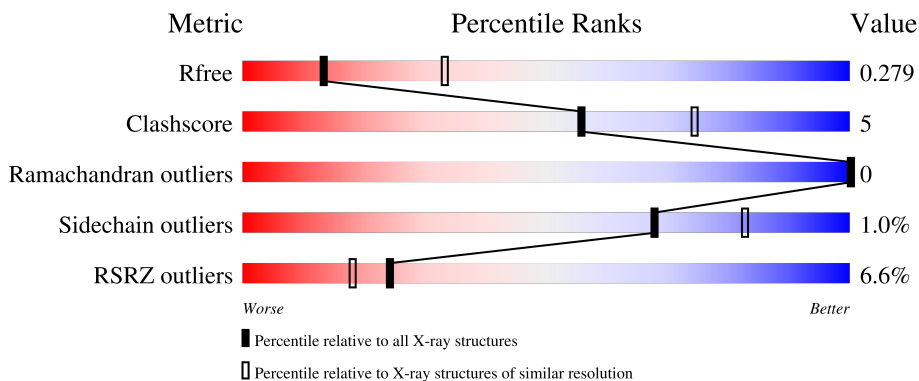
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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  $\geq 3$ , 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	465	 5% 62% 9% 29%
1	B	465	 5% 64% 8% 29%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 5055 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 Plasmepepsin X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	2518	1628	400	474	16	0	0	0
1	B	332	2471	1595	391	469	16	0	0	0

