



## Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:50 AM UTC

PDB ID : 4PY6 / pdb\_00004py6  
Title : Crystal Structure of bromodomain of PFA0510w from Plasmodium Falciparum  
Authors : Fonseca, M.; Tallant, C.; Hutchinson, A.; Savitsky, P.; Krojer, T.; Filipakopoulos, P.; Loppnau, P.; Brennan, P.E.; von Delft, F.; Dong, A.; Josling, G.A.; Duffy, M.F.; Arrowsmith, C.H.; Bountra, C.; Hui, R.; Knapp, S.; Wernimont, A.K.; Structural Genomics Consortium (SGC)  
Deposited on : 2014-03-26  
Resolution : 2.50 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>.

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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)  
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

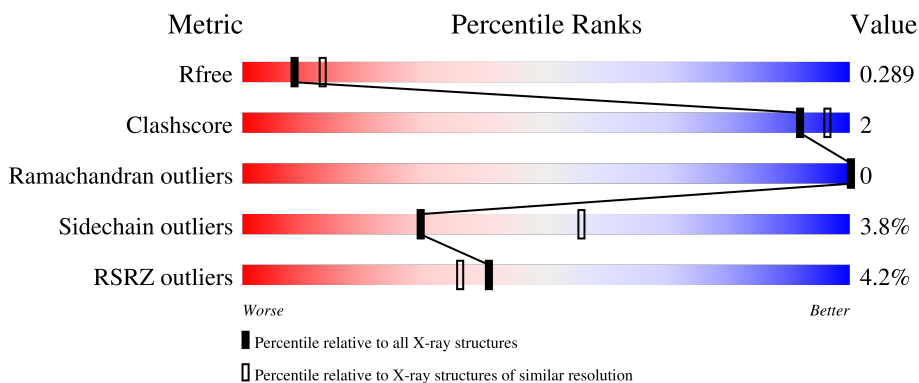
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	145	 2% 81% 10% 9%
1	B	145	 3% 86% 5% 10%
1	C	145	 3% 82% 6% 12%
1	D	145	 8% 77% 11% 12%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4733 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.

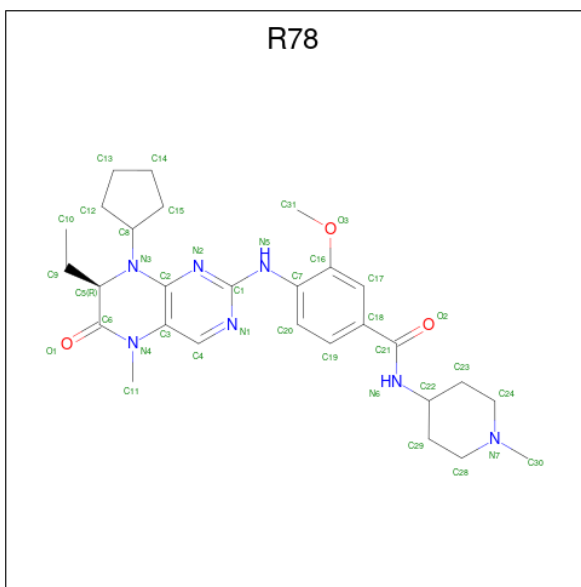
- Molecule 1 is a protein called Bromodomain protein, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	132	1138	734	189	210	5	0	1	0
1	B	131	1119	722	185	207	5	0	0	0
1	C	127	1092	707	179	201	5	0	1	0
1	D	128	1092	706	178	203	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

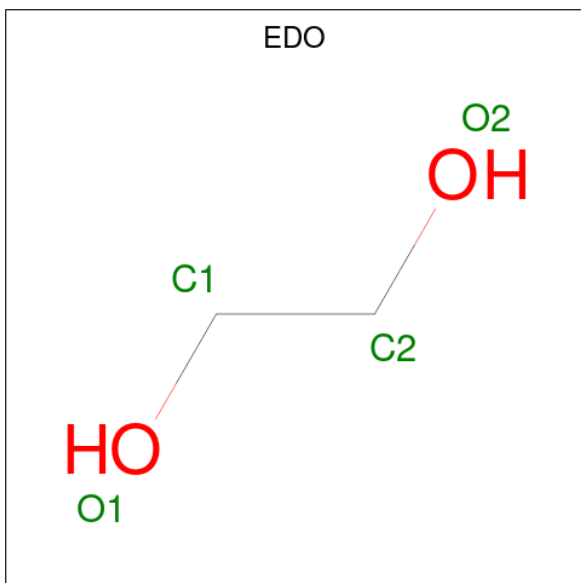
Chain	Residue	Modelled	Actual	Comment	Reference
A	1174	GLY	-	expression tag	UNP Q8I240
B	1174	GLY	-	expression tag	UNP Q8I240
C	1174	GLY	-	expression tag	UNP Q8I240
D	1174	GLY	-	expression tag	UNP Q8I240

- Molecule 2 is 4-{{(7R)-8-cyclopentyl-7-ethyl-5-methyl-6-oxo-5,6,7,8-tetrahydropteridin-2-yl}amino}-3-methoxy-N-(1-methylpiperidin-4-yl)benzamide (CCD ID: R78) (formula: C<sub>28</sub>H<sub>39</sub>N<sub>7</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	58	44	10	4	0	1
2	B	1	29	22	5	2	0	0
2	C	1	29	22	5	2	0	0
2	D	1	29	22	5	2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

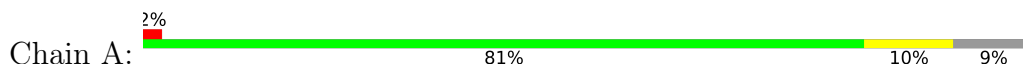
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	40	Total O 41 41	0	1
4	C	28	Total O 28 28	0	0
4	D	20	Total O 20 20	0	0

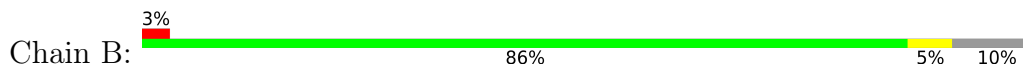
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

