



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:03 AM UTC

PDB ID : 8DUK / pdb_00008duk
Title : Estrogen Receptor Alpha Ligand Binding Domain in Complex with (6'-hydroxy-1'-(4-(2-(methylamino)ethoxy)phenyl)-1',4'-dihydro-2'-H-spiro[cyclopropane-1,3'-isoquinolin]-2'-yl)(phenyl)methanone
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Deposited on : 2022-07-27
Resolution : 1.70 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

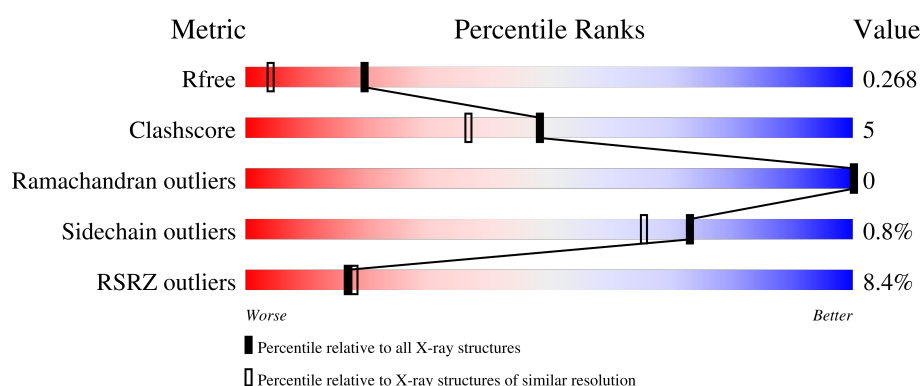
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	255	 9% 82% 11% • 7%
1	B	255	 9% 81% 7% • 11%
1	C	255	 7% 81% 13% 7%
1	D	255	 5% 79% 8% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8170 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.

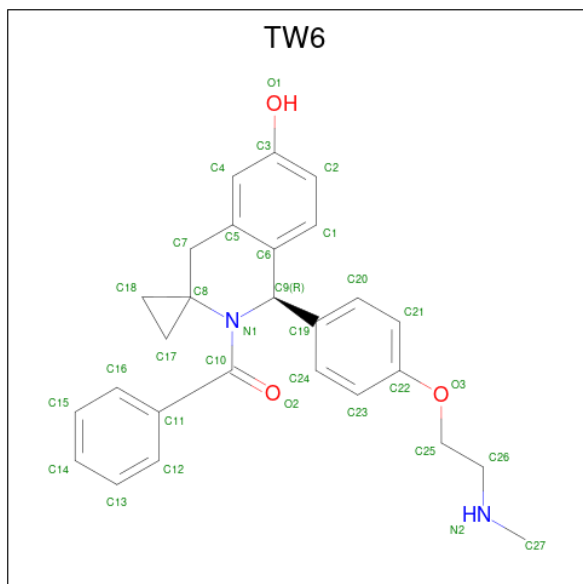
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	5	0
			1899	1218	322	343	16			
1	B	226	Total	C	N	O	S	0	4	0
			1793	1153	307	319	14			
1	C	238	Total	C	N	O	S	0	4	0
			1881	1208	317	341	15			
1	D	226	Total	C	N	O	S	0	5	0
			1813	1167	311	320	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	MET	-	initiating methionine	UNP P03372
A	381	SER	CYS	engineered mutation	UNP P03372
A	417	SER	CYS	engineered mutation	UNP P03372
A	530	SER	CYS	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	300	MET	-	initiating methionine	UNP P03372
B	381	SER	CYS	engineered mutation	UNP P03372
B	417	SER	CYS	engineered mutation	UNP P03372
B	530	SER	CYS	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	300	MET	-	initiating methionine	UNP P03372
C	381	SER	CYS	engineered mutation	UNP P03372
C	417	SER	CYS	engineered mutation	UNP P03372
C	530	SER	CYS	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
D	300	MET	-	initiating methionine	UNP P03372
D	381	SER	CYS	engineered mutation	UNP P03372
D	417	SER	CYS	engineered mutation	UNP P03372
D	530	SER	CYS	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is [(1'R)-6'-hydroxy-1'-{4-[2-(methylamino)ethoxy]phenyl}-1',4'-dihydro-2'H-spiro[cyclopropane-1,3'-isoquinolin]-2'-yl](phenyl)methanone (CCD ID: TW6) (formula: C₂₇H₂₈N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	27	2	3		
2	B	1	Total	C	N	O	0	0
			32	27	2	3		
2	C	1	Total	C	N	O	0	0
			32	27	2	3		
2	D	1	Total	C	N	O	0	0
			32	27	2	3		

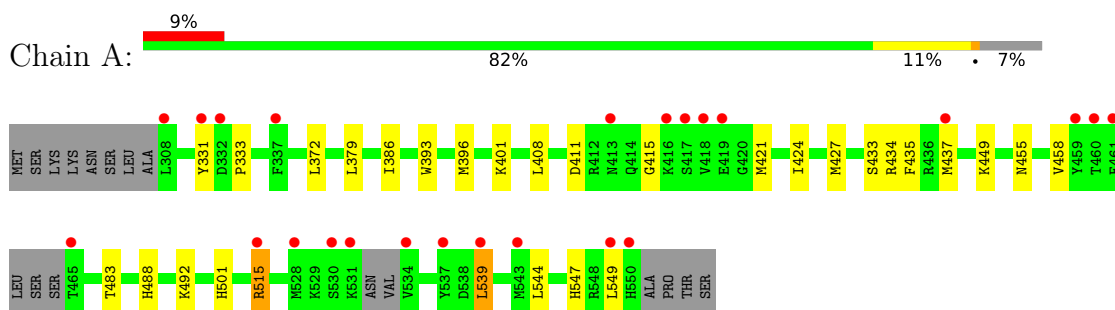
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total	O	0	0
			166	166		
3	B	160	Total	O	0	0
			160	160		
3	C	164	Total	O	0	0
			164	164		
3	D	166	Total	O	0	0
			166	166		

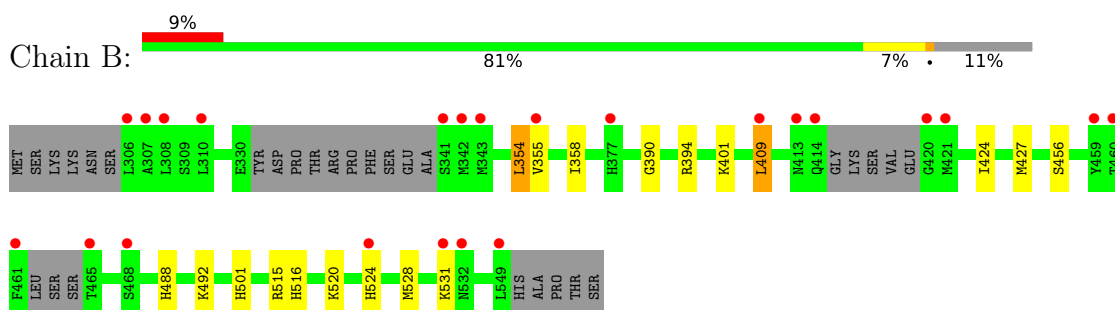
3 Residue-property plots [i](#)

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.

