



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 01:04 AM UTC

PDB ID : 9TPH / pdb\_00009tph  
Title : Survivin 1-127 in complex with a molecular tweezer-Histone-H3-peptide conjugate  
Authors : Vetter, I.R.; Bier, D.  
Deposited on : 2025-12-18  
Resolution : 2.00 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)
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

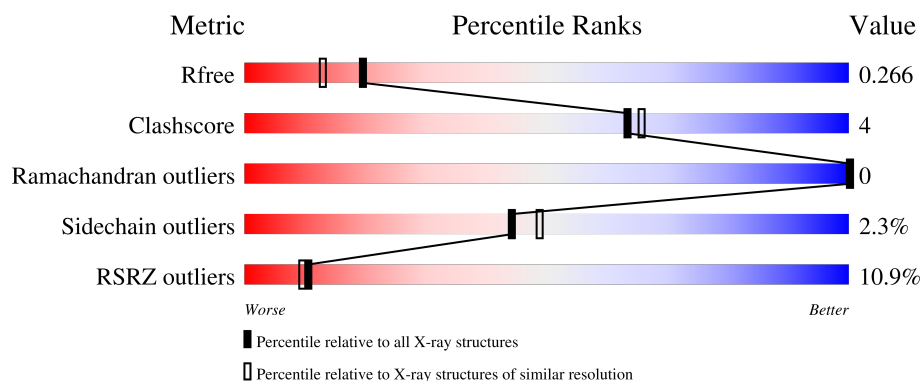
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	126	<div> <div>13%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> </div>
1	B	126	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>
2	C	6	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	D	6	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	A1JXR	C	101	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2282 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 Baculoviral IAP repeat-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	1	0
			1010	645	170	188	7			
1	B	120	Total	C	N	O	S	0	2	0
			990	633	167	182	8			

- Molecule 2 is a protein called Histone-H3-peptide conjugated to molecular tweezer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	1
			44	24	10	9	1			
2	D	6	Total	C	N	O	P	0	0	1
			44	24	10	9	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

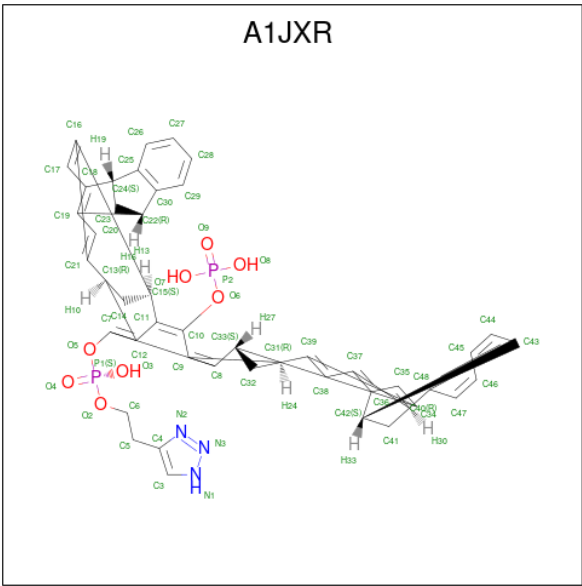
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is Molecular tweezer (BIRC5) (CCD ID: A1JXR) (formula: C<sub>46</sub>H<sub>37</sub>N<sub>3</sub>O<sub>8</sub>P<sub>2</sub>) (la-

beled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			59	46	3	8	2		
5	D	1	Total	C	N	O	P	0	0
			59	46	3	8	2		


- Molecule 6 is water.

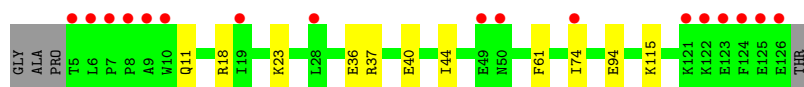
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total	O	0	0
			24	24		
6	B	25	Total	O	0	0
			25	25		
6	C	10	Total	O	0	0
			10	10		
6	D	12	Total	O	0	0
			12	12		

### 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: Baculoviral IAP repeat-containing protein 5

Chain A: 



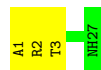
- Molecule 1: Baculoviral IAP repeat-containing protein 5

Chain B: 



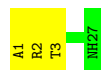
- Molecule 2: Histone-H3-peptide conjugated to molecular tweezer

Chain C: 



- Molecule 2: Histone-H3-peptide conjugated to molecular tweezer

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.55Å 64.09Å 75.87Å 90.00° 141.42° 90.00°	Depositor
Resolution (Å)	49.97 – 2.00 49.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.97-2.00) 98.0 (49.97-2.00)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.214 , 0.263 0.219 , 0.266	Depositor DCC
$R_{free}$ test set	1011 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 25.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.28% 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: TPO, A1JXR, CA, NH2, ZN, EE0

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	1.01	0/1042	1.37	0/1402
1	B	1.00	0/1026	1.39	0/1382
2	C	3.96	4/23 (17.4%)	2.09	0/26
2	D	3.38	2/23 (8.7%)	2.76	2/26 (7.7%)
All	All	1.13	6/2114 (0.3%)	1.41	2/2836 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	ARG	NE-CZ	12.03	1.46	1.33
2	C	1	ALA	C-N	11.22	1.49	1.33
2	D	2	ARG	NE-CZ	11.08	1.45	1.33
2	D	1	ALA	C-N	9.44	1.46	1.33
2	C	2	ARG	CZ-NH2	-6.04	1.25	1.33
2	C	2	ARG	CZ-NH1	-5.48	1.25	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	ARG	NE-CZ-NH1	-8.18	113.32	121.50
2	D	2	ARG	NH1-CZ-NH2	5.92	127.00	119.30

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	1010	0	968	5	0
1	B	990	0	954	8	0
2	C	44	0	39	0	0
2	D	44	0	39	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	59	0	0	2	0
5	D	59	0	0	2	0
6	A	24	0	0	0	0
6	B	25	0	0	1	1
6	C	10	0	0	0	0
6	D	12	0	0	0	1
All	All	2282	0	2000	17	1

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 4.