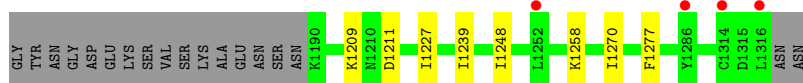
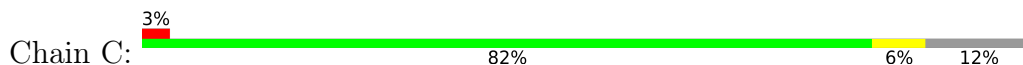
- Molecule 1: Bromodomain protein, putative



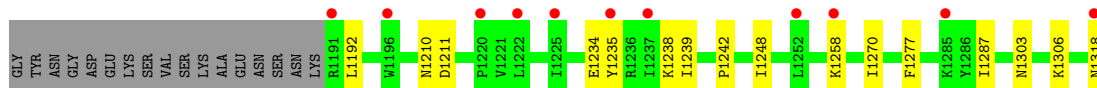
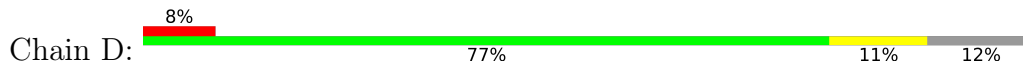
- Molecule 1: Bromodomain protein, putative



- Molecule 1: Bromodomain protein, putative



- Molecule 1: Bromodomain protein, putative



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.32Å 84.27Å 219.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.41 – 2.50 29.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.41-2.50) 99.7 (29.41-2.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.51Å)	Xtrriage
Refinement program	BUSTER-TNT, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.237 , 0.268 0.255 , 0.289	Depositor DCC
$R_{free}$ test set	1254 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtrriage
Anisotropy	0.080	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: EDO, R78

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	0.70	0/1165	1.33	1/1565 (0.1%)
1	B	0.70	0/1143	1.37	1/1538 (0.1%)
1	C	0.71	0/1116	1.38	1/1501 (0.1%)
1	D	0.71	0/1116	1.35	3/1502 (0.2%)
All	All	0.70	0/4540	1.36	6/6106 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1211	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	1211	ASP	CA-CB-CG	5.78	118.38	112.60
1	D	1211	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	1306	LYS	N-CA-C	5.20	117.62	111.33
1	D	1306	LYS	N-CA-C	5.05	118.21	111.75
1	D	1287	ILE	N-CA-C	5.02	115.75	110.62

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	1138	0	1137	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1119	0	1108	1	0
1	C	1092	0	1080	3	0
1	D	1092	0	1078	3	0
2	A	58	0	52	2	0
2	B	29	0	26	0	0
2	C	29	0	26	2	0
2	D	29	0	26	1	0
3	A	4	0	6	1	0
3	B	8	0	12	0	0
4	A	46	0	0	0	0
4	B	41	0	0	0	0
4	C	28	0	0	0	0
4	D	20	0	0	0	0
All	All	4733	0	4551	15	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 2.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1248:ILE:HD12	1:D:1270:ILE:HD11	1.83	0.61
1:A:1239:ILE:HD11	1:A:1277:PHE:HB2	1.86	0.56
1:A:1196:TRP:HE1	3:A:1402:EDO:H21	1.75	0.52
1:C:1239:ILE:HD11	1:C:1277:PHE:HB2	1.92	0.50
1:A:1248:ILE:HD12	1:A:1270:ILE:HD11	1.95	0.49
1:C:1248:ILE:HD12	1:C:1270:ILE:HD11	1.96	0.48
1:A:1235:TYR:HE1	1:A:1242:PRO:HB3	1.81	0.45
1:D:1239:ILE:HD11	1:D:1277:PHE:HB2	1.98	0.45
1:C:1227:ILE:HG12	2:C:1401:R78:HN5	1.82	0.45
2:A:1401[B]:R78:H4	2:A:1401[B]:R78:H11	1.86	0.43
2:D:1401:R78:N1	2:D:1401:R78:H20	2.33	0.43
2:A:1401[A]:R78:H4	2:A:1401[A]:R78:H11	1.85	0.42
2:C:1401:R78:H12	2:C:1401:R78:H5	1.88	0.42
1:D:1235:TYR:HE2	1:D:1242:PRO:HB3	1.84	0.41
1:B:1200:LEU:HD22	1:B:1263:PHE:CE1	2.56	0.41

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	131/145 (90%)	127 (97%)	4 (3%)	0	100	100
1	B	129/145 (89%)	125 (97%)	4 (3%)	0	100	100
1	C	126/145 (87%)	123 (98%)	3 (2%)	0	100	100
1	D	126/145 (87%)	122 (97%)	4 (3%)	0	100	100
All	All	512/580 (88%)	497 (97%)	15 (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	128/138 (93%)	122 (95%)	6 (5%)	23	47
1	B	125/138 (91%)	121 (97%)	4 (3%)	34	62
1	C	121/138 (88%)	119 (98%)	2 (2%)	53	78
1	D	122/138 (88%)	115 (94%)	7 (6%)	18	39
All	All	496/552 (90%)	477 (96%)	19 (4%)	29	56

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1188	SER
1	A	1190	LYS

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Mol	Chain	Res	Type
1	A	1193	LEU
1	A	1206	LYS
1	A	1246	ILE
1	A	1303	ASN
1	B	1192	LEU
1	B	1230	ASN
1	B	1234	GLU
1	B	1312	ASN
1	C	1209	LYS
1	C	1258	LYS
1	D	1192	LEU
1	D	1210	ASN
1	D	1234	GLU
1	D	1238	LYS
1	D	1258	LYS
1	D	1303	ASN
1	D	1318	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1195	GLN
1	A	1212	ASN
1	B	1228	ASN
1	B	1251	ASN
1	B	1312	ASN
1	C	1195	GLN
1	C	1203	ASN
1	C	1212	ASN
1	C	1312	ASN
1	D	1212	ASN
1	D	1226	ASN
1	D	1228	ASN
1	D	1318	ASN