There are 232 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	TYR	-	expression tag	UNP Q8IAS0
A	126	LYS	-	expression tag	UNP Q8IAS0
A	127	ILE	-	expression tag	UNP Q8IAS0
A	128	GLY	-	expression tag	UNP Q8IAS0
A	129	THR	-	expression tag	UNP Q8IAS0
A	130	LYS	-	expression tag	UNP Q8IAS0
A	131	ALA	-	expression tag	UNP Q8IAS0
A	132	LEU	-	expression tag	UNP Q8IAS0
A	133	PRO	-	expression tag	UNP Q8IAS0
A	134	CYS	-	expression tag	UNP Q8IAS0
A	135	SER	-	expression tag	UNP Q8IAS0
A	136	GLU	-	expression tag	UNP Q8IAS0
A	137	CYS	-	expression tag	UNP Q8IAS0
A	138	HIS	-	expression tag	UNP Q8IAS0
A	139	ASP	-	expression tag	UNP Q8IAS0
A	140	VAL	-	expression tag	UNP Q8IAS0
A	141	PHE	-	expression tag	UNP Q8IAS0
A	142	ASP	-	expression tag	UNP Q8IAS0
A	143	CYS	-	expression tag	UNP Q8IAS0
A	144	THR	-	expression tag	UNP Q8IAS0
A	145	GLY	-	expression tag	UNP Q8IAS0
A	146	CYS	-	expression tag	UNP Q8IAS0
A	147	LEU	-	expression tag	UNP Q8IAS0
A	148	PHE	-	expression tag	UNP Q8IAS0
A	149	GLU	-	expression tag	UNP Q8IAS0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	GLU	-	expression tag	UNP Q8IAS0
A	151	LYS	-	expression tag	UNP Q8IAS0
A	152	GLU	-	expression tag	UNP Q8IAS0
A	153	SER	-	expression tag	UNP Q8IAS0
A	154	SER	-	expression tag	UNP Q8IAS0
A	155	HIS	-	expression tag	UNP Q8IAS0
A	156	VAL	-	expression tag	UNP Q8IAS0
A	157	ILE	-	expression tag	UNP Q8IAS0
A	158	PRO	-	expression tag	UNP Q8IAS0
A	159	LEU	-	expression tag	UNP Q8IAS0
A	160	LYS	-	expression tag	UNP Q8IAS0
A	161	LEU	-	expression tag	UNP Q8IAS0
A	162	ASN	-	expression tag	UNP Q8IAS0
A	163	LYS	-	expression tag	UNP Q8IAS0
A	164	LYS	-	expression tag	UNP Q8IAS0
A	165	ASN	-	expression tag	UNP Q8IAS0
A	166	PRO	-	expression tag	UNP Q8IAS0
A	167	ASN	-	expression tag	UNP Q8IAS0
A	168	ASP	-	expression tag	UNP Q8IAS0
A	169	HIS	-	expression tag	UNP Q8IAS0
A	170	LYS	-	expression tag	UNP Q8IAS0
A	171	LYS	-	expression tag	UNP Q8IAS0
A	172	LEU	-	expression tag	UNP Q8IAS0
A	173	GLN	-	expression tag	UNP Q8IAS0
A	174	LYS	-	expression tag	UNP Q8IAS0
A	175	HIS	-	expression tag	UNP Q8IAS0
A	176	HIS	-	expression tag	UNP Q8IAS0
A	177	GLU	-	expression tag	UNP Q8IAS0
A	178	SER	-	expression tag	UNP Q8IAS0
A	179	LEU	-	expression tag	UNP Q8IAS0
A	180	LYS	-	expression tag	UNP Q8IAS0
A	181	LEU	-	expression tag	UNP Q8IAS0
A	182	GLY	-	expression tag	UNP Q8IAS0
A	183	ASP	-	expression tag	UNP Q8IAS0
A	184	VAL	-	expression tag	UNP Q8IAS0
A	185	LYS	-	expression tag	UNP Q8IAS0
A	186	TYR	-	expression tag	UNP Q8IAS0
A	187	TYR	-	expression tag	UNP Q8IAS0
A	188	VAL	-	expression tag	UNP Q8IAS0
A	189	ASN	-	expression tag	UNP Q8IAS0
A	190	ARG	-	expression tag	UNP Q8IAS0
A	191	GLY	-	expression tag	UNP Q8IAS0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	GLU	-	expression tag	UNP Q8IAS0
A	193	GLY	-	expression tag	UNP Q8IAS0
A	194	ILE	-	expression tag	UNP Q8IAS0
A	195	SER	-	expression tag	UNP Q8IAS0
A	196	GLY	-	expression tag	UNP Q8IAS0
A	197	SER	-	expression tag	UNP Q8IAS0
A	198	LEU	-	expression tag	UNP Q8IAS0
A	199	GLY	-	expression tag	UNP Q8IAS0
A	200	THR	-	expression tag	UNP Q8IAS0
A	201	SER	-	expression tag	UNP Q8IAS0
A	202	SER	-	expression tag	UNP Q8IAS0
A	203	GLY	-	expression tag	UNP Q8IAS0
A	204	ASN	-	expression tag	UNP Q8IAS0
A	205	THR	-	expression tag	UNP Q8IAS0
A	206	LEU	-	expression tag	UNP Q8IAS0
A	207	ASP	-	expression tag	UNP Q8IAS0
A	208	ASP	-	expression tag	UNP Q8IAS0
A	209	MET	-	expression tag	UNP Q8IAS0
A	210	ASP	-	expression tag	UNP Q8IAS0
A	211	LEU	-	expression tag	UNP Q8IAS0
A	212	ILE	-	expression tag	UNP Q8IAS0
A	213	ASN	-	expression tag	UNP Q8IAS0
A	214	GLU	-	expression tag	UNP Q8IAS0
A	215	GLU	-	expression tag	UNP Q8IAS0
A	216	ILE	-	expression tag	UNP Q8IAS0
A	217	ASN	-	expression tag	UNP Q8IAS0
A	218	LYS	-	expression tag	UNP Q8IAS0
A	219	LYS	-	expression tag	UNP Q8IAS0
A	220	ARG	-	expression tag	UNP Q8IAS0
A	221	THR	-	expression tag	UNP Q8IAS0
A	222	ASN	-	expression tag	UNP Q8IAS0
A	223	ALA	-	expression tag	UNP Q8IAS0
A	224	GLN	-	expression tag	UNP Q8IAS0
A	574	GLU	-	expression tag	UNP Q8IAS0
A	575	ASN	-	expression tag	UNP Q8IAS0
A	576	LEU	-	expression tag	UNP Q8IAS0
A	577	TYR	-	expression tag	UNP Q8IAS0
A	578	PHE	-	expression tag	UNP Q8IAS0
A	579	GLN	-	expression tag	UNP Q8IAS0
A	580	GLY	-	expression tag	UNP Q8IAS0
A	581	SER	-	expression tag	UNP Q8IAS0
A	582	HIS	-	expression tag	UNP Q8IAS0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	583	HIS	-	expression tag	UNP Q8IAS0
A	584	HIS	-	expression tag	UNP Q8IAS0
A	585	HIS	-	expression tag	UNP Q8IAS0
A	586	HIS	-	expression tag	UNP Q8IAS0
A	587	HIS	-	expression tag	UNP Q8IAS0
A	588	HIS	-	expression tag	UNP Q8IAS0