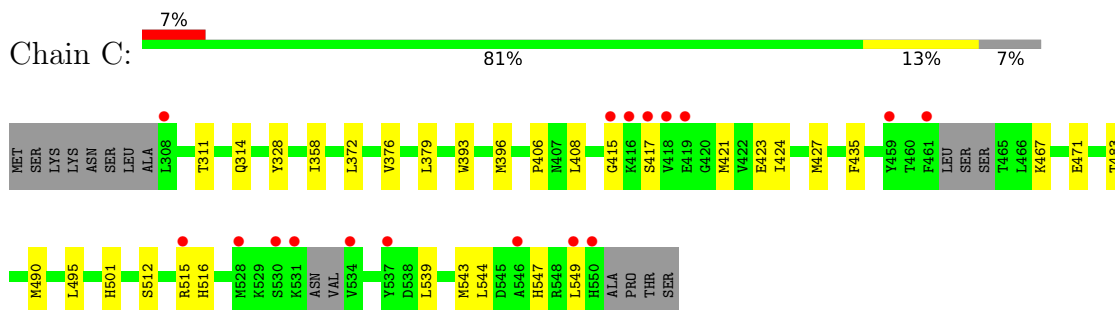
- Molecule 1: Estrogen receptor



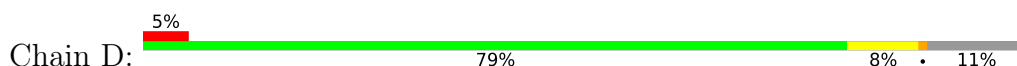
- Molecule 1: Estrogen receptor

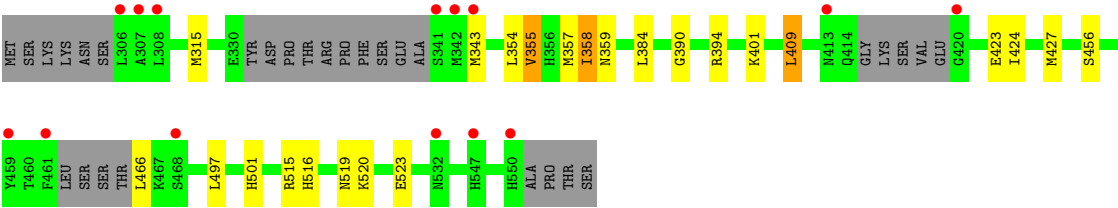


- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.03Å 57.66Å 174.52Å 90.00° 102.51° 90.00°	Depositor
Resolution (Å)	49.91 – 1.70 49.91 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.91-1.70) 96.0 (49.91-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.231 , 0.268 0.232 , 0.268	Depositor DCC
R_{free} test set	5193 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8170	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 97.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8502e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TW6

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	0.66	1/1938 (0.1%)	0.72	0/2622
1	B	0.66	2/1826 (0.1%)	0.73	2/2468 (0.1%)
1	C	0.77	3/1920 (0.2%)	0.82	1/2601 (0.0%)
1	D	0.80	4/1847 (0.2%)	0.79	0/2494
All	All	0.73	10/7531 (0.1%)	0.77	3/10185 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	515	ARG	C-O	-7.43	1.15	1.24
1	D	384	LEU	C-O	-6.39	1.16	1.24
1	D	359	ASN	C-O	-6.28	1.16	1.24
1	D	357	MET	C-O	-5.62	1.17	1.24
1	C	512	SER	C-O	-5.49	1.17	1.24
1	C	516	HIS	CE1-NE2	-5.41	1.27	1.32
1	D	355	VAL	C-O	-5.25	1.18	1.24
1	A	515	ARG	C-O	-5.08	1.18	1.24
1	B	354	LEU	C-O	-5.04	1.18	1.24
1	B	355	VAL	C-O	-5.02	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	531	LYS	CA-C-N	-5.75	113.53	122.67
1	B	531	LYS	C-N-CA	-5.75	113.53	122.67
1	C	423	GLU	CB-CG-CD	5.47	121.91	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1899	0	1904	29	0
1	B	1793	0	1814	16	0
1	C	1881	0	1873	27	0
1	D	1813	0	1841	19	0
2	A	32	0	0	1	0
2	B	32	0	0	0	0
2	C	32	0	0	1	0
2	D	32	0	0	0	0
3	A	166	0	0	1	0
3	B	160	0	0	0	0
3	C	164	0	0	0	0
3	D	166	0	0	0	0
All	All	8170	0	7432	82	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 (82) 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:415:GLY:HA2	1:A:421:MET:HE2	1.26	1.07
1:C:415:GLY:HA2	1:C:421:MET:HE2	1.11	1.07
1:A:372:LEU:HD23	1:C:372:LEU:HD23	1.55	0.86
1:A:379:LEU:HD12	1:A:544:LEU:HD11	1.65	0.78
1:A:393:TRP:CE3	1:A:396:MET:HE1	2.18	0.78
1:C:415:GLY:CA	1:C:421:MET:HE2	2.05	0.77
1:C:393:TRP:CE3	1:C:396:MET:HE1	2.21	0.75
1:C:539:LEU:HD23	1:C:539:LEU:O	1.88	0.72
1:C:358:ILE:HG13	1:C:543:MET:HE2	1.75	0.69
1:C:396:MET:HE2	1:C:435:PHE:HD2	1.59	0.66
1:C:379:LEU:HD12	1:C:544:LEU:HD11	1.77	0.66
1:A:396:MET:HE2	1:A:435:PHE:HD2	1.63	0.63
1:D:424:ILE:HD13	1:D:427:MET:HE2	1.84	0.60
1:A:539:LEU:O	1:A:539:LEU:HD23	2.01	0.59
1:D:424:ILE:HD13	1:D:427:MET:CE	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:HIS:NE2	1:D:520:LYS:HE2	2.19	0.58
1:C:424:ILE:HA	1:C:427:MET:HE3	1.86	0.57
1:A:501:HIS:CD2	1:B:501[B]:HIS:CD2	2.93	0.57
1:B:516:HIS:NE2	1:B:520:LYS:HE2	2.20	0.56
1:B:516:HIS:CE1	1:B:520:LYS:HE2	2.40	0.56
1:C:539:LEU:HD23	1:C:539:LEU:C	2.31	0.56
1:A:424:ILE:HA	1:A:427:MET:HE3	1.88	0.55
1:B:401:LYS:HB3	1:B:409:LEU:HD22	1.88	0.55
1:B:424:ILE:HD11	1:B:520:LYS:HB2	1.89	0.55
1:C:501:HIS:CD2	1:D:501[B]:HIS:CD2	2.96	0.54
1:C:415:GLY:HA2	1:C:421:MET:CE	2.07	0.54
1:C:424:ILE:HA	1:C:427:MET:CE	2.38	0.53
1:A:401:LYS:NZ	3:A:705:HOH:O	2.42	0.53
1:D:354:LEU:O	1:D:358:ILE:HD13	2.11	0.51
1:C:396:MET:HE2	1:C:435:PHE:CD2	2.44	0.50
1:C:539:LEU:C	1:C:539:LEU:CD2	2.85	0.50
1:A:424:ILE:HA	1:A:427:MET:CE	2.42	0.49
1:C:501:HIS:NE2	1:D:501[B]:HIS:NE2	2.60	0.49
1:C:421:MET:HG3	2:C:601:TW6:C13	2.42	0.49
1:A:515:ARG:NH1	1:B:516:HIS:CE1	2.79	0.49
1:A:331:TYR:O	1:A:333:PRO:HD3	2.13	0.49
1:A:396:MET:HE2	1:A:435:PHE:CD2	2.46	0.48
1:B:456[A]:SER:HA	1:B:515:ARG:NH2	2.27	0.48
1:C:379:LEU:CD1	1:C:544:LEU:HD11	2.44	0.48
1:D:343:MET:HE3	1:D:343:MET:HA	1.95	0.48
1:B:456[B]:SER:HA	1:B:515:ARG:NH2	2.30	0.47
1:A:393:TRP:CZ3	1:A:396:MET:HE1	2.49	0.47
1:B:488:HIS:NE2	1:B:492:LYS:HD2	2.29	0.47
1:D:456[A]:SER:HA	1:D:515:ARG:NH2	2.30	0.46
1:A:539:LEU:CD2	1:A:539:LEU:C	2.88	0.46
1:A:421:MET:HG3	2:A:601:TW6:C13	2.45	0.46
1:A:515:ARG:NH1	1:B:516:HIS:ND1	2.63	0.46
1:A:547:HIS:CE1	1:A:549:LEU:HB2	2.51	0.45
1:B:390:GLY:O	1:B:394:ARG:HG3	2.17	0.45
1:C:393:TRP:CZ3	1:C:396:MET:HE1	2.50	0.45
1:D:390:GLY:O	1:D:394:ARG:HG3	2.16	0.45
1:A:539:LEU:HD23	1:A:539:LEU:C	2.41	0.45
1:D:456[B]:SER:HA	1:D:515:ARG:NH2	2.31	0.45
1:A:434:ARG:HH11	1:A:437:MET:HE3	1.82	0.44
1:D:401:LYS:HB3	1:D:409:LEU:HD22	1.99	0.44
1:B:524:HIS:CE1	1:B:528:MET:CE	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:MET:HB3	1:C:495:LEU:HD22	1.99	0.44
1:D:424:ILE:HD11	1:D:520:LYS:HB2	1.98	0.44
1:A:488:HIS:NE2	1:A:492:LYS:HD2	2.33	0.44
1:A:455:ASN:O	1:A:458:VAL:HG12	2.18	0.43
1:C:408:LEU:HD12	1:C:408:LEU:HA	1.86	0.43
1:C:467:LYS:O	1:C:471:GLU:HG2	2.18	0.43
1:A:483:THR:HG22	1:B:501[A]:HIS:CD2	2.54	0.43
1:C:311:THR:OG1	1:C:314:GLN:HG3	2.18	0.43
1:A:433:SER:O	1:A:437:MET:HG3	2.19	0.43
1:C:328:TYR:CE2	1:C:406:PRO:HB2	2.54	0.43
1:D:423:GLU:O	1:D:427:MET:HG3	2.19	0.43
1:C:547:HIS:CE1	1:C:549:LEU:HB2	2.54	0.42
1:D:315:MET:HE2	1:D:315:MET:HB2	1.94	0.42
1:B:424:ILE:HD13	1:B:427:MET:CE	2.50	0.42
1:A:386[B]:ILE:HD12	1:A:449:LYS:HG3	2.02	0.42
1:B:354:LEU:O	1:B:358:ILE:HG12	2.19	0.42
1:D:519:ASN:O	1:D:523:GLU:HG3	2.20	0.42
1:A:501:HIS:NE2	1:B:501[B]:HIS:NE2	2.66	0.41
1:D:497:LEU:HD23	1:D:497:LEU:HA	1.79	0.41
1:A:408:LEU:HD12	1:A:408:LEU:HA	1.88	0.41
1:D:516:HIS:CE1	1:D:520:LYS:HE2	2.55	0.41
1:C:376:VAL:HG22	1:C:544:LEU:HD12	2.02	0.41
1:A:379:LEU:CD1	1:A:544:LEU:HD11	2.42	0.40
1:A:411:ASP:OD1	1:A:411:ASP:C	2.64	0.40
1:C:483:THR:HG22	1:D:501[A]:HIS:CD2	2.56	0.40
1:D:466:LEU:HD23	1:D:466:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	237/255 (93%)	234 (99%)	3 (1%)	0	100	100
1	B	222/255 (87%)	220 (99%)	2 (1%)	0	100	100
1	C	236/255 (92%)	235 (100%)	1 (0%)	0	100	100
1	D	223/255 (88%)	220 (99%)	3 (1%)	0	100	100
All	All	918/1020 (90%)	909 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	209/230 (91%)	208 (100%)	1 (0%)	81	76
1	B	195/230 (85%)	194 (100%)	1 (0%)	81	76
1	C	205/230 (89%)	204 (100%)	1 (0%)	81	76
1	D	198/230 (86%)	195 (98%)	3 (2%)	57	43
All	All	807/920 (88%)	801 (99%)	6 (1%)	73	69