### 5.3.3 RNA

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](#)

8 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	R78	B	1401	-	30,32,42	1.84	7 (23%)	36,46,60	1.96	6 (16%)
3	EDO	B	1403	-	3,3,3	0.50	0	2,2,2	0.37	0
2	R78	D	1401	-	30,32,42	1.85	7 (23%)	36,46,60	1.94	8 (22%)
2	R78	A	1401[A]	-	30,32,42	1.83	7 (23%)	36,46,60	2.01	9 (25%)
2	R78	C	1401	-	30,32,42	1.87	8 (26%)	36,46,60	1.89	8 (22%)
3	EDO	B	1402	-	3,3,3	0.50	0	2,2,2	0.31	0
2	R78	A	1401[B]	-	30,32,42	1.85	7 (23%)	36,46,60	1.85	8 (22%)
3	EDO	A	1402	-	3,3,3	0.48	0	2,2,2	0.37	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	R78	B	1401	-	-	2/12/39/57	0/4/4/5
3	EDO	B	1403	-	-	0/1/1/1	-
2	R78	D	1401	-	-	4/12/39/57	0/4/4/5
2	R78	A	1401[A]	-	-	5/12/39/57	0/4/4/5
2	R78	C	1401	-	-	5/12/39/57	0/4/4/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1402	-	-	0/1/1/1	-
2	R78	A	1401[B]	-	-	6/12/39/57	0/4/4/5
3	EDO	A	1402	-	-	0/1/1/1	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1401	R78	C5-C6	-5.46	1.41	1.51
2	A	1401[A]	R78	C5-C6	-5.39	1.41	1.51
2	B	1401	R78	C5-C6	-5.32	1.41	1.51
2	A	1401[B]	R78	C5-C6	-5.31	1.41	1.51
2	C	1401	R78	C5-C6	-5.31	1.41	1.51
2	C	1401	R78	C21-C18	-3.96	1.39	1.51
2	D	1401	R78	C21-C18	-3.94	1.39	1.51
2	A	1401[B]	R78	C21-C18	-3.92	1.39	1.51
2	A	1401[A]	R78	C21-C18	-3.90	1.39	1.51
2	B	1401	R78	C21-C18	-3.88	1.39	1.51
2	C	1401	R78	C4-N1	3.59	1.41	1.34
2	B	1401	R78	C4-N1	3.54	1.41	1.34
2	D	1401	R78	C4-N1	3.36	1.41	1.34
2	A	1401[B]	R78	C4-N1	3.31	1.41	1.34
2	A	1401[A]	R78	C4-N1	3.20	1.40	1.34
2	B	1401	R78	C14-C15	-3.00	1.39	1.51
2	A	1401[A]	R78	C14-C15	-2.99	1.39	1.51
2	A	1401[B]	R78	C14-C15	-2.96	1.39	1.51
2	C	1401	R78	C14-C15	-2.96	1.39	1.51
2	D	1401	R78	C14-C15	-2.96	1.39	1.51
2	D	1401	R78	C13-C12	-2.95	1.39	1.51
2	A	1401[A]	R78	C13-C12	-2.94	1.39	1.51
2	B	1401	R78	C13-C12	-2.94	1.39	1.51
2	A	1401[B]	R78	C13-C12	-2.92	1.40	1.51
2	C	1401	R78	C13-C12	-2.92	1.40	1.51
2	B	1401	R78	C11-N4	2.31	1.50	1.46
2	A	1401[B]	R78	C11-N4	2.31	1.50	1.46
2	A	1401[A]	R78	C11-N4	2.31	1.50	1.46
2	C	1401	R78	C14-C13	-2.26	1.34	1.48
2	D	1401	R78	C14-C13	-2.26	1.34	1.48
2	B	1401	R78	C14-C13	-2.25	1.34	1.48
2	A	1401[A]	R78	C14-C13	-2.25	1.34	1.48
2	A	1401[B]	R78	C14-C13	-2.25	1.34	1.48
2	C	1401	R78	C11-N4	2.24	1.50	1.46
2	D	1401	R78	C11-N4	2.20	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1401	R78	C7-N5	-2.07	1.34	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1401	R78	N1-C1-N2	-7.83	118.85	126.42
2	D	1401	R78	N1-C1-N2	-7.67	119.01	126.42
2	A	1401[A]	R78	N1-C1-N2	-7.58	119.09	126.42
2	C	1401	R78	N1-C1-N2	-7.16	119.50	126.42
2	A	1401[B]	R78	N1-C1-N2	-6.86	119.79	126.42
2	D	1401	R78	C4-N1-C1	3.76	120.97	115.81
2	A	1401[A]	R78	C4-N1-C1	3.72	120.91	115.81
2	B	1401	R78	C4-N1-C1	3.43	120.52	115.81
2	A	1401[B]	R78	C4-N1-C1	3.14	120.11	115.81
2	C	1401	R78	C4-N1-C1	3.10	120.06	115.81
2	C	1401	R78	C5-C6-N4	3.09	121.23	116.28
2	B	1401	R78	C5-C6-N4	3.01	121.10	116.28
2	B	1401	R78	C1-N2-C2	3.00	123.63	113.99
2	A	1401[B]	R78	C5-C6-N4	2.85	120.84	116.28
2	A	1401[A]	R78	C1-N2-C2	2.83	123.07	113.99
2	C	1401	R78	C1-N2-C2	2.82	123.03	113.99
2	A	1401[A]	R78	C5-C6-N4	2.77	120.72	116.28
2	D	1401	R78	C1-N2-C2	2.75	122.82	113.99
2	D	1401	R78	C5-C6-N4	2.75	120.69	116.28
2	A	1401[B]	R78	C1-N2-C2	2.74	122.77	113.99
2	B	1401	R78	O1-C6-N4	-2.63	119.79	122.35
2	C	1401	R78	O1-C6-N4	-2.59	119.82	122.35
2	A	1401[B]	R78	C3-C2-N2	-2.55	119.27	123.32
2	A	1401[A]	R78	C3-C2-N2	-2.52	119.33	123.32
2	A	1401[B]	R78	O3-C16-C7	2.52	117.95	114.81
2	A	1401[A]	R78	C31-O3-C16	-2.50	113.84	117.51
2	C	1401	R78	O3-C16-C7	2.48	117.91	114.81
2	A	1401[A]	R78	O3-C16-C7	2.45	117.86	114.81
2	A	1401[A]	R78	N5-C1-N1	2.39	123.06	116.29
2	A	1401[B]	R78	O1-C6-N4	-2.36	120.05	122.35
2	C	1401	R78	C31-O3-C16	-2.35	114.06	117.51
2	A	1401[A]	R78	O1-C6-N4	-2.32	120.09	122.35
2	B	1401	R78	C3-C2-N2	-2.28	119.70	123.32
2	D	1401	R78	N5-C1-N1	2.27	122.73	116.29
2	C	1401	R78	C3-C2-N2	-2.27	119.72	123.32
2	D	1401	R78	O3-C16-C7	2.25	117.61	114.81
2	D	1401	R78	O1-C6-N4	-2.16	120.24	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1401	R78	C3-C2-N2	-2.04	120.09	123.32
2	A	1401[B]	R78	C7-N5-C1	-2.00	123.11	129.22