All (17) 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)
5:D:101:A1JXR:C9	5:D:101:A1JXR:C8	1.79	1.48
5:C:101:A1JXR:C8	5:C:101:A1JXR:C9	1.79	1.48
5:D:101:A1JXR:C12	5:D:101:A1JXR:C11	1.78	1.45
5:C:101:A1JXR:C12	5:C:101:A1JXR:C11	1.80	1.43
1:A:18:ARG:HG2	1:A:44:ILE:HD11	1.61	0.82
1:B:18:ARG:HG2	1:B:44:ILE:HD11	1.79	0.64
1:A:61:PHE:O	1:A:115:LYS:HE3	2.04	0.57
1:B:21:THR:HG21	1:B:44:ILE:HG23	1.86	0.56
1:A:37[B]:ARG:NH2	1:A:40:GLU:HG2	2.25	0.52
1:B:37:ARG:NH2	1:B:40:GLU:HG2	2.25	0.52
1:B:62:LYS:HE2	1:B:80:HIS:O	2.11	0.51
1:B:11:GLN:N	1:B:12:PRO:CD	2.76	0.48
1:A:36:GLU:OE2	1:A:37[B]:ARG:HD3	2.14	0.48
1:A:37[B]:ARG:HD2	1:A:37[B]:ARG:HA	1.59	0.45
1:B:110:LYS:HE3	6:B:321:HOH:O	2.15	0.45
1:B:68:GLU:HB3	1:B:69:PRO:HD2	2.01	0.42

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:321:HOH:O	6:D:209:HOH:O[4_555]	2.16	0.04

## 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	121/126 (96%)	118 (98%)	3 (2%)	0	100	100
1	B	120/126 (95%)	116 (97%)	4 (3%)	0	100	100
2	C	2/6 (33%)	2 (100%)	0	0	100	100
2	D	2/6 (33%)	2 (100%)	0	0	100	100
All	All	245/264 (93%)	238 (97%)	7 (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	110/111 (99%)	106 (96%)	4 (4%)	31	31
1	B	109/111 (98%)	108 (99%)	1 (1%)	70	78
2	C	2/2 (100%)	2 (100%)	0	100	100
2	D	2/2 (100%)	2 (100%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	223/226 (99%)	218 (98%)	5 (2%)	44 50

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

Mol	Chain	Res	Type
1	A	11	GLN
1	A	23	LYS
1	A	74	ILE
1	A	94	GLU
1	B	78	LYS

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

Mol	Chain	Res	Type
1	A	11	GLN
1	A	92	GLN

### 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
2	TPO	D	3	2	8,10,11	1.59	1 (12%)	10,14,16	1.24	2 (20%)
2	TPO	C	3	2	8,10,11	1.55	2 (25%)	10,14,16	1.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	D	3	2	-	1/9/11/13	-
2	TPO	C	3	2	-	2/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	TPO	P-OG1	3.77	1.66	1.59
2	C	3	TPO	P-OG1	3.04	1.64	1.59
2	C	3	TPO	P-O3P	-2.05	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	TPO	P-OG1-CB	-2.45	116.67	123.33
2	D	3	TPO	O2P-P-OG1	2.08	113.96	105.85

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	TPO	CB-OG1-P-O3P
2	C	3	TPO	CB-OG1-P-O1P
2	D	3	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	A1JXR	D	101	2	72,72,72	9.65	55 (76%)	114,118,118	3.70	61 (53%)
5	A1JXR	C	101	2	72,72,72	9.78	55 (76%)	114,118,118	3.75	67 (58%)

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
5	A1JXR	D	101	2	-	3/17/97/97	0/1/14/14
5	A1JXR	C	101	2	-	4/17/97/97	0/1/14/14