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	539	LEU
1	B	409	LEU
1	C	417	SER
1	D	355	VAL
1	D	358	ILE
1	D	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	375	GLN

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Mol	Chain	Res	Type
1	A	398	HIS
1	B	455	ASN
1	C	359	ASN
1	D	373	HIS
1	D	455	ASN
1	D	476	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	TW6	B	601	-	35,36,36	4.80	23 (65%)	40,52,52	2.12	15 (37%)
2	TW6	C	601	-	35,36,36	4.74	26 (74%)	40,52,52	2.55	17 (42%)
2	TW6	D	601	-	35,36,36	4.83	23 (65%)	40,52,52	1.94	15 (37%)
2	TW6	A	601	-	35,36,36	4.66	24 (68%)	40,52,52	2.60	22 (55%)

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	TW6	B	601	-	-	5/17/40/40	0/5/5/5
2	TW6	C	601	-	-	6/17/40/40	0/5/5/5
2	TW6	D	601	-	-	5/17/40/40	0/5/5/5
2	TW6	A	601	-	-	6/17/40/40	0/5/5/5

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TW6	C1-C6	11.24	1.53	1.39
2	D	601	TW6	C1-C6	10.16	1.52	1.39
2	C	601	TW6	C16-C11	9.66	1.54	1.39
2	B	601	TW6	C16-C11	9.60	1.54	1.39
2	A	601	TW6	C16-C11	9.53	1.53	1.39
2	D	601	TW6	C16-C11	9.31	1.53	1.39
2	A	601	TW6	C21-C20	9.21	1.53	1.38
2	D	601	TW6	C13-C12	9.15	1.54	1.38
2	B	601	TW6	C4-C5	9.14	1.53	1.39
2	A	601	TW6	C1-C6	9.11	1.50	1.39
2	C	601	TW6	C1-C6	9.10	1.50	1.39
2	C	601	TW6	C21-C20	9.07	1.53	1.38
2	A	601	TW6	C24-C19	8.83	1.53	1.39
2	D	601	TW6	C21-C20	8.58	1.52	1.38
2	D	601	TW6	C24-C19	8.55	1.52	1.39
2	D	601	TW6	C4-C5	8.48	1.52	1.39
2	B	601	TW6	C13-C12	8.43	1.53	1.38
2	C	601	TW6	C24-C19	8.20	1.52	1.39
2	B	601	TW6	C21-C20	8.08	1.51	1.38
2	C	601	TW6	C4-C5	8.02	1.52	1.39
2	A	601	TW6	C23-C22	7.80	1.53	1.38
2	D	601	TW6	C23-C22	7.77	1.53	1.38
2	B	601	TW6	C24-C19	7.74	1.51	1.39
2	C	601	TW6	C23-C22	7.46	1.52	1.38
2	C	601	TW6	C13-C12	7.42	1.51	1.38
2	A	601	TW6	C4-C5	7.42	1.51	1.39
2	A	601	TW6	C13-C12	7.24	1.51	1.38
2	D	601	TW6	C14-C15	7.14	1.53	1.38
2	C	601	TW6	C2-C3	7.13	1.52	1.39
2	B	601	TW6	C14-C15	7.00	1.53	1.38
2	A	601	TW6	C14-C15	6.41	1.52	1.38
2	C	601	TW6	C14-C15	6.38	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TW6	C2-C3	6.31	1.50	1.39
2	A	601	TW6	C2-C3	6.09	1.50	1.39
2	B	601	TW6	C23-C22	6.04	1.50	1.38
2	D	601	TW6	C2-C3	6.02	1.50	1.39
2	C	601	TW6	C17-C8	4.77	1.57	1.50
2	C	601	TW6	C2-C1	-4.75	1.31	1.38
2	A	601	TW6	C12-C11	-4.74	1.32	1.39
2	A	601	TW6	C10-N1	4.70	1.46	1.36
2	C	601	TW6	C12-C11	-4.53	1.32	1.39
2	B	601	TW6	C9-N1	-4.45	1.41	1.47
2	B	601	TW6	C10-N1	4.45	1.46	1.36
2	C	601	TW6	C10-N1	4.44	1.46	1.36
2	D	601	TW6	C5-C6	-4.27	1.32	1.40
2	D	601	TW6	C2-C1	-4.25	1.31	1.38
2	B	601	TW6	C12-C11	-4.21	1.33	1.39
2	D	601	TW6	C10-N1	4.14	1.45	1.36
2	B	601	TW6	C18-C8	3.87	1.56	1.50
2	A	601	TW6	C8-N1	-3.76	1.45	1.51
2	B	601	TW6	C2-C1	-3.76	1.32	1.38
2	B	601	TW6	C8-N1	-3.70	1.45	1.51
2	A	601	TW6	C2-C1	-3.69	1.32	1.38
2	D	601	TW6	C9-N1	-3.66	1.42	1.47
2	A	601	TW6	C15-C16	-3.64	1.32	1.38
2	A	601	TW6	C18-C8	3.62	1.55	1.50
2	B	601	TW6	C23-C24	-3.55	1.33	1.38
2	C	601	TW6	C18-C8	3.55	1.55	1.50
2	B	601	TW6	C17-C8	3.54	1.55	1.50
2	A	601	TW6	C4-C3	-3.48	1.34	1.39
2	D	601	TW6	C15-C16	-3.47	1.33	1.38
2	D	601	TW6	C21-C22	-3.45	1.32	1.38
2	D	601	TW6	C20-C19	-3.43	1.33	1.39
2	D	601	TW6	C17-C8	3.43	1.55	1.50
2	D	601	TW6	C12-C11	-3.41	1.34	1.39
2	C	601	TW6	C5-C6	-3.40	1.34	1.40
2	D	601	TW6	C8-N1	-3.36	1.46	1.51
2	C	601	TW6	C8-N1	-3.35	1.46	1.51
2	B	601	TW6	C5-C6	-3.35	1.34	1.40
2	A	601	TW6	C17-C8	3.23	1.55	1.50
2	C	601	TW6	C15-C16	-3.22	1.33	1.38
2	B	601	TW6	C20-C19	-3.20	1.34	1.39
2	D	601	TW6	C23-C24	-3.13	1.33	1.38
2	C	601	TW6	C4-C3	-3.08	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	TW6	C18-C8	2.94	1.54	1.50
2	A	601	TW6	O3-C22	2.92	1.44	1.37
2	B	601	TW6	C15-C16	-2.88	1.34	1.38
2	C	601	TW6	O3-C22	2.65	1.43	1.37
2	A	601	TW6	C20-C19	-2.59	1.35	1.39