A	589	HIS	-	expression tag	UNP Q8IAS0
B	125	TYR	-	expression tag	UNP Q8IAS0
B	126	LYS	-	expression tag	UNP Q8IAS0
B	127	ILE	-	expression tag	UNP Q8IAS0
B	128	GLY	-	expression tag	UNP Q8IAS0
B	129	THR	-	expression tag	UNP Q8IAS0
B	130	LYS	-	expression tag	UNP Q8IAS0
B	131	ALA	-	expression tag	UNP Q8IAS0
B	132	LEU	-	expression tag	UNP Q8IAS0
B	133	PRO	-	expression tag	UNP Q8IAS0
B	134	CYS	-	expression tag	UNP Q8IAS0
B	135	SER	-	expression tag	UNP Q8IAS0
B	136	GLU	-	expression tag	UNP Q8IAS0
B	137	CYS	-	expression tag	UNP Q8IAS0
B	138	HIS	-	expression tag	UNP Q8IAS0
B	139	ASP	-	expression tag	UNP Q8IAS0
B	140	VAL	-	expression tag	UNP Q8IAS0
B	141	PHE	-	expression tag	UNP Q8IAS0
B	142	ASP	-	expression tag	UNP Q8IAS0
B	143	CYS	-	expression tag	UNP Q8IAS0
B	144	THR	-	expression tag	UNP Q8IAS0
B	145	GLY	-	expression tag	UNP Q8IAS0
B	146	CYS	-	expression tag	UNP Q8IAS0
B	147	LEU	-	expression tag	UNP Q8IAS0
B	148	PHE	-	expression tag	UNP Q8IAS0
B	149	GLU	-	expression tag	UNP Q8IAS0
B	150	GLU	-	expression tag	UNP Q8IAS0
B	151	LYS	-	expression tag	UNP Q8IAS0
B	152	GLU	-	expression tag	UNP Q8IAS0
B	153	SER	-	expression tag	UNP Q8IAS0
B	154	SER	-	expression tag	UNP Q8IAS0
B	155	HIS	-	expression tag	UNP Q8IAS0
B	156	VAL	-	expression tag	UNP Q8IAS0
B	157	ILE	-	expression tag	UNP Q8IAS0
B	158	PRO	-	expression tag	UNP Q8IAS0
B	159	LEU	-	expression tag	UNP Q8IAS0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	160	LYS	-	expression tag	UNP Q8IAS0
B	161	LEU	-	expression tag	UNP Q8IAS0
B	162	ASN	-	expression tag	UNP Q8IAS0
B	163	LYS	-	expression tag	UNP Q8IAS0
B	164	LYS	-	expression tag	UNP Q8IAS0
B	165	ASN	-	expression tag	UNP Q8IAS0
B	166	PRO	-	expression tag	UNP Q8IAS0
B	167	ASN	-	expression tag	UNP Q8IAS0
B	168	ASP	-	expression tag	UNP Q8IAS0
B	169	HIS	-	expression tag	UNP Q8IAS0
B	170	LYS	-	expression tag	UNP Q8IAS0
B	171	LYS	-	expression tag	UNP Q8IAS0
B	172	LEU	-	expression tag	UNP Q8IAS0
B	173	GLN	-	expression tag	UNP Q8IAS0
B	174	LYS	-	expression tag	UNP Q8IAS0
B	175	HIS	-	expression tag	UNP Q8IAS0
B	176	HIS	-	expression tag	UNP Q8IAS0
B	177	GLU	-	expression tag	UNP Q8IAS0
B	178	SER	-	expression tag	UNP Q8IAS0
B	179	LEU	-	expression tag	UNP Q8IAS0
B	180	LYS	-	expression tag	UNP Q8IAS0
B	181	LEU	-	expression tag	UNP Q8IAS0
B	182	GLY	-	expression tag	UNP Q8IAS0
B	183	ASP	-	expression tag	UNP Q8IAS0
B	184	VAL	-	expression tag	UNP Q8IAS0
B	185	LYS	-	expression tag	UNP Q8IAS0
B	186	TYR	-	expression tag	UNP Q8IAS0
B	187	TYR	-	expression tag	UNP Q8IAS0
B	188	VAL	-	expression tag	UNP Q8IAS0
B	189	ASN	-	expression tag	UNP Q8IAS0
B	190	ARG	-	expression tag	UNP Q8IAS0
B	191	GLY	-	expression tag	UNP Q8IAS0
B	192	GLU	-	expression tag	UNP Q8IAS0
B	193	GLY	-	expression tag	UNP Q8IAS0
B	194	ILE	-	expression tag	UNP Q8IAS0
B	195	SER	-	expression tag	UNP Q8IAS0
B	196	GLY	-	expression tag	UNP Q8IAS0
B	197	SER	-	expression tag	UNP Q8IAS0
B	198	LEU	-	expression tag	UNP Q8IAS0
B	199	GLY	-	expression tag	UNP Q8IAS0
B	200	THR	-	expression tag	UNP Q8IAS0
B	201	SER	-	expression tag	UNP Q8IAS0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	SER	-	expression tag	UNP Q8IAS0
B	203	GLY	-	expression tag	UNP Q8IAS0
B	204	ASN	-	expression tag	UNP Q8IAS0
B	205	THR	-	expression tag	UNP Q8IAS0
B	206	LEU	-	expression tag	UNP Q8IAS0
B	207	ASP	-	expression tag	UNP Q8IAS0
B	208	ASP	-	expression tag	UNP Q8IAS0
B	209	MET	-	expression tag	UNP Q8IAS0
B	210	ASP	-	expression tag	UNP Q8IAS0
B	211	LEU	-	expression tag	UNP Q8IAS0
B	212	ILE	-	expression tag	UNP Q8IAS0
B	213	ASN	-	expression tag	UNP Q8IAS0
B	214	GLU	-	expression tag	UNP Q8IAS0
B	215	GLU	-	expression tag	UNP Q8IAS0
B	216	ILE	-	expression tag	UNP Q8IAS0
B	217	ASN	-	expression tag	UNP Q8IAS0
B	218	LYS	-	expression tag	UNP Q8IAS0
B	219	LYS	-	expression tag	UNP Q8IAS0
B	220	ARG	-	expression tag	UNP Q8IAS0
B	221	THR	-	expression tag	UNP Q8IAS0
B	222	ASN	-	expression tag	UNP Q8IAS0
B	223	ALA	-	expression tag	UNP Q8IAS0
B	224	GLN	-	expression tag	UNP Q8IAS0
B	574	GLU	-	expression tag	UNP Q8IAS0
B	575	ASN	-	expression tag	UNP Q8IAS0
B	576	LEU	-	expression tag	UNP Q8IAS0
B	577	TYR	-	expression tag	UNP Q8IAS0
B	578	PHE	-	expression tag	UNP Q8IAS0
B	579	GLN	-	expression tag	UNP Q8IAS0
B	580	GLY	-	expression tag	UNP Q8IAS0
B	581	SER	-	expression tag	UNP Q8IAS0
B	582	HIS	-	expression tag	UNP Q8IAS0
B	583	HIS	-	expression tag	UNP Q8IAS0
B	584	HIS	-	expression tag	UNP Q8IAS0
B	585	HIS	-	expression tag	UNP Q8IAS0
B	586	HIS	-	expression tag	UNP Q8IAS0
B	587	HIS	-	expression tag	UNP Q8IAS0
B	588	HIS	-	expression tag	UNP Q8IAS0
B	589	HIS	-	expression tag	UNP Q8IAS0