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	101	A1JXR	C48-C43	-22.21	1.01	1.40
5	C	101	A1JXR	C12-C11	21.49	1.80	1.40
5	D	101	A1JXR	C30-C25	-21.05	1.03	1.40
5	C	101	A1JXR	C9-C8	20.93	1.79	1.40
5	C	101	A1JXR	C48-C43	-20.89	1.04	1.40
5	C	101	A1JXR	C30-C25	-20.88	1.04	1.40
5	D	101	A1JXR	C9-C8	20.77	1.79	1.40
5	D	101	A1JXR	C12-C11	20.53	1.78	1.40
5	D	101	A1JXR	C35-C34	19.57	1.70	1.39
5	C	101	A1JXR	C20-C21	19.50	1.70	1.39
5	C	101	A1JXR	C17-C16	19.32	1.70	1.39
5	C	101	A1JXR	C38-C39	19.31	1.70	1.39
5	C	101	A1JXR	C35-C34	19.29	1.70	1.39
5	D	101	A1JXR	C20-C21	19.20	1.70	1.39
5	D	101	A1JXR	C38-C39	18.29	1.68	1.39
5	D	101	A1JXR	C17-C16	18.05	1.68	1.39
5	C	101	A1JXR	C44-C43	17.42	1.60	1.39
5	D	101	A1JXR	C26-C25	17.07	1.60	1.39
5	C	101	A1JXR	C41-C42	-16.97	1.34	1.55
5	D	101	A1JXR	C29-C30	16.04	1.59	1.39
5	D	101	A1JXR	C41-C42	-15.98	1.35	1.55
5	D	101	A1JXR	C23-C22	-15.88	1.35	1.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	101	A1JXR	C29-C30	15.84	1.58	1.39
5	C	101	A1JXR	C23-C22	-15.84	1.35	1.55
5	C	101	A1JXR	C26-C25	15.61	1.58	1.39
5	C	101	A1JXR	C41-C40	-15.50	1.36	1.55
5	C	101	A1JXR	C47-C48	15.10	1.58	1.39
5	D	101	A1JXR	C41-C40	-15.07	1.36	1.55
5	D	101	A1JXR	C44-C43	15.05	1.58	1.39
5	C	101	A1JXR	C23-C24	-15.00	1.36	1.55
5	D	101	A1JXR	C23-C24	-14.73	1.37	1.55
5	D	101	A1JXR	C47-C48	14.66	1.57	1.39
5	C	101	A1JXR	C19-C18	13.05	1.62	1.40
5	D	101	A1JXR	C37-C36	12.80	1.62	1.40
5	D	101	A1JXR	C19-C18	12.56	1.61	1.40
5	C	101	A1JXR	C16-C15	-10.98	1.33	1.52
5	D	101	A1JXR	C16-C15	-10.90	1.34	1.52
5	C	101	A1JXR	C21-C13	-10.71	1.34	1.52
5	C	101	A1JXR	C37-C36	10.43	1.58	1.40
5	D	101	A1JXR	C21-C13	-10.40	1.34	1.52
5	C	101	A1JXR	C34-C33	-10.38	1.34	1.52
5	D	101	A1JXR	C34-C33	-9.95	1.35	1.52
5	C	101	A1JXR	C39-C31	-9.91	1.35	1.52
5	D	101	A1JXR	C39-C31	-9.53	1.36	1.52
5	C	101	A1JXR	C39-C34	-9.25	1.24	1.40
5	C	101	A1JXR	C21-C16	-8.58	1.25	1.40
5	D	101	A1JXR	C21-C16	-8.47	1.25	1.40
5	D	101	A1JXR	C39-C34	-7.83	1.26	1.40
5	D	101	A1JXR	C10-C11	7.21	1.52	1.39
5	C	101	A1JXR	C7-C8	7.06	1.51	1.39
5	C	101	A1JXR	C10-C11	6.67	1.51	1.39
5	D	101	A1JXR	C7-C8	6.66	1.51	1.39
5	C	101	A1JXR	C14-C13	-6.57	1.47	1.55
5	D	101	A1JXR	C32-C33	-6.50	1.47	1.55
5	C	101	A1JXR	C14-C15	-6.44	1.47	1.55
5	C	101	A1JXR	C10-C9	6.10	1.50	1.39
5	D	101	A1JXR	C48-C40	-6.01	1.42	1.52
5	D	101	A1JXR	C14-C15	-5.95	1.48	1.55
5	D	101	A1JXR	C14-C13	-5.95	1.48	1.55
5	C	101	A1JXR	C43-C42	-5.94	1.42	1.52
5	C	101	A1JXR	C32-C31	-5.90	1.48	1.55
5	C	101	A1JXR	C7-C12	5.90	1.49	1.39
5	C	101	A1JXR	C32-C33	-5.88	1.48	1.55
5	D	101	A1JXR	C18-C24	5.55	1.61	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	101	A1JXR	C30-C22	-5.50	1.43	1.52
5	C	101	A1JXR	C25-C24	-5.48	1.43	1.52
5	D	101	A1JXR	C7-C12	5.33	1.48	1.39
5	D	101	A1JXR	C43-C42	-5.33	1.43	1.52
5	C	101	A1JXR	C48-C40	-5.32	1.43	1.52
5	D	101	A1JXR	C32-C31	-5.26	1.49	1.55
5	C	101	A1JXR	C37-C40	5.18	1.61	1.52
5	D	101	A1JXR	C10-C9	5.10	1.48	1.39
5	D	101	A1JXR	C25-C24	-5.04	1.43	1.52
5	C	101	A1JXR	C19-C22	4.93	1.60	1.52
5	C	101	A1JXR	C18-C24	4.91	1.60	1.52
5	D	101	A1JXR	N2-N3	4.86	1.41	1.32
5	D	101	A1JXR	C37-C40	4.85	1.60	1.52
5	D	101	A1JXR	C30-C22	-4.71	1.44	1.52
5	D	101	A1JXR	O6-C10	-4.58	1.33	1.40
5	C	101	A1JXR	N2-N3	4.56	1.40	1.32
5	C	101	A1JXR	C36-C42	4.55	1.60	1.52
5	C	101	A1JXR	C35-C36	-4.33	1.32	1.39
5	D	101	A1JXR	C19-C22	4.31	1.59	1.52
5	D	101	A1JXR	C17-C18	-4.14	1.33	1.39
5	D	101	A1JXR	C38-C37	-4.07	1.33	1.39
5	C	101	A1JXR	O6-C10	-3.92	1.34	1.40
5	D	101	A1JXR	C20-C19	-3.76	1.33	1.39
5	D	101	A1JXR	C36-C42	3.68	1.58	1.52
5	C	101	A1JXR	C38-C37	-3.64	1.33	1.39
5	D	101	A1JXR	C3-N1	3.53	1.39	1.34
5	C	101	A1JXR	C3-N1	3.48	1.39	1.34
5	D	101	A1JXR	C8-C33	3.39	1.57	1.52
5	C	101	A1JXR	C20-C19	-3.30	1.34	1.39
5	D	101	A1JXR	C5-C4	3.12	1.56	1.50
5	C	101	A1JXR	C17-C18	-3.10	1.34	1.39
5	D	101	A1JXR	C35-C36	-3.04	1.34	1.39
5	D	101	A1JXR	C46-C45	-2.94	1.31	1.38
5	C	101	A1JXR	C8-C33	2.87	1.57	1.52
5	C	101	A1JXR	P2-O6	2.80	1.64	1.59
5	D	101	A1JXR	C46-C47	-2.68	1.34	1.38
5	D	101	A1JXR	C28-C27	-2.67	1.32	1.38
5	C	101	A1JXR	P1-O2	2.52	1.69	1.59
5	C	101	A1JXR	C5-C4	2.50	1.55	1.50
5	C	101	A1JXR	C9-C31	2.45	1.56	1.52
5	C	101	A1JXR	C28-C27	-2.23	1.33	1.38
5	D	101	A1JXR	P1-O2	2.22	1.68	1.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	101	A1JXR	P1-O5	2.19	1.64	1.60
5	D	101	A1JXR	P2-O7	-2.14	1.46	1.54
5	C	101	A1JXR	C46-C45	-2.10	1.33	1.38
5	C	101	A1JXR	P1-O5	2.06	1.64	1.60