2	C	601	TW6	C11-C10	2.50	1.54	1.50
2	A	601	TW6	C21-C22	-2.47	1.34	1.38
2	C	601	TW6	C23-C24	-2.46	1.34	1.38
2	C	601	TW6	C20-C19	-2.45	1.35	1.39
2	A	601	TW6	C5-C6	-2.45	1.35	1.40
2	C	601	TW6	C21-C22	-2.37	1.34	1.38
2	C	601	TW6	C14-C13	-2.31	1.33	1.38
2	B	601	TW6	C7-C5	2.31	1.55	1.50
2	C	601	TW6	C7-C5	2.31	1.55	1.50
2	D	601	TW6	C4-C3	-2.31	1.35	1.39
2	B	601	TW6	C14-C13	-2.22	1.33	1.38
2	A	601	TW6	C7-C5	2.21	1.54	1.50
2	D	601	TW6	C11-C10	2.08	1.53	1.50
2	C	601	TW6	C6-C9	2.06	1.54	1.51
2	A	601	TW6	C23-C24	-2.04	1.35	1.38
2	A	601	TW6	O2-C10	-2.02	1.18	1.22
2	B	601	TW6	C6-C9	2.01	1.54	1.51

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	TW6	C13-C12-C11	-6.31	114.16	120.36
2	A	601	TW6	C23-C24-C19	-5.61	115.59	121.18
2	C	601	TW6	C3-C4-C5	-5.60	114.48	120.77
2	C	601	TW6	C13-C12-C11	-4.95	115.50	120.36
2	A	601	TW6	C14-C15-C16	-4.47	114.73	120.24
2	A	601	TW6	C16-C11-C12	4.41	124.18	118.57
2	C	601	TW6	C25-O3-C22	-4.40	106.50	117.93
2	C	601	TW6	C23-C24-C19	-4.28	116.91	121.18
2	D	601	TW6	C21-C20-C19	-4.26	116.93	121.18
2	B	601	TW6	C20-C21-C22	-4.18	114.95	119.73
2	A	601	TW6	C16-C11-C10	-4.18	109.57	120.28
2	B	601	TW6	C23-C24-C19	-4.15	117.04	121.18
2	C	601	TW6	C24-C19-C20	3.86	123.08	118.30
2	C	601	TW6	C7-C5-C4	-3.82	113.08	121.18
2	A	601	TW6	C24-C19-C20	3.77	122.97	118.30
2	C	601	TW6	C17-C18-C8	3.75	62.24	59.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	TW6	C24-C19-C20	3.73	122.93	118.30
2	A	601	TW6	C11-C10-N1	3.67	124.59	117.83
2	B	601	TW6	O2-C10-N1	-3.53	116.78	121.84
2	D	601	TW6	C16-C11-C12	3.48	123.00	118.57
2	B	601	TW6	C16-C11-C12	3.43	122.93	118.57
2	A	601	TW6	C5-C6-C9	3.39	127.11	121.32
2	D	601	TW6	O2-C10-N1	-3.37	117.01	121.84
2	C	601	TW6	C16-C11-C12	3.35	122.82	118.57
2	B	601	TW6	C11-C10-N1	3.31	123.93	117.83
2	C	601	TW6	C16-C11-C10	-3.29	111.85	120.28
2	B	601	TW6	C3-C4-C5	-3.26	117.10	120.77
2	D	601	TW6	C24-C19-C20	3.19	122.26	118.30
2	C	601	TW6	C11-C10-N1	3.16	123.64	117.83
2	B	601	TW6	C13-C12-C11	-3.09	117.33	120.36
2	B	601	TW6	C25-O3-C22	-3.06	109.98	117.93
2	C	601	TW6	C4-C5-C6	3.04	123.31	119.49
2	A	601	TW6	C7-C5-C4	-3.02	114.77	121.18
2	C	601	TW6	C1-C6-C9	-3.02	113.83	121.22
2	D	601	TW6	C24-C23-C22	-2.99	116.32	119.73
2	A	601	TW6	C3-C4-C5	-2.92	117.49	120.77
2	A	601	TW6	C1-C6-C9	-2.89	114.16	121.22
2	C	601	TW6	O2-C10-N1	-2.87	117.73	121.84
2	D	601	TW6	C3-C4-C5	-2.81	117.61	120.77
2	C	601	TW6	C5-C6-C9	2.76	126.04	121.32
2	C	601	TW6	C14-C15-C16	-2.76	116.83	120.24
2	B	601	TW6	C1-C6-C9	-2.74	114.51	121.22
2	D	601	TW6	C19-C9-N1	2.71	115.80	112.60
2	B	601	TW6	C16-C11-C10	-2.67	113.44	120.28
2	A	601	TW6	C18-C17-C8	2.65	61.49	59.67
2	B	601	TW6	C23-C22-C21	2.63	123.99	120.16
2	A	601	TW6	C25-O3-C22	-2.61	111.15	117.93
2	A	601	TW6	C1-C2-C3	2.58	122.61	119.88
2	D	601	TW6	C7-C5-C4	-2.56	115.75	121.18
2	D	601	TW6	C5-C6-C9	2.47	125.54	121.32
2	B	601	TW6	C24-C19-C9	-2.39	115.68	120.67
2	D	601	TW6	C12-C11-C10	-2.39	114.16	120.28
2	B	601	TW6	C5-C6-C9	2.38	125.39	121.32
2	A	601	TW6	C4-C5-C6	2.37	122.47	119.49
2	A	601	TW6	C20-C21-C22	-2.35	117.05	119.73
2	D	601	TW6	C1-C6-C9	-2.34	115.49	121.22
2	D	601	TW6	C25-O3-C22	-2.33	111.87	117.93
2	A	601	TW6	C15-C14-C13	2.27	122.98	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	TW6	C15-C16-C11	-2.22	118.18	120.36
2	A	601	TW6	C12-C11-C10	2.20	125.92	120.28
2	A	601	TW6	O2-C10-N1	-2.20	118.69	121.84
2	D	601	TW6	C17-C18-C8	2.11	61.12	59.67
2	C	601	TW6	C14-C13-C12	2.09	122.82	120.24
2	D	601	TW6	C11-C10-N1	2.09	121.68	117.83
2	C	601	TW6	C2-C3-C4	2.07	122.46	120.19
2	A	601	TW6	O2-C10-C11	-2.07	116.19	120.29
2	B	601	TW6	C18-C17-C8	2.06	61.08	59.67
2	A	601	TW6	C17-C18-C8	2.02	61.06	59.67
2	A	601	TW6	C24-C23-C22	2.01	122.03	119.73