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401[B]	R78	N1-C1-N5-C7
2	A	1401[B]	R78	N2-C1-N5-C7
2	C	1401	R78	N1-C1-N5-C7
2	C	1401	R78	N2-C1-N5-C7
2	D	1401	R78	N1-C1-N5-C7
2	B	1401	R78	C7-C16-O3-C31
2	D	1401	R78	C7-C16-O3-C31
2	D	1401	R78	N2-C1-N5-C7
2	A	1401[A]	R78	C7-C16-O3-C31
2	C	1401	R78	C7-C16-O3-C31
2	B	1401	R78	C17-C16-O3-C31
2	A	1401[B]	R78	C7-C16-O3-C31
2	A	1401[B]	R78	C17-C16-O3-C31
2	C	1401	R78	C17-C16-O3-C31
2	D	1401	R78	C17-C16-O3-C31
2	A	1401[A]	R78	C17-C16-O3-C31
2	A	1401[A]	R78	N1-C1-N5-C7
2	A	1401[A]	R78	C15-C8-N3-C5
2	A	1401[A]	R78	C15-C8-N3-C2
2	A	1401[B]	R78	C15-C8-N3-C5
2	A	1401[B]	R78	C15-C8-N3-C2
2	C	1401	R78	C20-C7-N5-C1

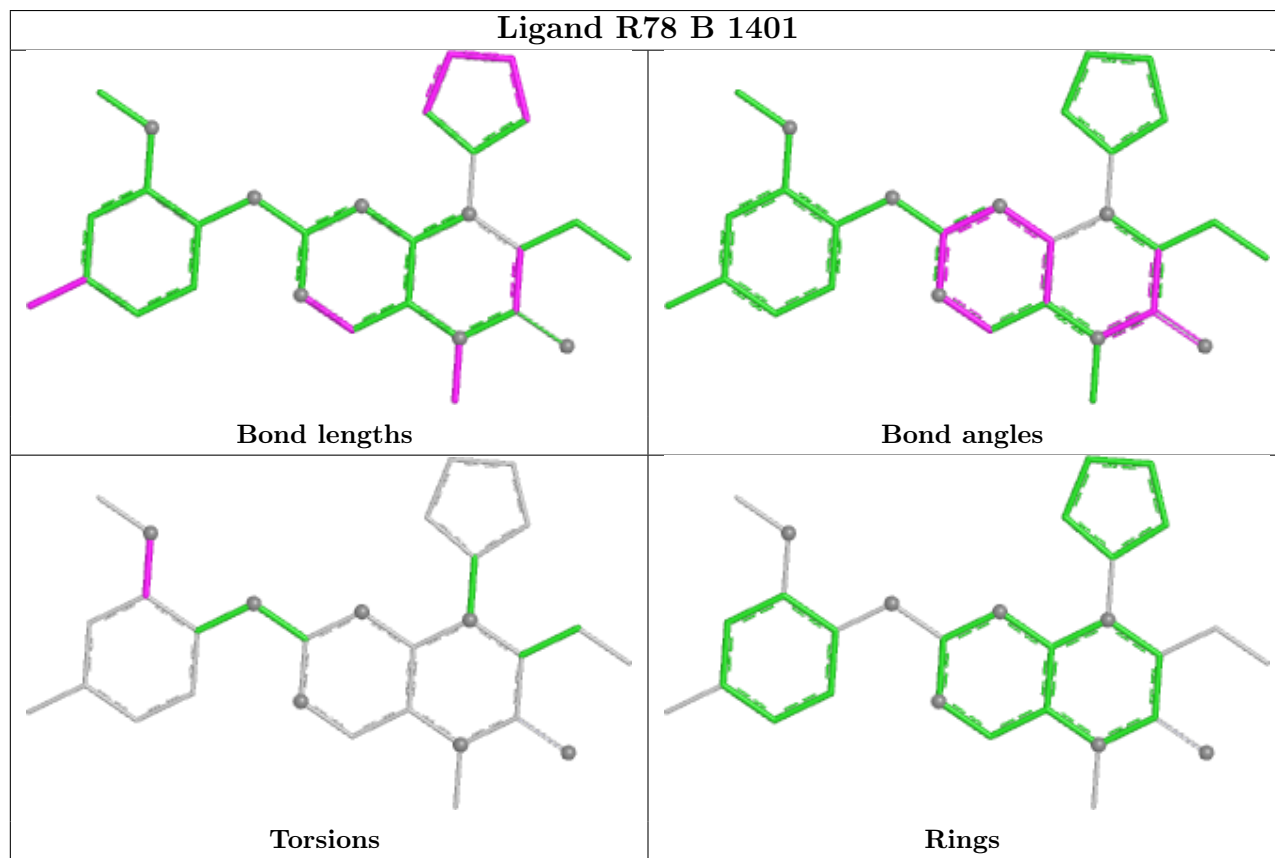
There are no ring outliers.