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	101	A1JXR	C11-C12-C13	-10.52	96.35	106.74
5	C	101	A1JXR	C9-C8-C33	-10.52	96.35	106.74
5	C	101	A1JXR	C19-C18-C24	-8.91	96.41	106.65
5	D	101	A1JXR	C9-C8-C33	-8.77	98.08	106.74
5	C	101	A1JXR	C36-C37-C40	-8.64	96.71	106.65
5	C	101	A1JXR	C24-C23-C22	8.51	99.68	94.42
5	D	101	A1JXR	C42-C41-C40	8.37	99.59	94.42
5	C	101	A1JXR	C42-C41-C40	8.22	99.50	94.42
5	D	101	A1JXR	C36-C37-C40	-8.19	97.23	106.65
5	D	101	A1JXR	C12-C11-C15	-8.17	98.67	106.74
5	C	101	A1JXR	C15-C14-C13	8.14	99.45	94.42
5	D	101	A1JXR	C11-C12-C13	-8.10	98.74	106.74
5	D	101	A1JXR	C8-C9-C31	-8.05	98.79	106.74
5	D	101	A1JXR	C15-C14-C13	7.84	99.27	94.42
5	D	101	A1JXR	C18-C19-C22	-7.73	97.76	106.65
5	D	101	A1JXR	C36-C35-C34	-7.55	110.59	123.16
5	D	101	A1JXR	C21-C20-C19	-7.32	110.97	123.16
5	D	101	A1JXR	C24-C23-C22	7.25	98.90	94.42
5	D	101	A1JXR	O5-C7-C8	7.20	126.40	118.34
5	D	101	A1JXR	C19-C18-C24	-7.10	98.48	106.65
5	D	101	A1JXR	C33-C32-C31	7.04	98.77	94.42
5	C	101	A1JXR	C8-C9-C31	-6.94	99.89	106.74
5	C	101	A1JXR	C18-C17-C16	-6.64	112.11	123.16
5	C	101	A1JXR	C12-C11-C15	-6.56	100.27	106.74
5	C	101	A1JXR	C21-C20-C19	-6.53	112.29	123.16
5	D	101	A1JXR	C18-C17-C16	-6.53	112.30	123.16
5	D	101	A1JXR	C37-C36-C42	-6.45	99.23	106.65
5	D	101	A1JXR	C39-C38-C37	-6.12	112.97	123.16
5	C	101	A1JXR	C36-C35-C34	-6.12	112.98	123.16
5	C	101	A1JXR	C18-C19-C22	-5.87	99.90	106.65
5	C	101	A1JXR	C33-C32-C31	5.86	98.04	94.42
5	C	101	A1JXR	C39-C34-C33	5.58	113.06	106.65
5	D	101	A1JXR	C21-C16-C15	5.50	112.97	106.65
5	C	101	A1JXR	C39-C38-C37	-5.44	114.10	123.16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	101	A1JXR	C38-C37-C40	5.43	139.65	130.65
5	C	101	A1JXR	C37-C36-C42	-5.27	100.59	106.65
5	C	101	A1JXR	O5-C7-C12	5.11	124.06	118.34
5	C	101	A1JXR	C16-C21-C13	5.01	112.41	106.65
5	D	101	A1JXR	O6-C10-C11	4.86	123.78	118.34
5	C	101	A1JXR	O5-C7-C8	4.84	123.76	118.34
5	D	101	A1JXR	C48-C43-C42	4.84	112.21	106.65
5	C	101	A1JXR	C20-C21-C13	-4.75	122.77	130.65
5	D	101	A1JXR	C48-C40-C37	4.71	110.51	105.39
5	D	101	A1JXR	C38-C37-C40	4.68	138.40	130.65
5	C	101	A1JXR	C17-C18-C24	4.58	138.24	130.65
5	C	101	A1JXR	C35-C34-C33	-4.57	123.07	130.65
5	C	101	A1JXR	P1-O5-C7	-4.52	113.13	124.10
5	C	101	A1JXR	C30-C25-C24	4.38	111.69	106.65
5	D	101	A1JXR	C25-C30-C22	4.36	111.66	106.65
5	C	101	A1JXR	O6-C10-C9	4.36	123.22	118.34
5	C	101	A1JXR	C12-C7-C8	-4.30	112.17	119.53
5	D	101	A1JXR	C43-C48-C40	4.23	111.52	106.65
5	D	101	A1JXR	C17-C16-C15	-4.19	123.69	130.65
5	D	101	A1JXR	C12-C7-C8	-4.15	112.43	119.53
5	D	101	A1JXR	C35-C34-C33	-4.11	123.83	130.65
5	C	101	A1JXR	C21-C16-C15	4.04	111.29	106.65
5	D	101	A1JXR	C39-C34-C33	4.03	111.28	106.65
5	D	101	A1JXR	C20-C19-C22	4.01	137.30	130.65
5	D	101	A1JXR	C10-C11-C15	4.01	140.22	131.67
5	D	101	A1JXR	C34-C39-C31	3.95	111.19	106.65
5	C	101	A1JXR	C43-C48-C40	3.94	111.18	106.65
5	D	101	A1JXR	C17-C18-C24	3.91	137.13	130.65
5	D	101	A1JXR	C43-C42-C36	3.91	109.64	105.39
5	C	101	A1JXR	C25-C30-C22	3.86	111.09	106.65
5	C	101	A1JXR	C20-C19-C22	3.83	137.00	130.65
5	D	101	A1JXR	P1-O5-C7	-3.72	115.06	124.10
5	C	101	A1JXR	C45-C44-C43	-3.70	116.56	120.99
5	C	101	A1JXR	O6-P2-O9	-3.70	97.15	109.48
5	C	101	A1JXR	C48-C43-C42	3.69	110.89	106.65
5	C	101	A1JXR	C7-C8-C33	3.68	139.51	131.67
5	D	101	A1JXR	C16-C21-C13	3.68	110.87	106.65
5	C	101	A1JXR	O6-C10-C11	3.55	122.32	118.34
5	C	101	A1JXR	C7-C12-C13	3.46	139.05	131.67
5	C	101	A1JXR	C9-C31-C39	3.38	108.78	104.71
5	D	101	A1JXR	C20-C21-C13	-3.38	125.04	130.65
5	D	101	A1JXR	C30-C25-C24	3.34	110.49	106.65