- Molecule 2 is (2E,6S)-6-{2-chloro-3-[(2-cyclopropylpyrimidin-5-yl)amino]phenyl}-2-imino-6-methyl-3-[(2S,4S)-2-methyloxan-4-yl]-1,3-diazinan-4-one (CCD ID: TWU) (formula: C<sub>24</sub>H<sub>29</sub>ClN<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.71Å 61.43Å 143.98Å 90.00° 90.77° 90.00°	Depositor
Resolution (Å)	47.99 – 2.85 47.99 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.99-2.85) 99.6 (47.99-2.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.86Å)	Xtrriage
Refinement program	PHENIX 1.19 dev 4035	Depositor
R, $R_{free}$	0.234 , 0.280 0.234 , 0.279	Depositor DCC
$R_{free}$ test set	2037 reflections (9.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.8	Xtrriage
Anisotropy	0.708	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TWU

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	0.13	0/2581	0.33	0/3514
1	B	0.11	0/2532	0.30	0/3456
All	All	0.13	0/5113	0.31	0/6970

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	A	2518	0	2358	23	0
1	B	2471	0	2264	22	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0
All	All	5055	0	4622	45	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 5.

All (45) 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:B:447:CYS:SG	1:B:448:CYS:N	2.59	0.76
1:B:470:MET:HG3	1:B:527:GLN:HB3	1.68	0.75
1:A:447:CYS:SG	1:A:448:CYS:N	2.60	0.75
1:A:326:MET:HE3	1:A:329:LYS:HA	1.76	0.68
1:B:470:MET:HE1	1:B:525:TYR:HB3	1.75	0.68
1:B:455:ILE:HB	1:B:539:LEU:HD23	1.75	0.67
1:A:498:LYS:HG2	1:A:507:GLU:HG2	1.76	0.66
1:A:465:MET:HB2	1:A:470:MET:HE2	1.78	0.64
1:A:506:ILE:HD11	1:A:566:VAL:HG21	1.81	0.63
1:A:455:ILE:HB	1:A:539:LEU:HD23	1.81	0.62
1:B:542:SER:HA	1:B:546:MET:HB2	1.84	0.60
1:A:439:LEU:HB3	1:A:447:CYS:HB3	1.91	0.53
1:B:447:CYS:SG	1:B:538:TYR:OH	2.64	0.53
1:B:506:ILE:HD11	1:B:566:VAL:HG21	1.91	0.53
1:A:275:VAL:HA	1:A:340:VAL:HB	1.90	0.52
1:B:275:VAL:HA	1:B:340:VAL:HB	1.91	0.52
1:A:436:LEU:HB2	1:A:454:VAL:HG23	1.92	0.51
1:B:462:TYR:HD2	1:B:526:MET:HG3	1.74	0.51
1:B:462:TYR:HB2	1:B:526:MET:HE2	1.93	0.51
1:A:433:GLU:HG3	1:A:455:ILE:HG12	1.95	0.49
1:A:276:THR:HG22	1:A:290:TYR:HD2	1.78	0.48
1:A:246:SER:HB3	1:A:461:SER:HB2	1.96	0.47
1:B:271:ASN:HD21	1:B:373:SER:H	1.63	0.47
1:B:440:TYR:CE1	1:B:445:ARG:HB2	2.50	0.47
1:A:466:PRO:HG3	1:A:536:HIS:HB3	1.95	0.47
1:A:421:ILE:HG12	1:A:567:ALA:HB2	1.98	0.46
1:B:458:THR:HG22	1:B:546:MET:SD	2.56	0.45
1:B:436:LEU:HB2	1:B:454:VAL:HG23	1.98	0.44
1:B:433:GLU:HG2	1:B:453:TYR:HB3	2.00	0.44
1:A:266:ASP:O	1:A:366:LEU:N	2.48	0.43
1:B:466:PRO:HG3	1:B:536:HIS:HB3	1.99	0.43
1:A:271:ASN:HD21	1:A:373:SER:H	1.67	0.43
1:B:381:ASP:N	1:B:381:ASP:OD1	2.51	0.42
1:A:510:PRO:HA	1:A:513:TYR:CE2	2.54	0.42
1:A:464:THR:HG21	1:A:539:LEU:HD12	2.02	0.41
1:A:506:ILE:HG21	1:A:545:PHE:HE1	1.85	0.41
1:B:470:MET:HE3	1:B:526:MET:O	2.20	0.41
1:A:463:ASN:O	1:A:525:TYR:HA	2.21	0.41
1:A:462:TYR:HD2	1:A:526:MET:HG3	1.85	0.41
1:A:381:ASP:N	1:A:381:ASP:OD1	2.54	0.41
1:B:465:MET:HB2	1:B:470:MET:HE2	2.02	0.41
1:B:391:ASP:HA	1:B:392:PRO:HD3	1.97	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ILE:HG12	1:B:567:ALA:HB2	2.02	0.40
1:B:424:LEU:HD13	1:B:434:VAL:HG11	2.02	0.40
1:A:458:THR:HG22	1:A:546:MET:SD	2.60	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	328/465 (70%)	318 (97%)	10 (3%)	0	100	100
1	B	328/465 (70%)	316 (96%)	12 (4%)	0	100	100
All	All	656/930 (70%)	634 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	267/420 (64%)	264 (99%)	3 (1%)	65	81
1	B	256/420 (61%)	254 (99%)	2 (1%)	73	86
All	All	523/840 (62%)	518 (99%)	5 (1%)	68	83