There are no chirality outliers.

All (22) torsion outliers are listed below:

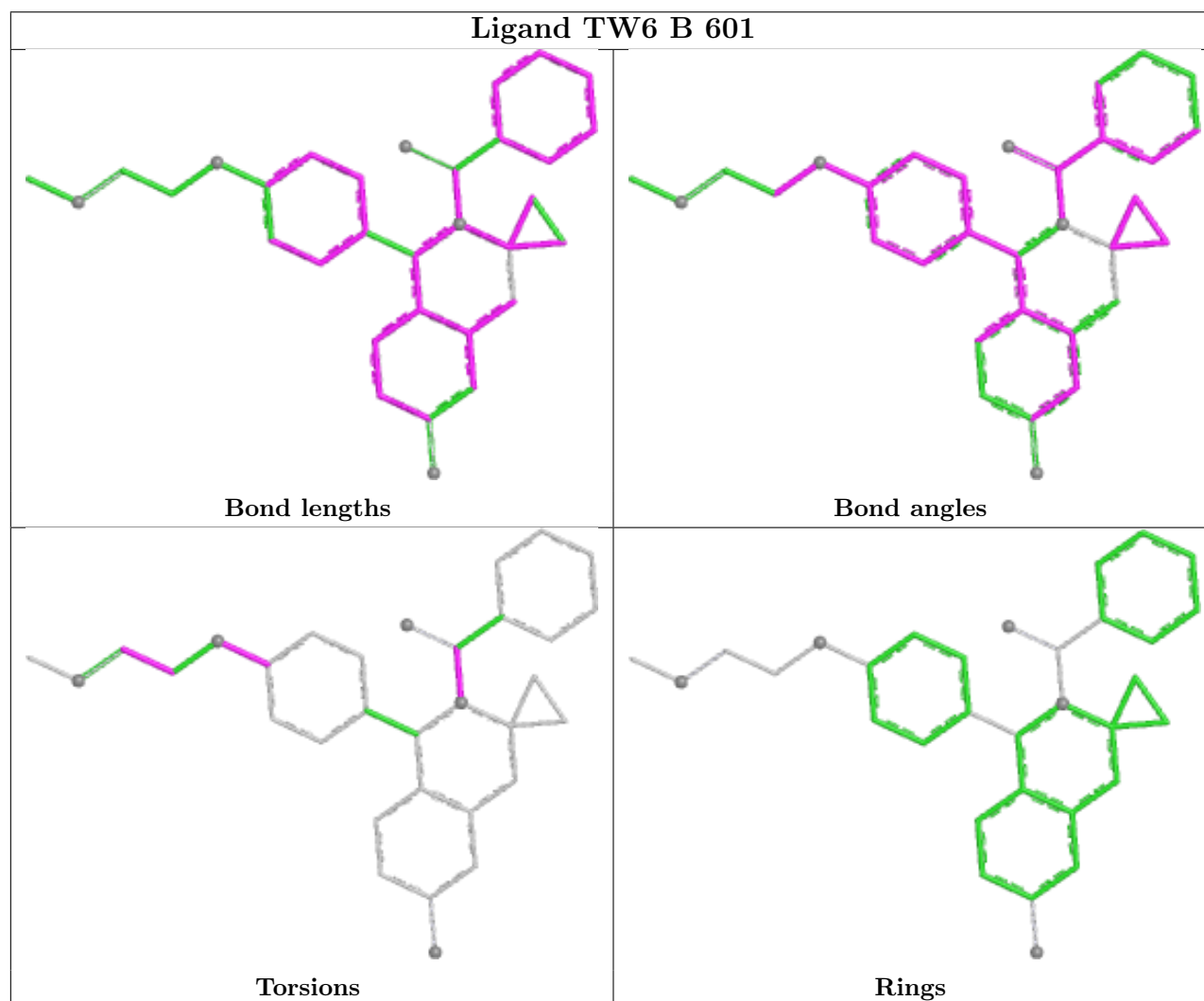
Mol	Chain	Res	Type	Atoms
2	A	601	TW6	C11-C10-N1-C8
2	A	601	TW6	O2-C10-N1-C8
2	A	601	TW6	C25-C26-N2-C27
2	B	601	TW6	C11-C10-N1-C8
2	B	601	TW6	O2-C10-N1-C8
2	C	601	TW6	C11-C10-N1-C8
2	C	601	TW6	O2-C10-N1-C8
2	C	601	TW6	C25-C26-N2-C27
2	D	601	TW6	C11-C10-N1-C8
2	D	601	TW6	O2-C10-N1-C8
2	C	601	TW6	C21-C22-O3-C25
2	C	601	TW6	C23-C22-O3-C25
2	A	601	TW6	C23-C22-O3-C25
2	A	601	TW6	C21-C22-O3-C25
2	A	601	TW6	O3-C25-C26-N2
2	C	601	TW6	O3-C25-C26-N2
2	B	601	TW6	C23-C22-O3-C25
2	B	601	TW6	O3-C25-C26-N2
2	D	601	TW6	O3-C25-C26-N2
2	B	601	TW6	C21-C22-O3-C25
2	D	601	TW6	C21-C22-O3-C25
2	D	601	TW6	C23-C22-O3-C25