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	101	A1JXR	C7-C8-C33	3.34	138.78	131.67
5	C	101	A1JXR	C17-C18-C19	3.29	125.35	121.37
5	D	101	A1JXR	P2-O6-C10	-3.18	111.79	124.05
5	D	101	A1JXR	O6-C10-C9	3.16	121.88	118.34
5	D	101	A1JXR	C35-C36-C42	3.15	135.87	130.65
5	D	101	A1JXR	C45-C44-C43	-3.13	117.23	120.99
5	C	101	A1JXR	C34-C39-C31	3.11	110.22	106.65
5	D	101	A1JXR	C11-C10-C9	-3.04	114.33	119.53
5	C	101	A1JXR	C11-C10-C9	-3.03	114.34	119.53
5	C	101	A1JXR	C8-C33-C34	2.97	108.29	104.71
5	C	101	A1JXR	C28-C29-C30	-2.95	117.45	120.99
5	D	101	A1JXR	C20-C19-C18	2.95	124.94	121.37
5	D	101	A1JXR	C41-C42-C43	-2.91	96.33	99.28
5	D	101	A1JXR	C35-C36-C37	2.90	124.89	121.37
5	C	101	A1JXR	C20-C21-C16	2.85	124.82	121.37
5	C	101	A1JXR	C10-C11-C15	2.83	137.71	131.67
5	D	101	A1JXR	C35-C34-C39	2.81	124.77	121.37
5	D	101	A1JXR	C10-C9-C31	2.79	137.60	131.67
5	C	101	A1JXR	C48-C40-C37	2.77	108.40	105.39
5	D	101	A1JXR	C47-C48-C40	-2.76	125.14	129.39
5	C	101	A1JXR	P2-O6-C10	-2.75	113.44	124.05
5	D	101	A1JXR	C7-C12-C11	2.75	125.47	120.95
5	C	101	A1JXR	C27-C26-C25	-2.74	117.70	120.99
5	C	101	A1JXR	C46-C47-C48	-2.72	117.73	120.99
5	C	101	A1JXR	C41-C40-C48	-2.71	96.53	99.28
5	D	101	A1JXR	C14-C15-C16	-2.71	96.54	99.28
5	C	101	A1JXR	C10-C9-C31	2.68	137.38	131.67
5	C	101	A1JXR	C35-C36-C42	2.67	135.07	130.65
5	C	101	A1JXR	O3-P1-O5	2.67	113.56	104.94
5	C	101	A1JXR	C17-C16-C15	-2.59	126.36	130.65
5	D	101	A1JXR	C47-C48-C43	2.54	123.32	120.62
5	C	101	A1JXR	C14-C13-C12	2.53	101.81	99.17
5	D	101	A1JXR	C38-C39-C31	-2.53	126.45	130.65
5	C	101	A1JXR	O5-P1-O4	-2.51	101.88	109.95
5	D	101	A1JXR	C41-C40-C48	-2.50	96.74	99.28
5	D	101	A1JXR	O5-C7-C12	2.49	121.13	118.34
5	D	101	A1JXR	C17-C18-C19	2.49	124.38	121.37
5	D	101	A1JXR	C38-C37-C36	2.47	124.37	121.37
5	C	101	A1JXR	O7-P2-O6	2.45	112.57	105.32
5	C	101	A1JXR	C35-C36-C37	2.45	124.33	121.37
5	C	101	A1JXR	C11-C15-C16	-2.37	101.86	104.71
5	C	101	A1JXR	O2-P1-O4	2.35	118.23	108.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	101	A1JXR	C20-C21-C16	2.23	124.08	121.37
5	C	101	A1JXR	C7-C12-C11	2.22	124.60	120.95
5	C	101	A1JXR	C23-C24-C18	2.20	101.52	99.28
5	C	101	A1JXR	C26-C25-C24	-2.17	126.04	129.39
5	D	101	A1JXR	O5-P1-O4	2.15	116.86	109.95
5	C	101	A1JXR	C12-C13-C21	-2.14	102.14	104.71
5	D	101	A1JXR	O7-P2-O6	2.05	111.39	105.32
5	C	101	A1JXR	C35-C34-C39	2.04	123.85	121.37
5	C	101	A1JXR	C23-C24-C25	-2.04	97.22	99.28
5	D	101	A1JXR	O6-P2-O9	-2.01	102.76	109.48

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	101	A1JXR	C12-C7-O5-P1
5	C	101	A1JXR	C8-C7-O5-P1
5	C	101	A1JXR	C10-O6-P2-O9
5	D	101	A1JXR	C10-O6-P2-O9
5	C	101	A1JXR	C7-O5-P1-O3
5	D	101	A1JXR	C7-O5-P1-O4
5	D	101	A1JXR	C7-O5-P1-O2