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

Mol	Chain	Res	Type
1	A	317	SER
1	A	381	ASP
1	A	533	GLU
1	B	381	ASP
1	B	533	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	A	308	HIS
1	A	393	GLN
1	B	247	GLN
1	B	271	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands 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
2	TWU	B	600	-	33,37,37	1.42	3 (9%)	35,55,55	1.80	5 (14%)
2	TWU	A	600	-	33,37,37	1.36	3 (9%)	35,55,55	1.86	5 (14%)

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	TWU	B	600	-	-	6/18/48/48	0/5/5/5
2	TWU	A	600	-	-	5/18/48/48	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	TWU	C32-CL33	5.70	1.84	1.72
2	A	600	TWU	C32-CL33	5.43	1.84	1.72
2	B	600	TWU	C15-N14	3.79	1.38	1.34
2	A	600	TWU	C15-N14	3.55	1.38	1.34
2	A	600	TWU	C15-N08	2.35	1.40	1.38
2	B	600	TWU	C15-N08	2.31	1.40	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	TWU	C21-C32-CL33	-8.73	113.14	119.50
2	B	600	TWU	C21-C32-CL33	-7.88	113.77	119.50
2	B	600	TWU	C20-C21-C32	-3.07	116.41	118.81
2	B	600	TWU	N27-C26-N25	-2.64	122.66	126.04
2	A	600	TWU	N27-C26-N25	-2.57	122.75	126.04
2	A	600	TWU	C23-C24-N25	-2.56	121.95	124.07
2	B	600	TWU	C23-C24-N25	-2.54	121.97	124.07
2	B	600	TWU	C23-C28-N27	-2.41	122.08	124.07
2	A	600	TWU	C23-C28-N27	-2.38	122.10	124.07
2	A	600	TWU	C20-C21-C32	-2.09	117.17	118.81

There are no chirality outliers.

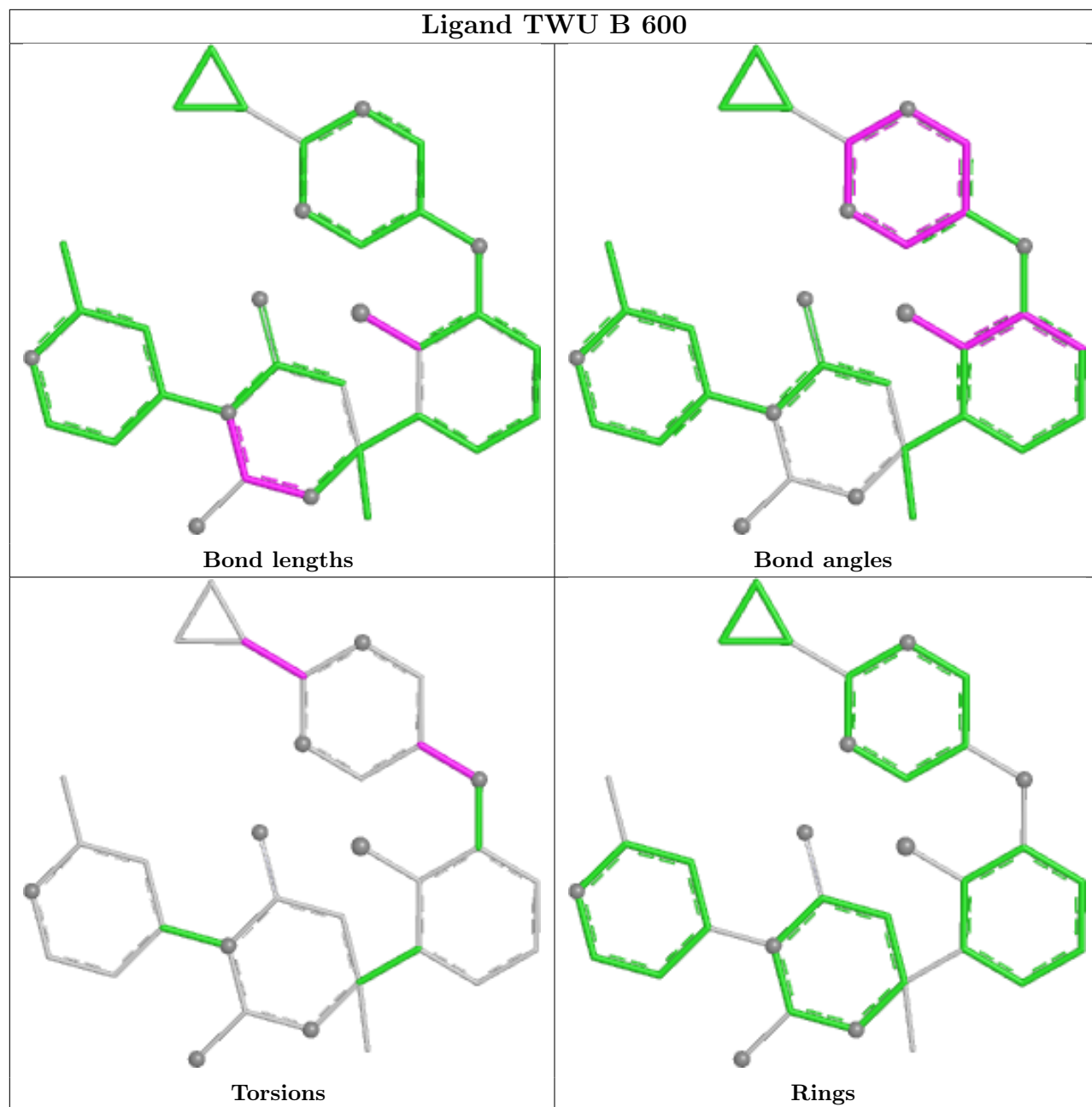
All (11) torsion outliers are listed below:

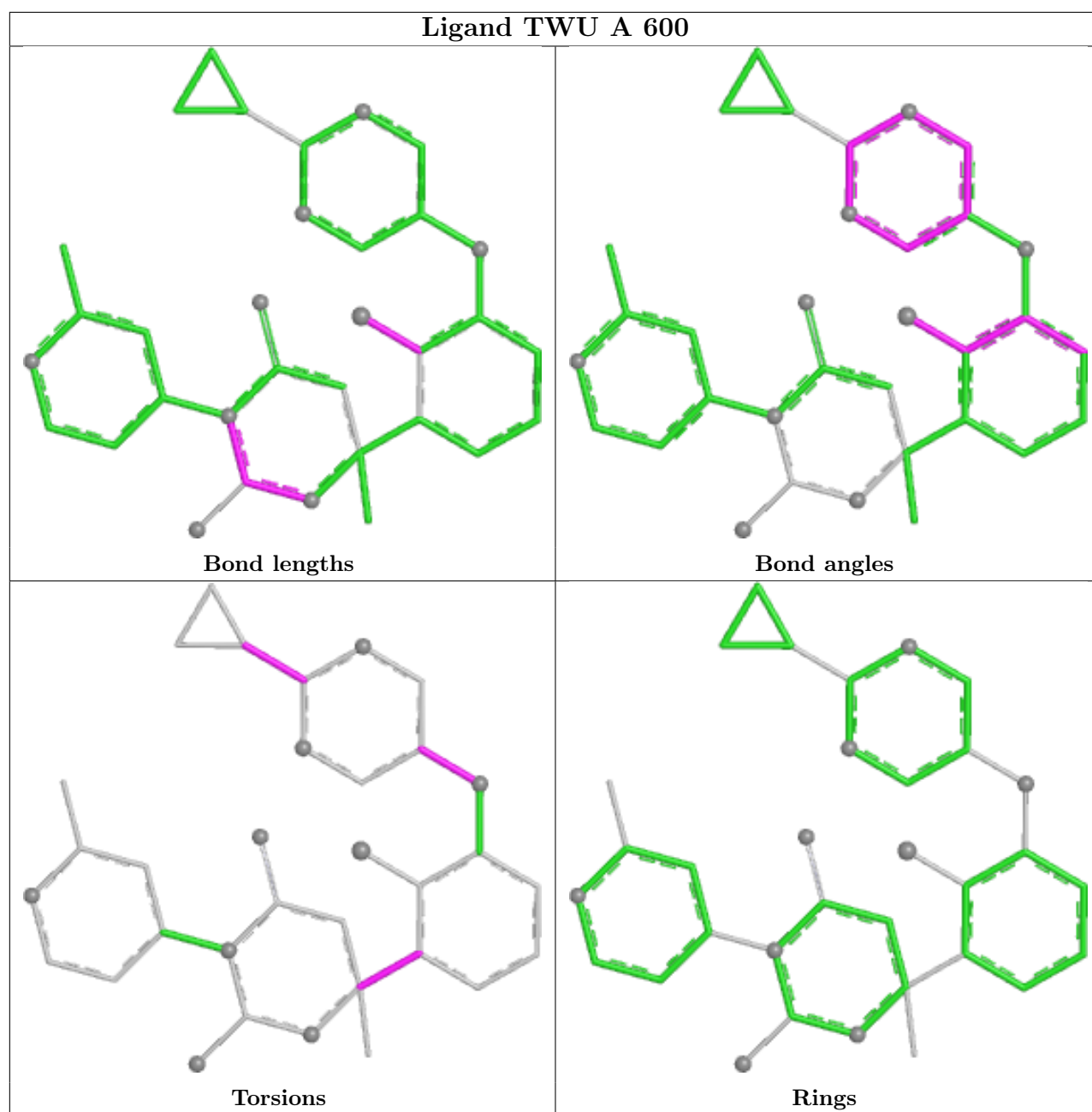
Mol	Chain	Res	Type	Atoms
2	A	600	TWU	N25-C26-C29-C31
2	A	600	TWU	N27-C26-C29-C31
2	B	600	TWU	N25-C26-C29-C30
2	B	600	TWU	N25-C26-C29-C31
2	B	600	TWU	C24-C23-N22-C21
2	B	600	TWU	C28-C23-N22-C21
2	A	600	TWU	C28-C23-N22-C21
2	A	600	TWU	C24-C23-N22-C21
2	B	600	TWU	N27-C26-C29-C31
2	B	600	TWU	N27-C26-C29-C30
2	A	600	TWU	C11-C12-C17-C18