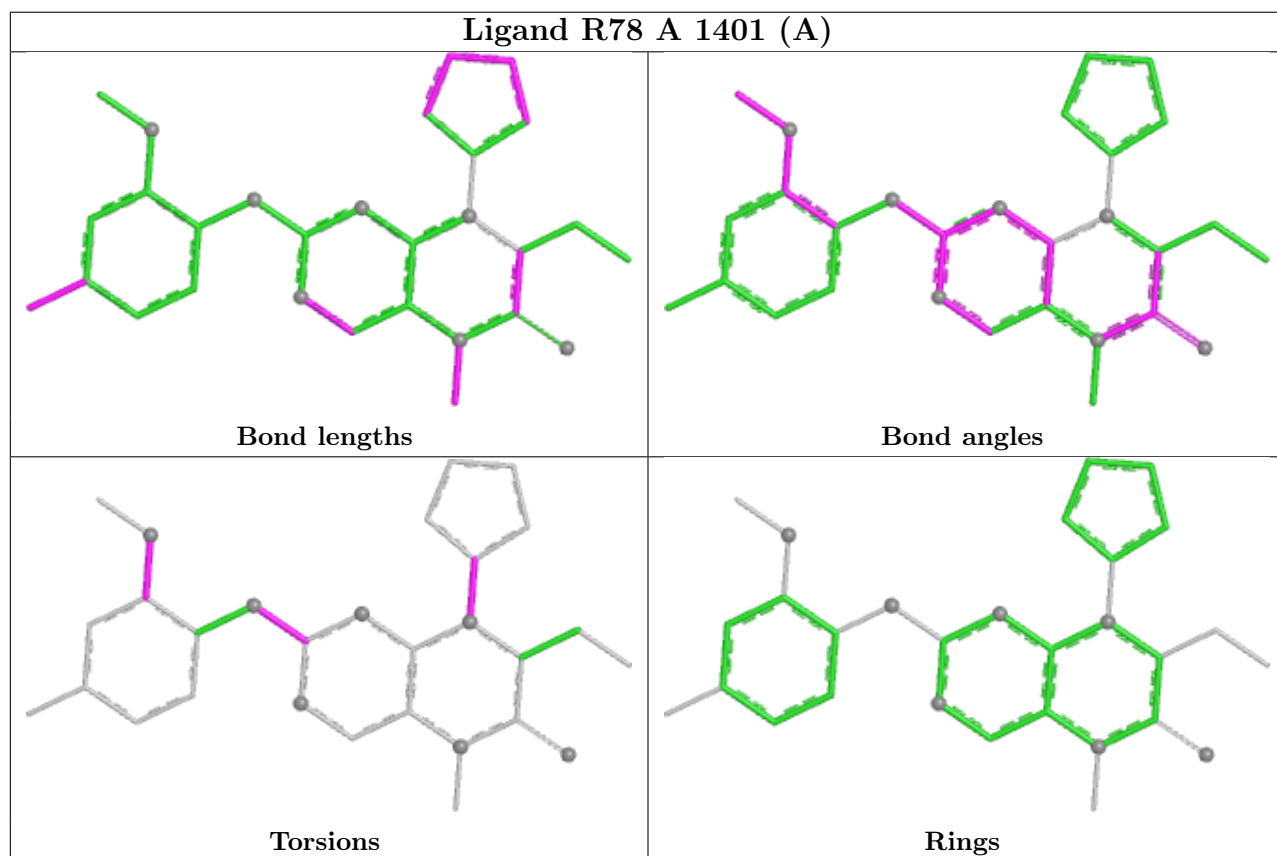
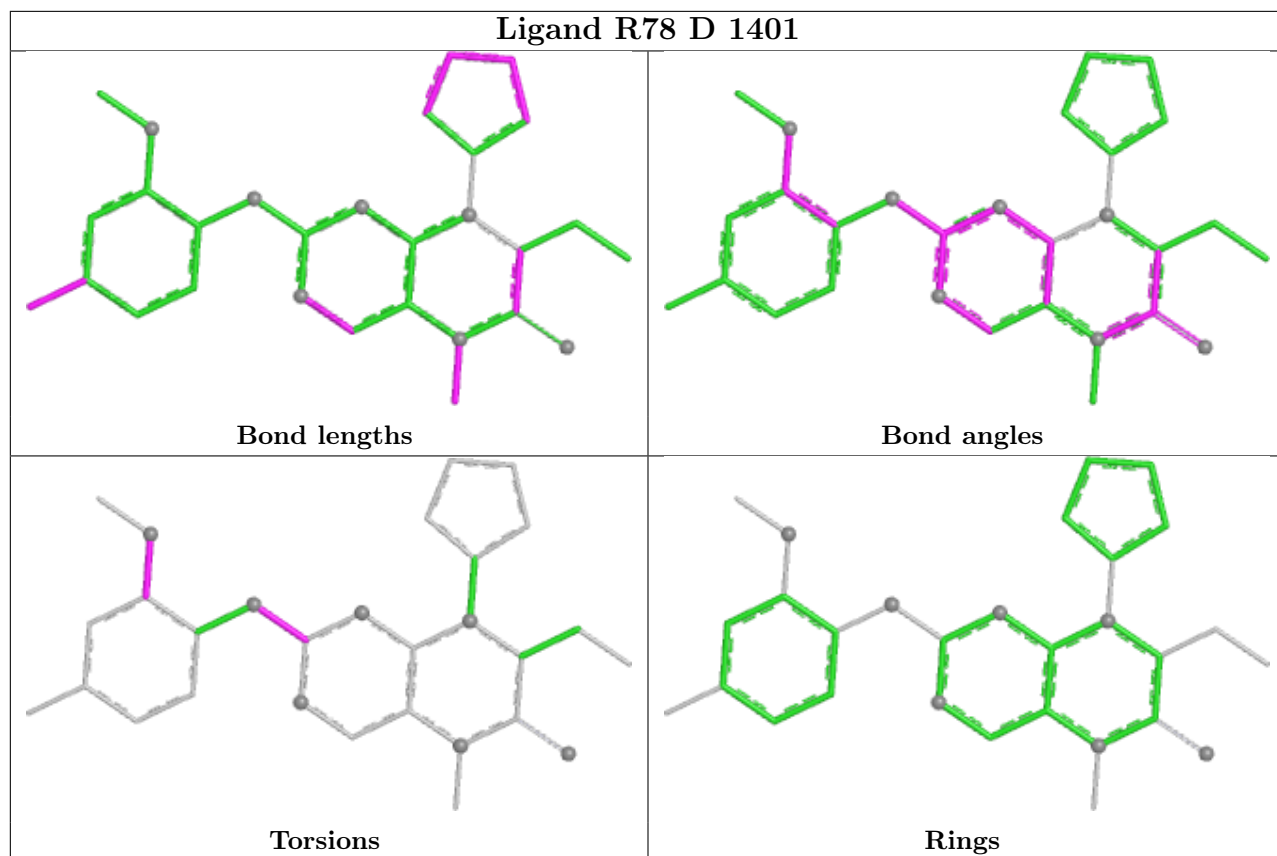
5 monomers are involved in 6 short contacts:

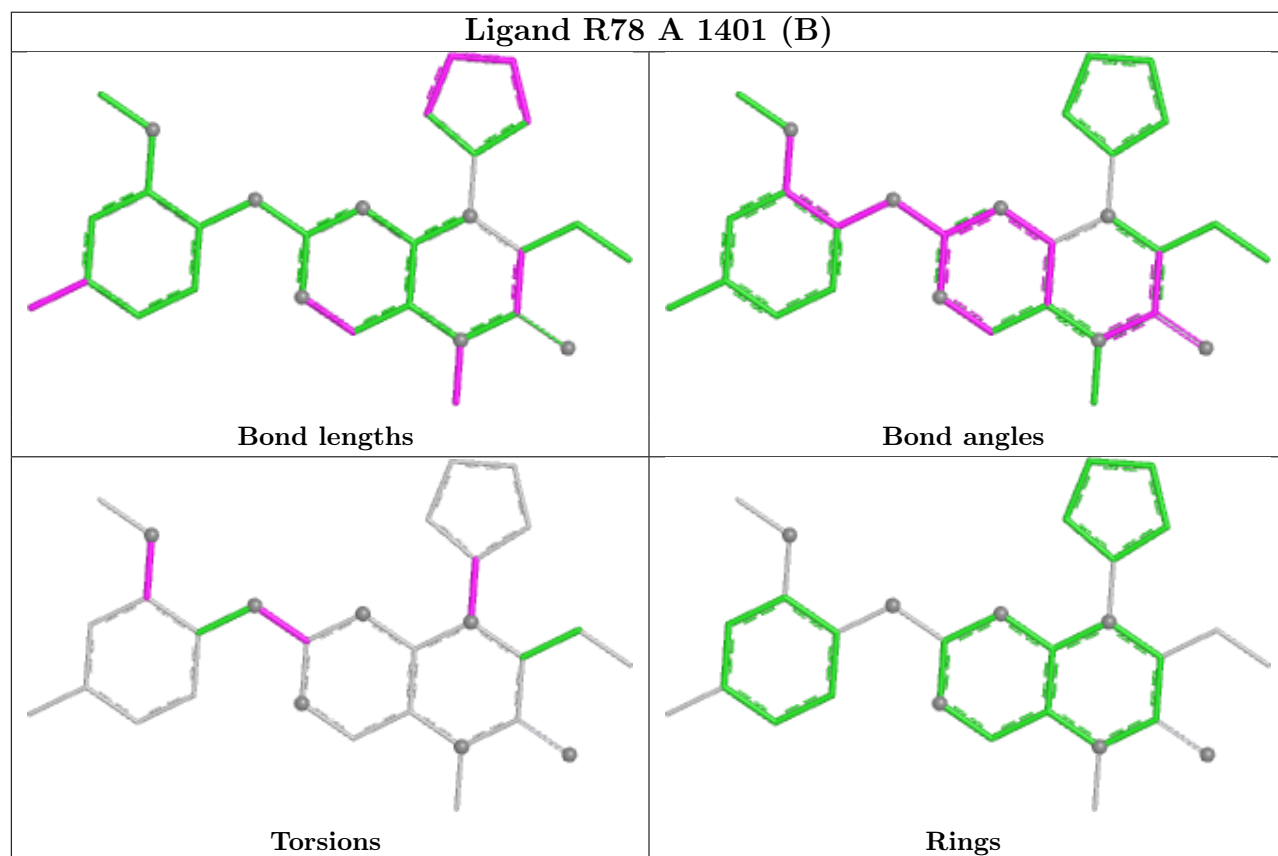
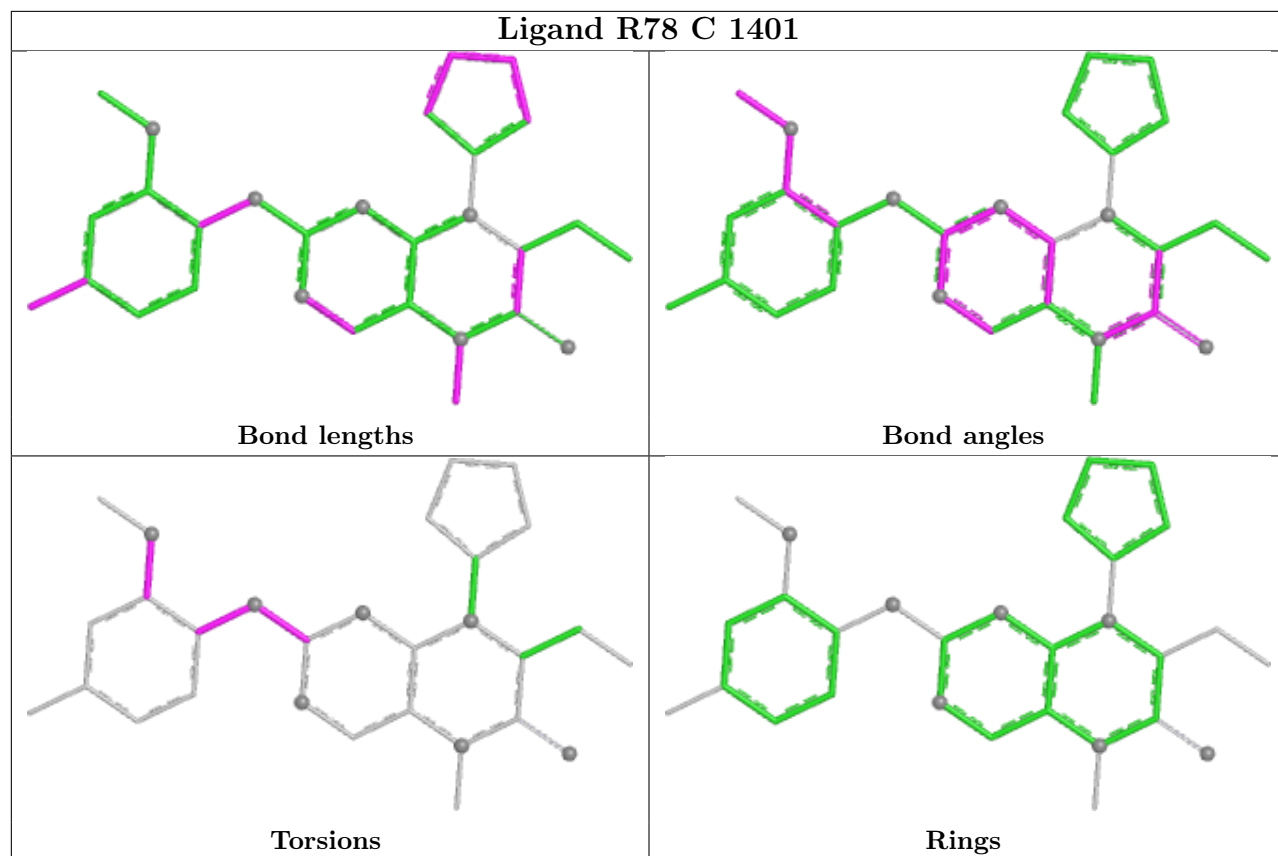
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1401	R78	1	0
2	A	1401[A]	R78	1	0
2	C	1401	R78	2	0
2	A	1401[B]	R78	1	0
3	A	1402	EDO	1	0