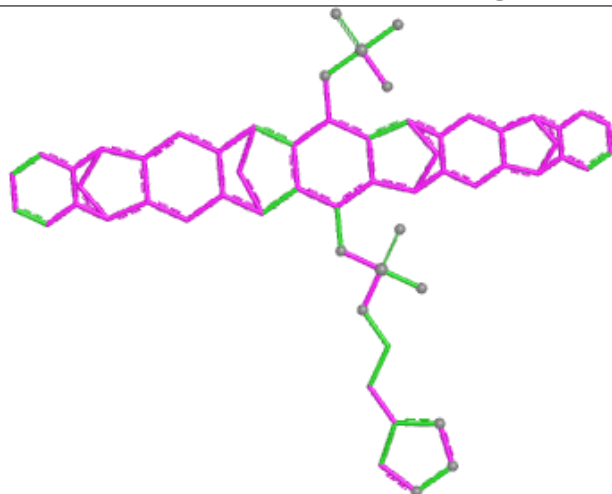
There are no ring outliers.

2 monomers are involved in 4 short contacts:

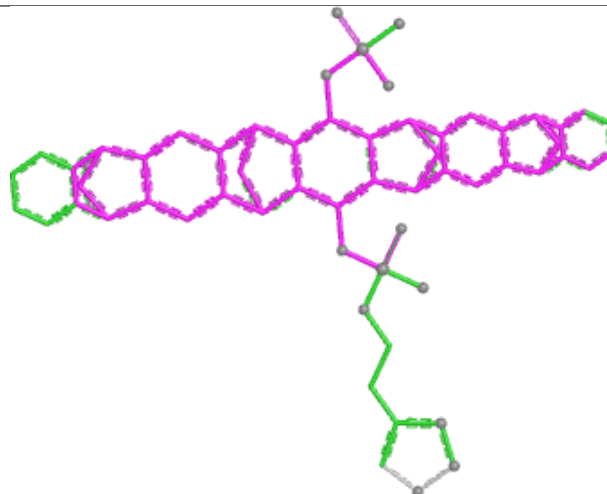
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	101	A1JXR	2	0
5	C	101	A1JXR	2	0

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.