There are no ring outliers.

No monomer is involved in short contacts.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	332/465 (71%)	0.44	21 (6%) 26 19	48, 66, 112, 170	0
1	B	332/465 (71%)	0.65	23 (6%) 23 17	54, 84, 131, 192	0
All	All	664/930 (71%)	0.55	44 (6%) 24 18	48, 73, 123, 192	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	SER	4.8
1	A	353	ASN	4.8
1	A	284	CYS	4.3
1	A	345	ASN	4.3
1	B	345	ASN	4.2
1	A	283	SER	4.1
1	A	282	GLU	4.0
1	B	353	ASN	3.9
1	A	247	GLN	3.8
1	A	516	LEU	3.4
1	B	245	ASP	3.1
1	A	536	HIS	3.1
1	B	516	LEU	3.0
1	A	245	ASP	2.9
1	B	243	LEU	2.8
1	B	536	HIS	2.7
1	A	246	SER	2.7
1	B	526	MET	2.7
1	B	518	ASP	2.7
1	B	313	SER	2.6
1	B	422	TYR	2.6
1	A	519	ASP	2.5
1	B	453	TYR	2.5
1	B	487	TYR	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	244	ARG	2.4
1	B	519	ASP	2.4
1	A	400	PRO	2.4
1	B	400	PRO	2.4
1	B	247	GLN	2.3
1	A	447	CYS	2.3
1	B	531	PRO	2.3
1	B	285	LYS	2.2
1	B	290	TYR	2.2
1	B	428	LYS	2.2
1	B	549	PHE	2.2
1	B	527	GLN	2.1
1	A	422	TYR	2.1
1	A	532	SER	2.1
1	A	281	GLU	2.1
1	A	306	ASN	2.1
1	A	285	LYS	2.1
1	B	283	SER	2.0
1	A	535	ASN	2.0
1	A	528	ILE	2.0

## 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](#)

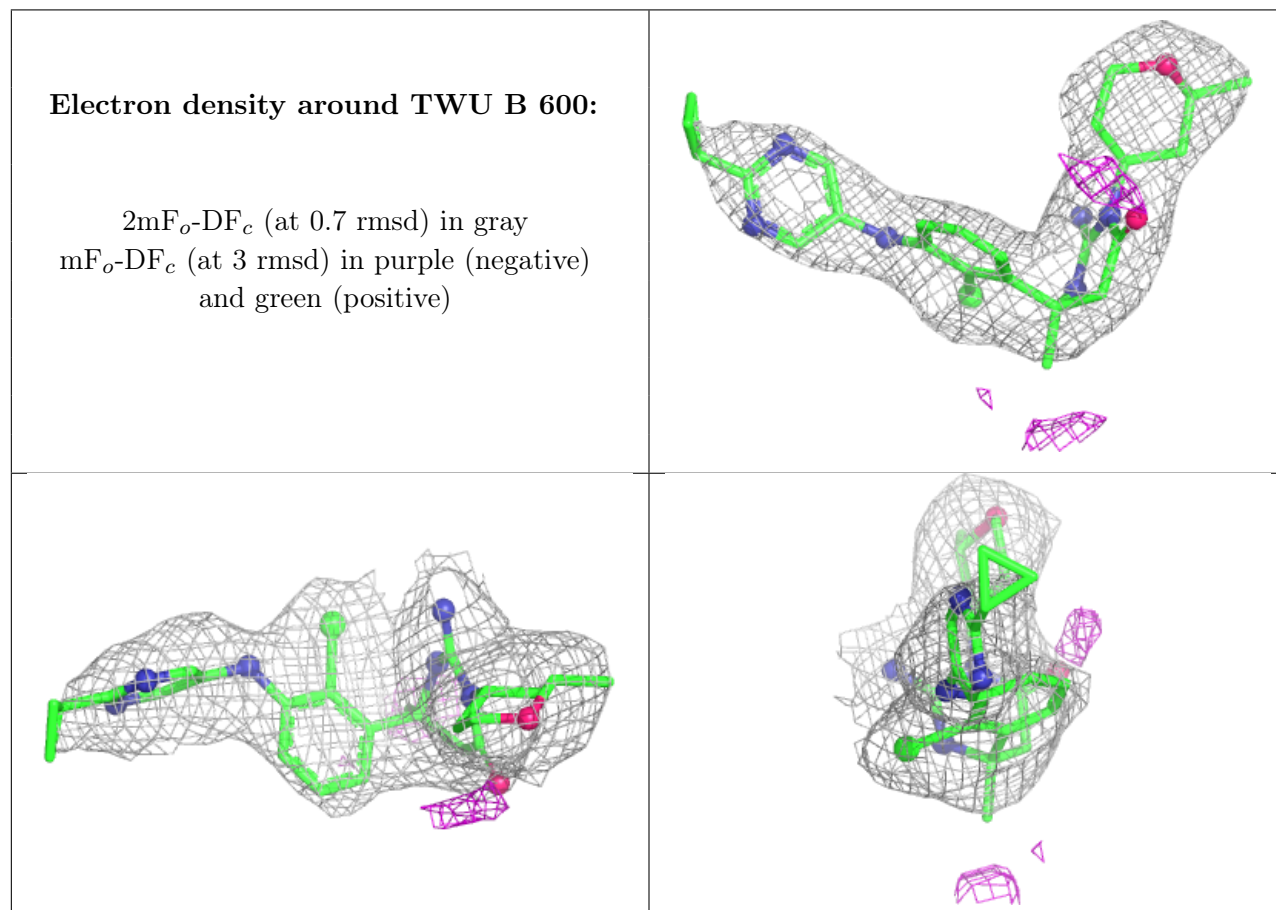
There are no oligosaccharides in this entry.