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, 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	132/145 (91%)	0.70	3 (2%) 61 57	21, 35, 60, 75	1 (0%)
1	B	131/145 (90%)	0.66	4 (3%) 51 47	24, 39, 63, 72	0
1	C	127/145 (87%)	0.85	4 (3%) 51 47	24, 46, 64, 88	1 (0%)
1	D	128/145 (88%)	1.05	11 (8%) 16 14	29, 51, 81, 89	0
All	All	518/580 (89%)	0.81	22 (4%) 40 36	21, 43, 69, 89	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1316	LEU	6.6
1	A	1317	ASN	5.9
1	D	1225	ILE	3.1
1	B	1312	ASN	3.0
1	D	1252	LEU	2.9
1	A	1316	LEU	2.9
1	D	1191	ARG	2.8
1	C	1252	LEU	2.6
1	B	1282	GLU	2.6
1	D	1285	LYS	2.4
1	A	1187	ASN	2.4
1	D	1258	LYS	2.4
1	D	1222	LEU	2.3
1	C	1314	CYS	2.3
1	B	1286	TYR	2.3
1	D	1237	ILE	2.2
1	D	1220	PRO	2.2
1	C	1286	TYR	2.2
1	D	1318	ASN	2.1
1	D	1235	TYR	2.1
1	D	1196	TRP	2.0
1	B	1258	LYS	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](#)

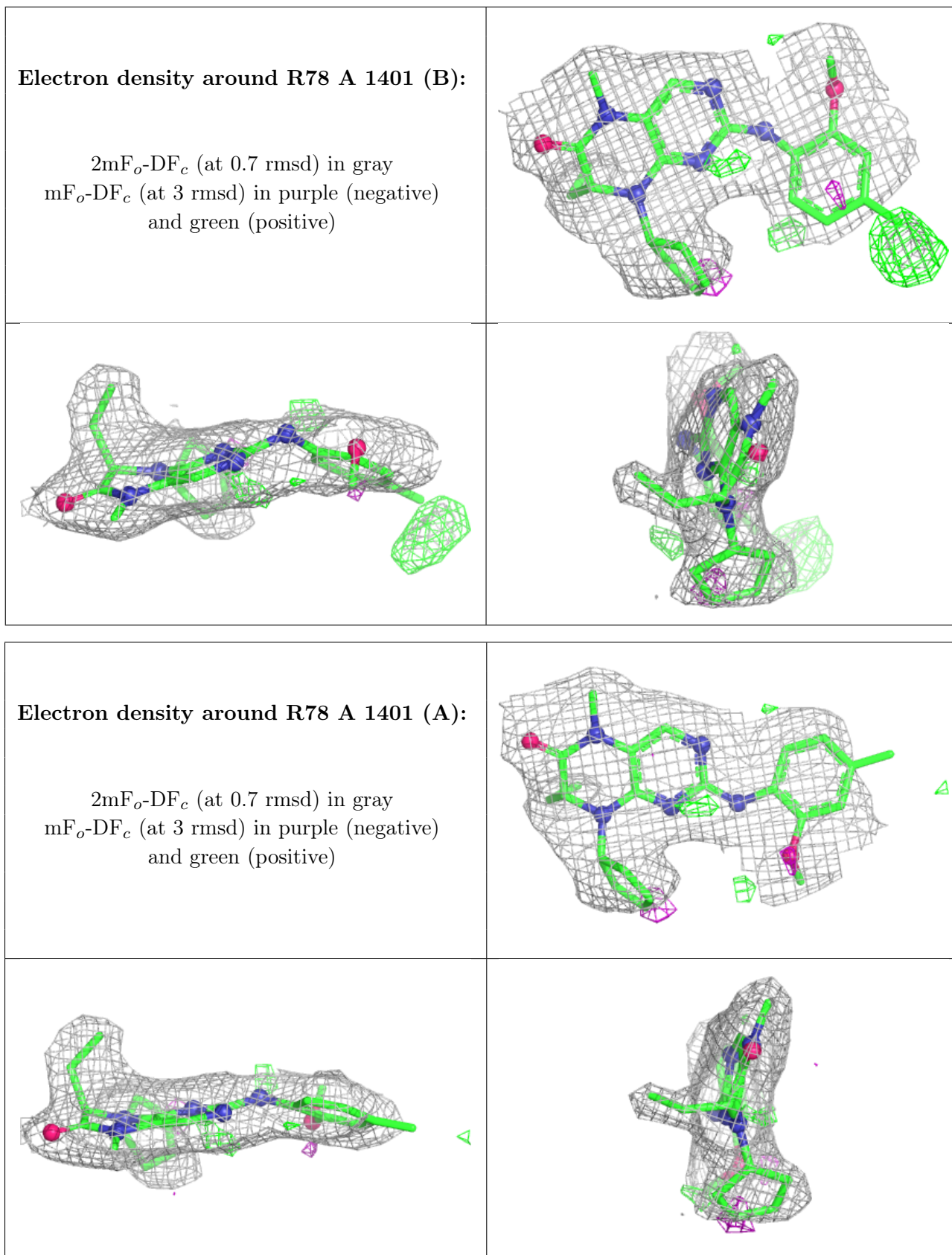
There are no oligosaccharides in this entry.