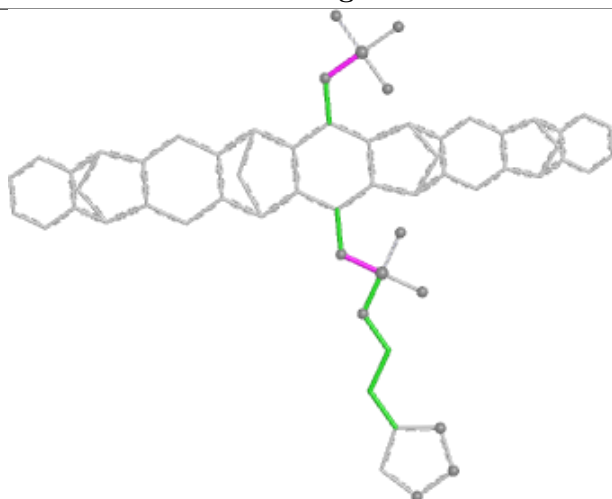
## Ligand A1JXR D 101



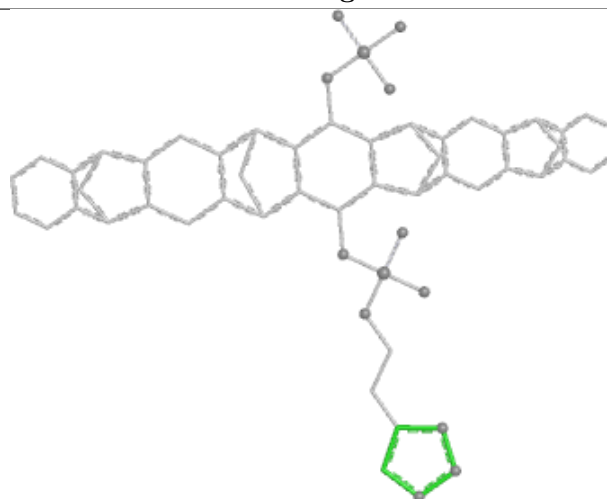
Bond lengths



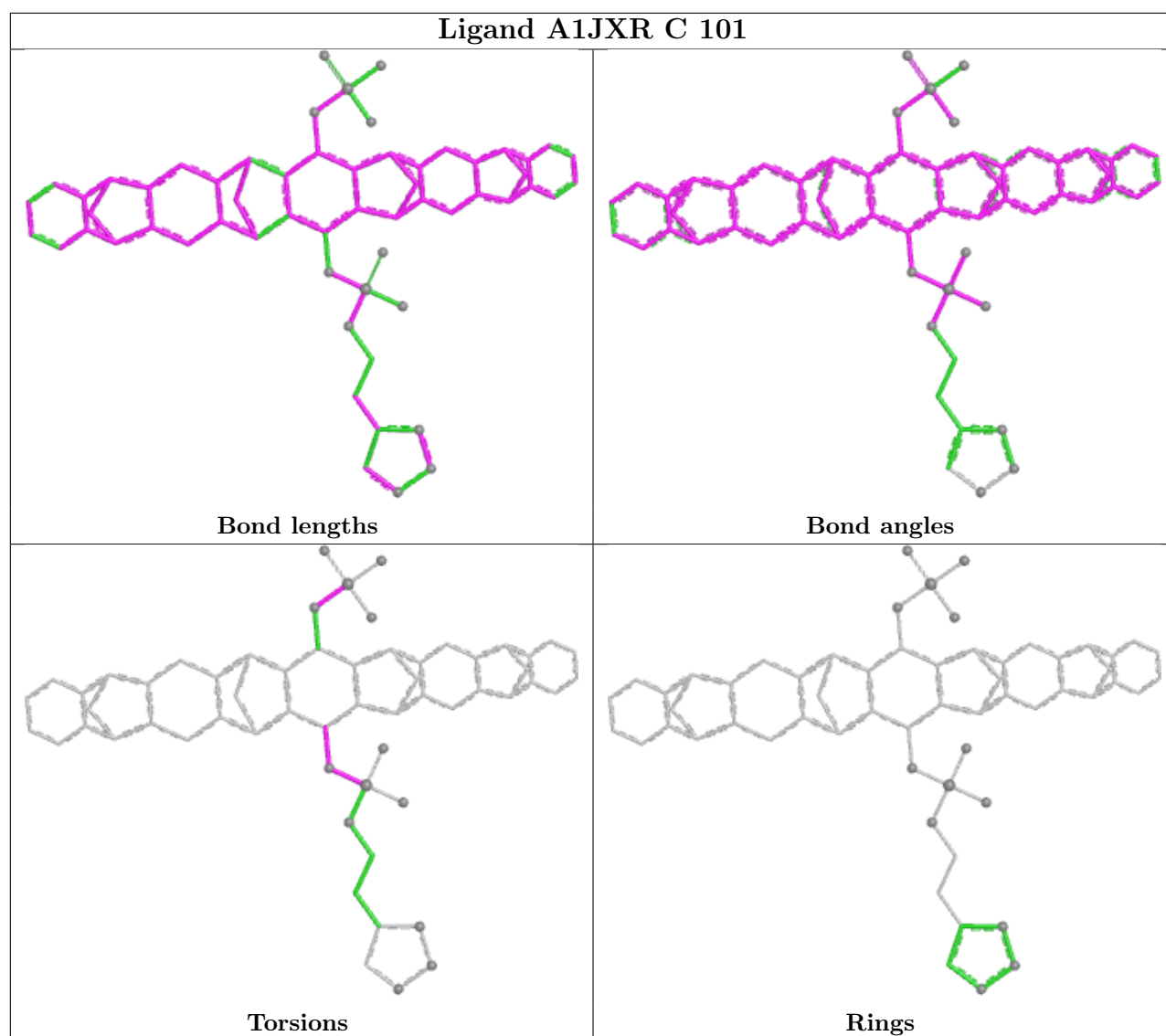
Bond angles



Torsions



Rings



## 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	122/126 (96%)	0.72	17 (13%) 6 5	24, 42, 88, 114	1 (0%)
1	B	120/126 (95%)	0.51	10 (8%) 17 16	26, 40, 85, 119	2 (1%)
2	C	3/6 (50%)	-0.29	0 100 100	29, 29, 33, 47	0
2	D	3/6 (50%)	-0.44	0 100 100	32, 32, 32, 41	0
All	All	248/264 (93%)	0.59	27 (10%) 10 9	24, 41, 88, 119	3 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	PRO	6.0
1	A	124	PHE	4.8
1	A	7	PRO	4.0
1	B	5	THR	3.7
1	A	5	THR	3.7
1	A	6	LEU	3.5
1	A	8	PRO	3.4
1	B	7	PRO	3.0
1	A	10	TRP	2.7
1	B	123	GLU	2.7
1	A	122	LYS	2.7
1	A	50	ASN	2.6
1	A	126	GLU	2.6
1	A	9	ALA	2.5
1	A	125	GLU	2.5
1	A	49	GLU	2.5
1	B	6	LEU	2.5
1	B	8	PRO	2.4
1	A	123	GLU	2.4
1	A	74	ILE	2.3
1	B	118	ASN	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	9	ALA	2.2
1	A	19	ILE	2.2
1	B	10	TRP	2.2
1	B	31	CYS	2.1
1	A	28	LEU	2.1
1	A	121	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	TPO	D	3	11/12	0.96	0.07	27,32,36,38	0
2	TPO	C	3	11/12	0.97	0.06	30,32,39,39	0

## 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
5	A1JXR	C	101	59/59	0.93	0.08	32,39,48,52	0
5	A1JXR	D	101	59/59	0.95	0.08	30,37,49,54	0
4	CA	D	102	1/1	0.96	0.09	70,70,70,70	0
4	CA	C	102	1/1	0.97	0.05	66,66,66,66	0
4	CA	A	202	1/1	0.99	0.07	31,31,31,31	0
3	ZN	B	200	1/1	1.00	0.03	30,30,30,30	0
3	ZN	A	201	1/1	1.00	0.04	32,32,32,32	0