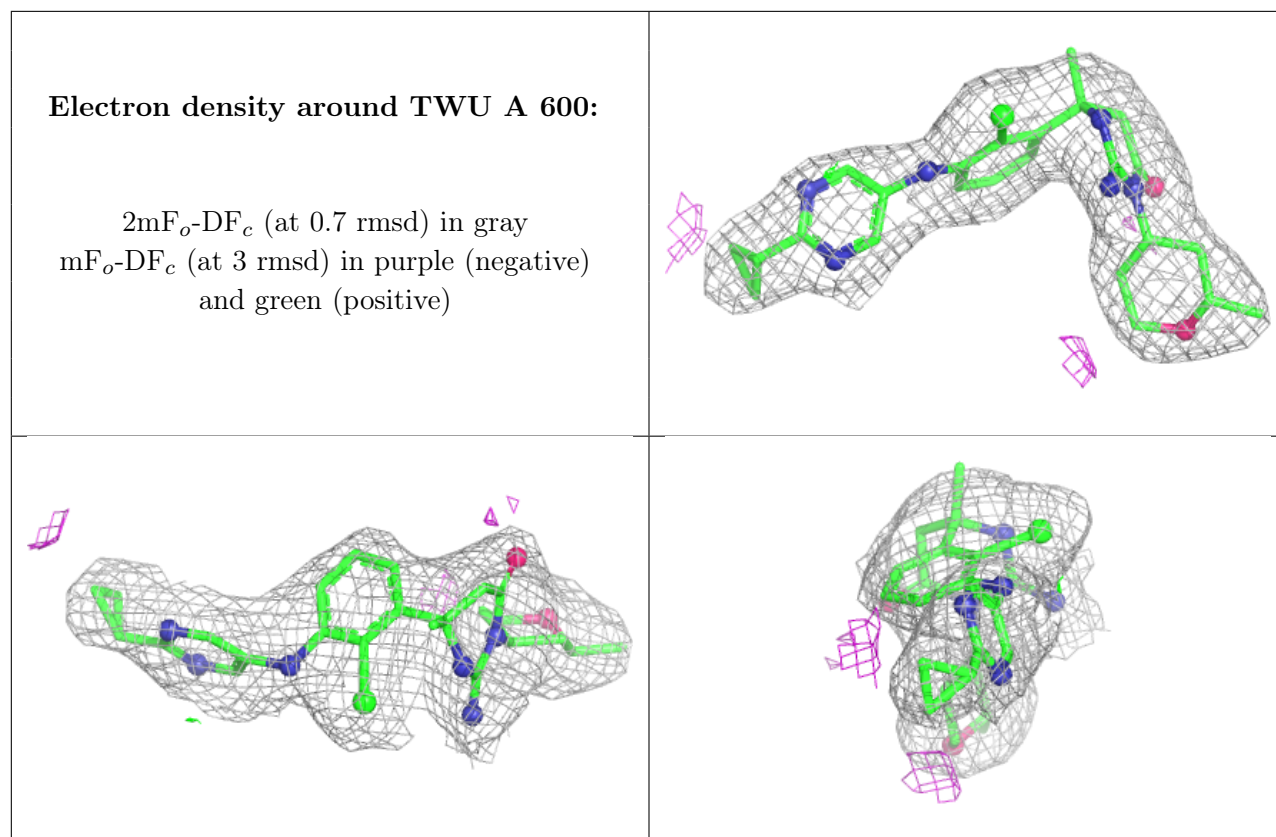
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	TWU	B	600	33/33	0.90	0.13	58,66,94,102	0
2	TWU	A	600	33/33	0.94	0.10	44,53,82,86	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.