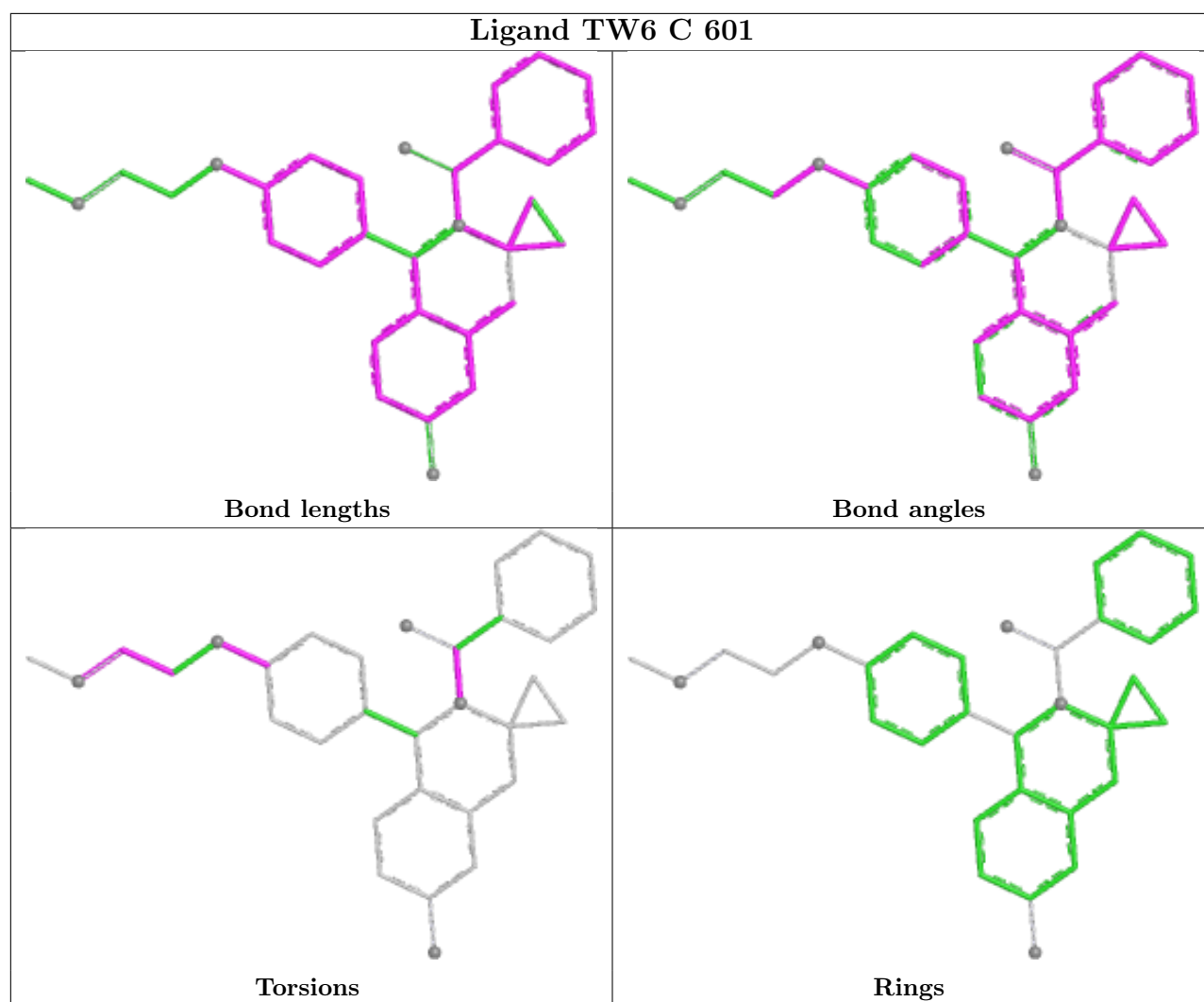
There are no ring outliers.

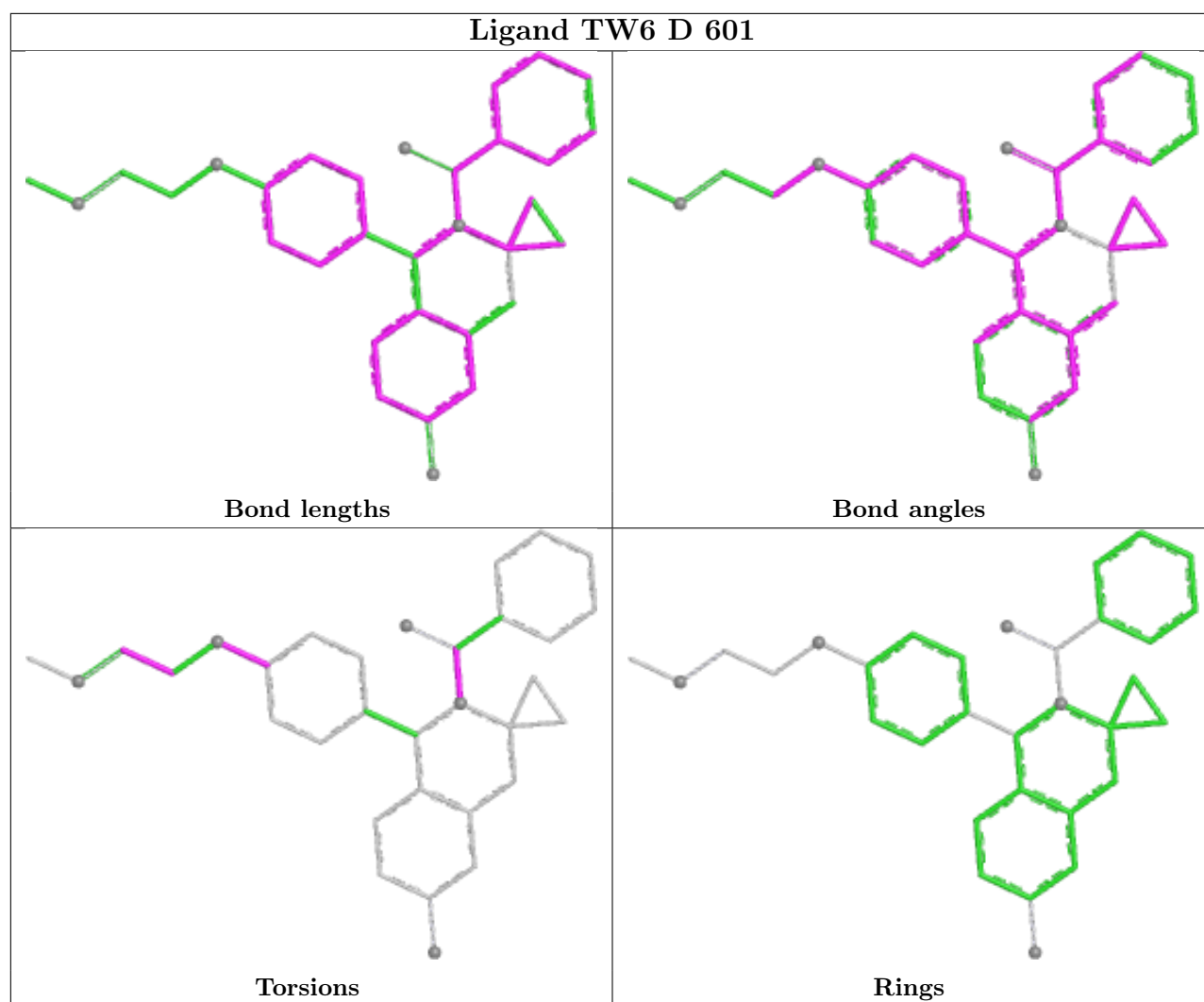
2 monomers are involved in 2 short contacts:

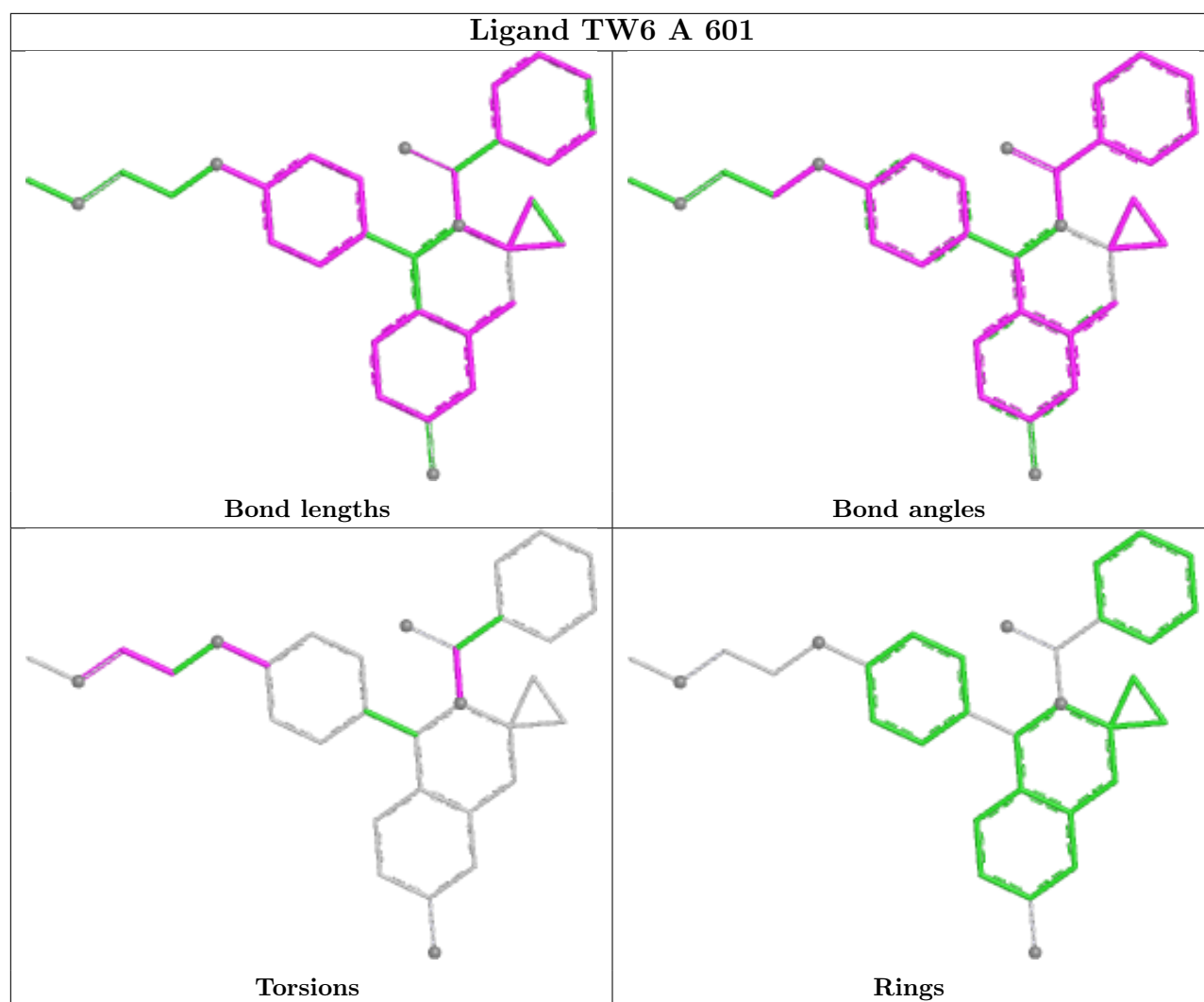
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	TW6	1	0
2	A	601	TW6	1	0

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 [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	238/255 (93%)	0.51	24 (10%)	12 13	5, 18, 41, 56	6 (2%)
1	B	226/255 (88%)	0.52	23 (10%)	12 12	6, 19, 36, 49	5 (2%)
1	C	238/255 (93%)	0.21	17 (7%)	22 24	3, 15, 40, 52	5 (2%)
1	D	226/255 (88%)	0.12	14 (6%)	26 29	3, 16, 35, 48	6 (2%)
All	All	928/1020 (90%)	0.34	78 (8%)	17 18	3, 17, 39, 56	22 (2%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	515	ARG	5.5
1	B	459	TYR	5.3
1	B	461	PHE	4.6
1	D	461	PHE	4.4
1	C	534	VAL	4.2
1	A	459	TYR	4.2
1	A	537	TYR	4.1
1	A	308	LEU	4.0
1	C	459	TYR	3.9
1	D	459	TYR	3.9
1	D	550	HIS	3.8
1	A	418	VAL	3.7
1	D	306	LEU	3.6
1	C	419	GLU	3.6
1	C	531	LYS	3.6
1	D	532	ASN	3.6
1	A	461	PHE	3.5
1	C	461	PHE	3.3
1	A	531	LYS	3.3
1	B	532	ASN	3.3
1	D	341	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	537	TYR	3.2
1	A	534	VAL	3.2
1	B	341	SER	3.1
1	D	343	MET	3.1
1	A	515	ARG	3.1
1	C	417	SER	3.1
1	C	418	VAL	3.0
1	A	549	LEU	3.0
1	C	308	LEU	3.0
1	B	465	THR	3.0
1	B	460	THR	3.0
1	A	417	SER	2.9
1	B	342	MET	2.9
1	A	419	GLU	2.9
1	A	530	SER	2.9
1	A	550	HIS	2.9
1	A	416	LYS	2.8
1	A	332	ASP	2.8
1	B	413	ASN	2.8
1	C	550	HIS	2.8
1	D	468	SER	2.7
1	A	437	MET	2.7
1	A	337	PHE	2.6
1	B	306	LEU	2.6
1	B	420	GLY	2.6
1	B	377	HIS	2.6
1	A	528	MET	2.6
1	B	468	SER	2.5
1	C	415	GLY	2.5
1	D	307	ALA	2.5
1	C	530	SER	2.5
1	B	308	LEU	2.5
1	B	549	LEU	2.5
1	B	355	VAL	2.5
1	C	549	LEU	2.4
1	C	528	MET	2.4
1	A	331	TYR	2.4
1	C	416	LYS	2.4
1	C	546	ALA	2.4
1	B	414	GLN	2.4
1	A	543	MET	2.4
1	D	420	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	342	MET	2.3
1	A	460	THR	2.3
1	D	308	LEU	2.3
1	B	409	LEU	2.2
1	B	307	ALA	2.2
1	D	413	ASN	2.2
1	A	465	THR	2.2
1	A	539	LEU	2.1
1	B	524	HIS	2.1
1	D	547	HIS	2.1
1	B	531	LYS	2.1
1	A	413	ASN	2.1
1	B	421	MET	2.1
1	B	310	LEU	2.1
1	B	343	MET	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](#)

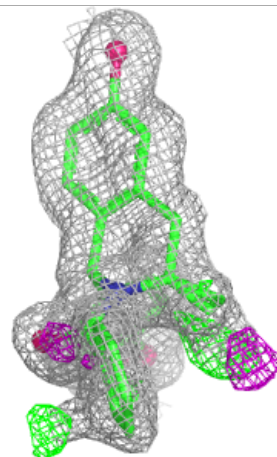
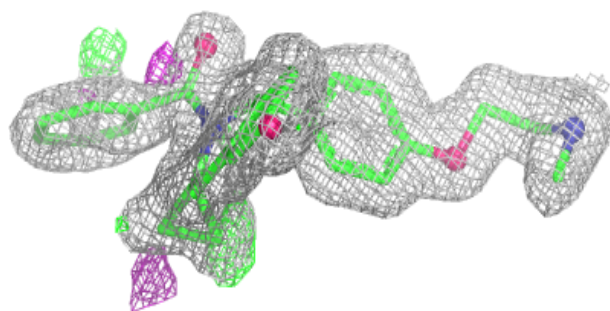
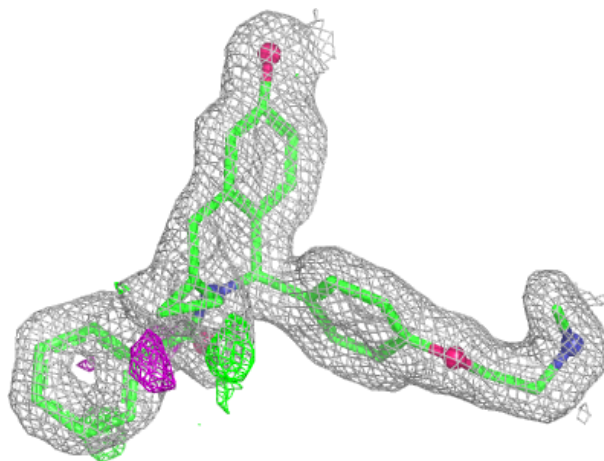
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TW6	D	601	32/32	0.94	0.09	7,14,30,32	0
2	TW6	C	601	32/32	0.95	0.08	7,13,32,34	0
2	TW6	B	601	32/32	0.95	0.09	7,14,33,38	0
2	TW6	A	601	32/32	0.96	0.07	5,15,31,33	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.