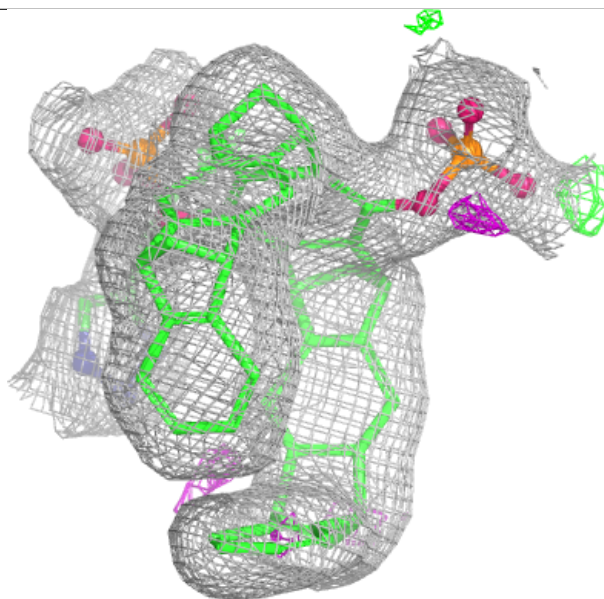
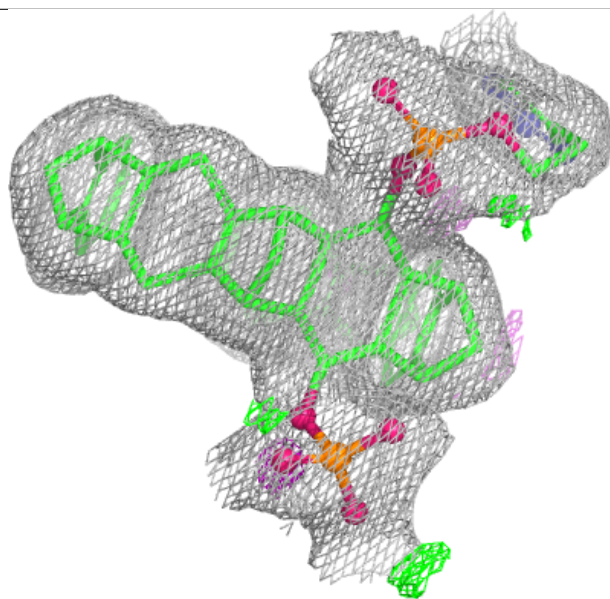
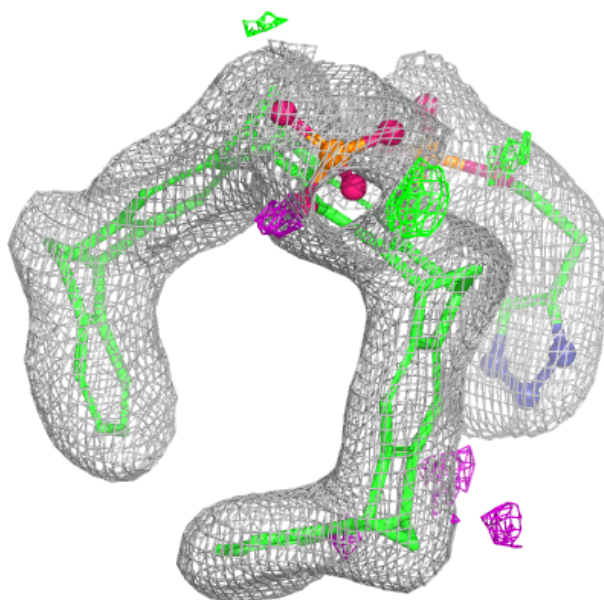
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different



orientation to approximate a three-dimensional view.

**Electron density around A1JXR C 101:**

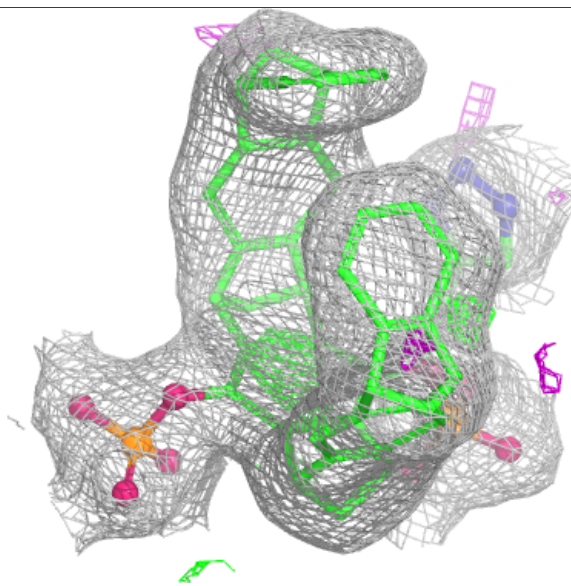
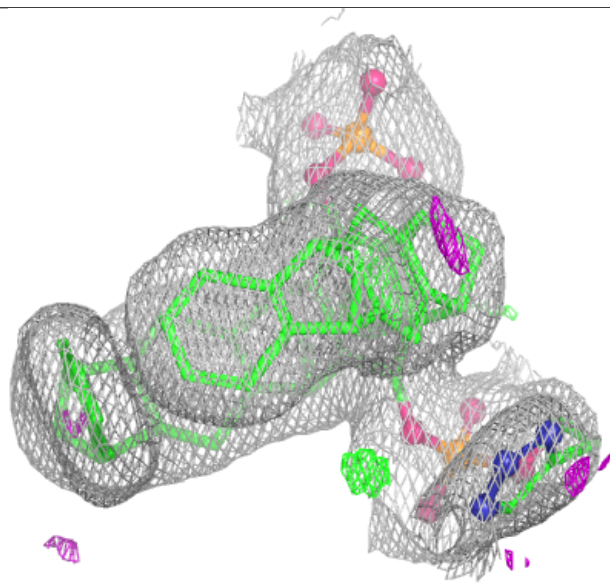
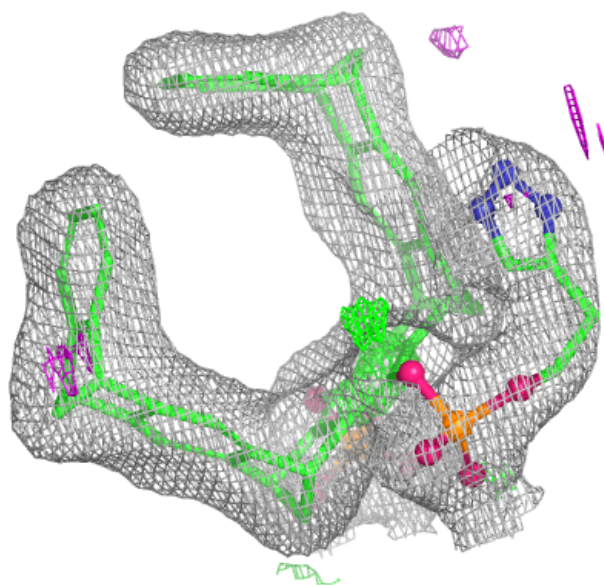
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around A1JXR D 101:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.