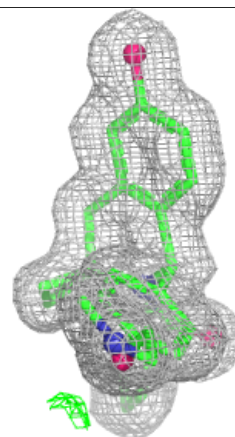
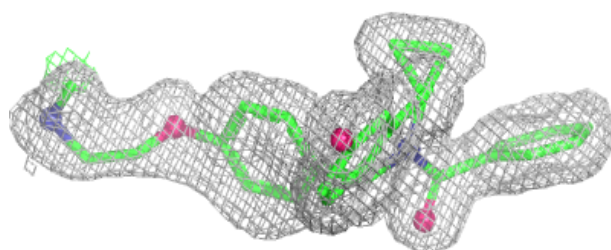
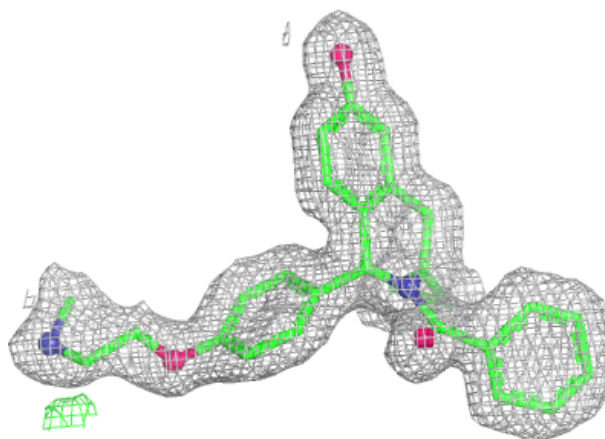
Electron density around TW6 D 601:

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



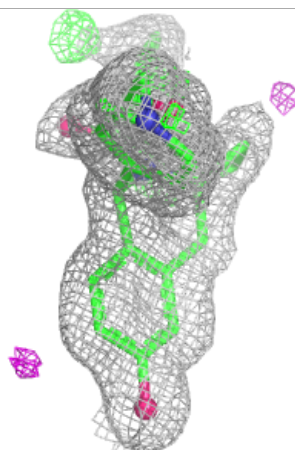
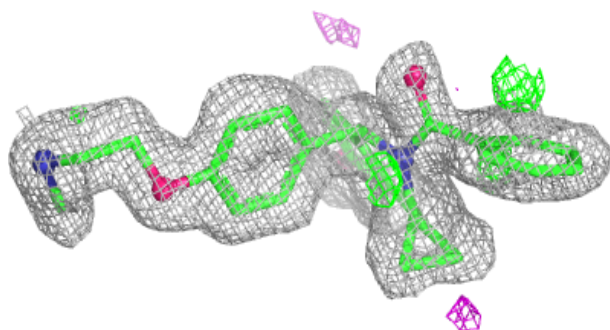
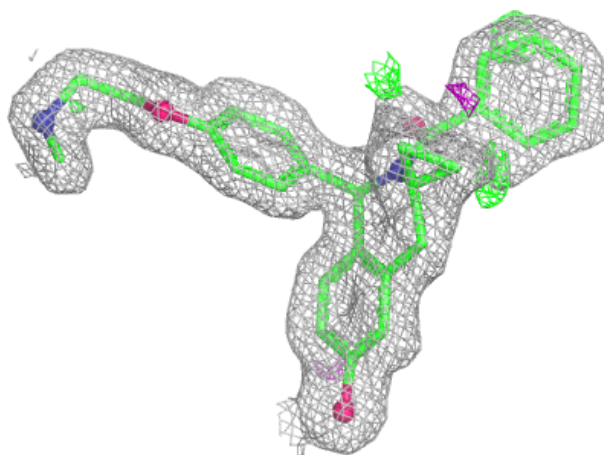
Electron density around TW6 C 601:

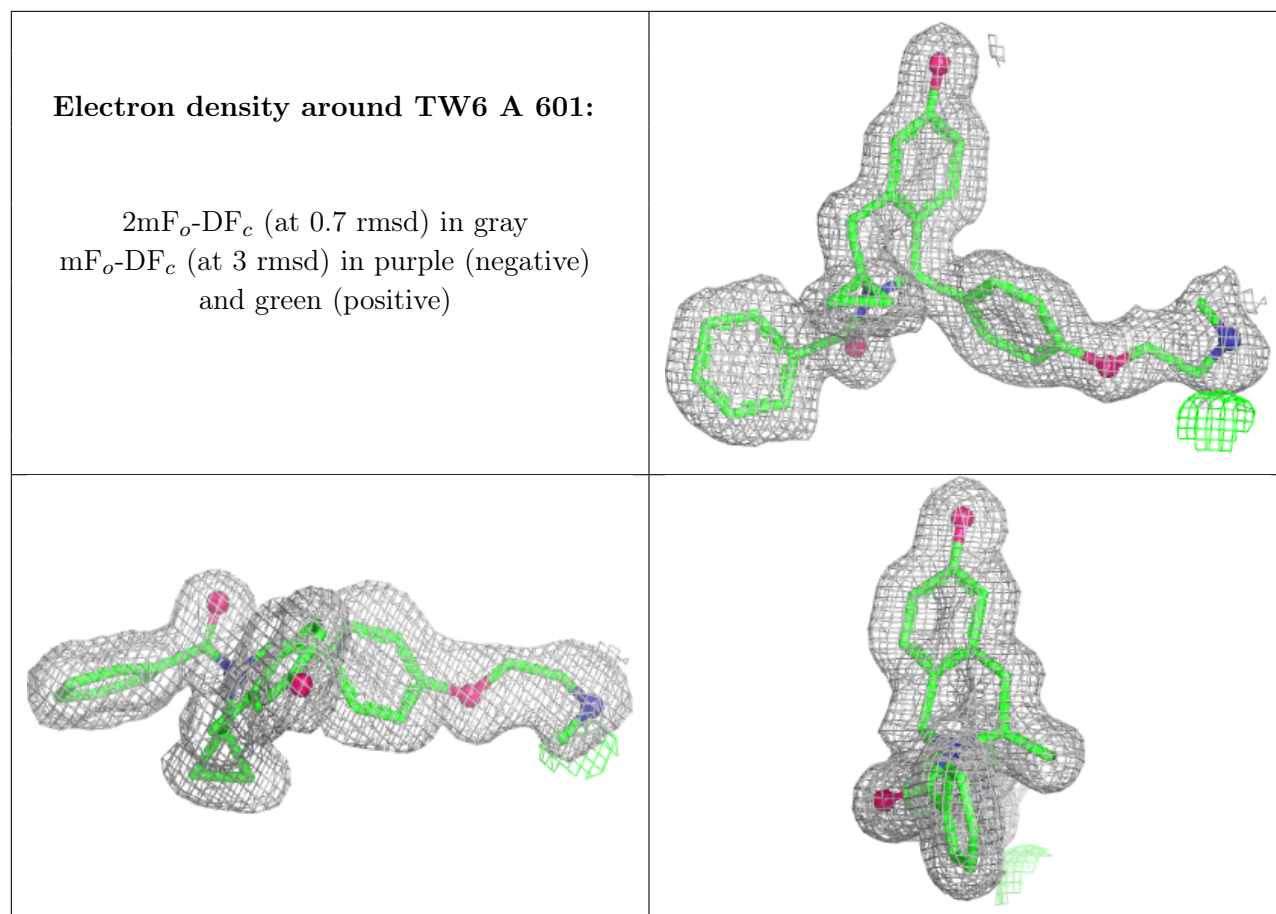
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TW6 B 601:

$2mF_o-DF_c$ (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.