## 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.

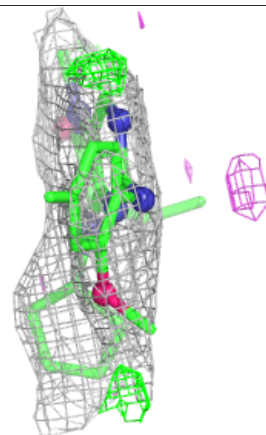
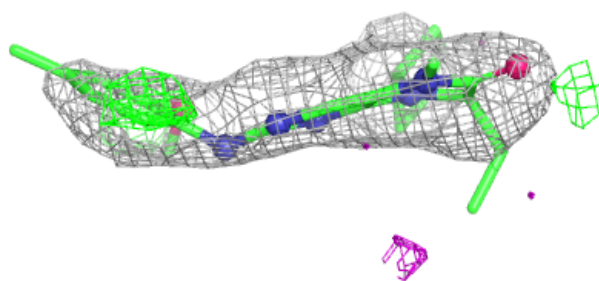
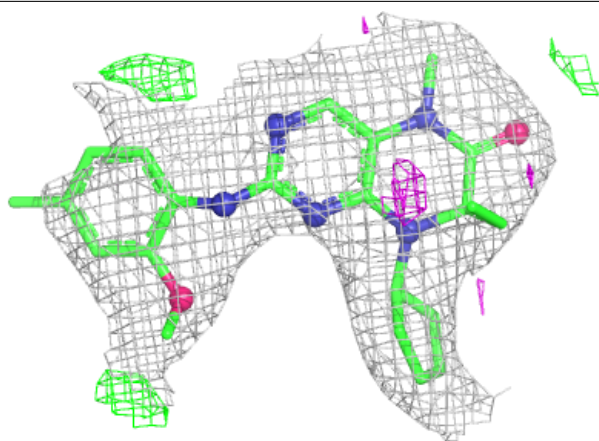
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	B	1402	4/4	0.72	0.21	44,44,44,44	0
3	EDO	B	1403	4/4	0.74	0.25	67,67,67,67	0
3	EDO	A	1402	4/4	0.77	0.15	53,53,53,53	0
2	R78	A	1401[B]	29/38	0.78	0.17	53,58,65,68	29
2	R78	A	1401[A]	29/38	0.78	0.17	40,45,52,53	29
2	R78	C	1401	29/38	0.82	0.19	67,79,90,93	0
2	R78	B	1401	29/38	0.83	0.15	47,56,66,68	0
2	R78	D	1401	29/38	0.86	0.18	77,91,100,102	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.

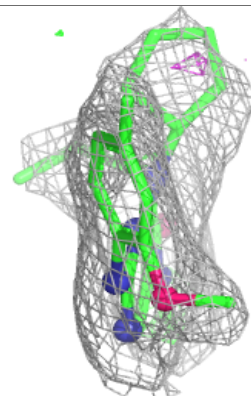
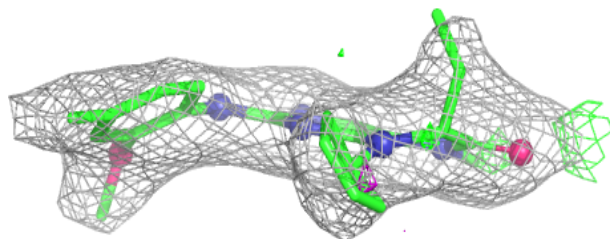
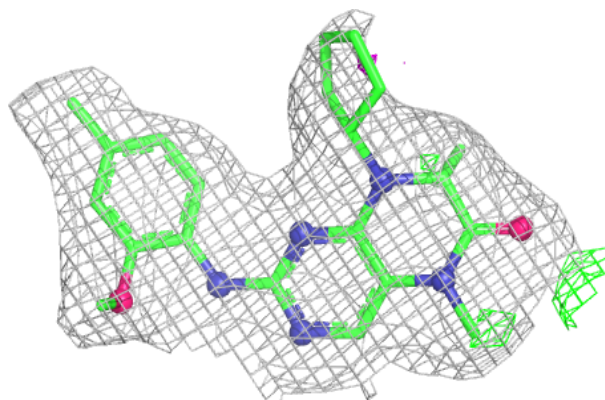


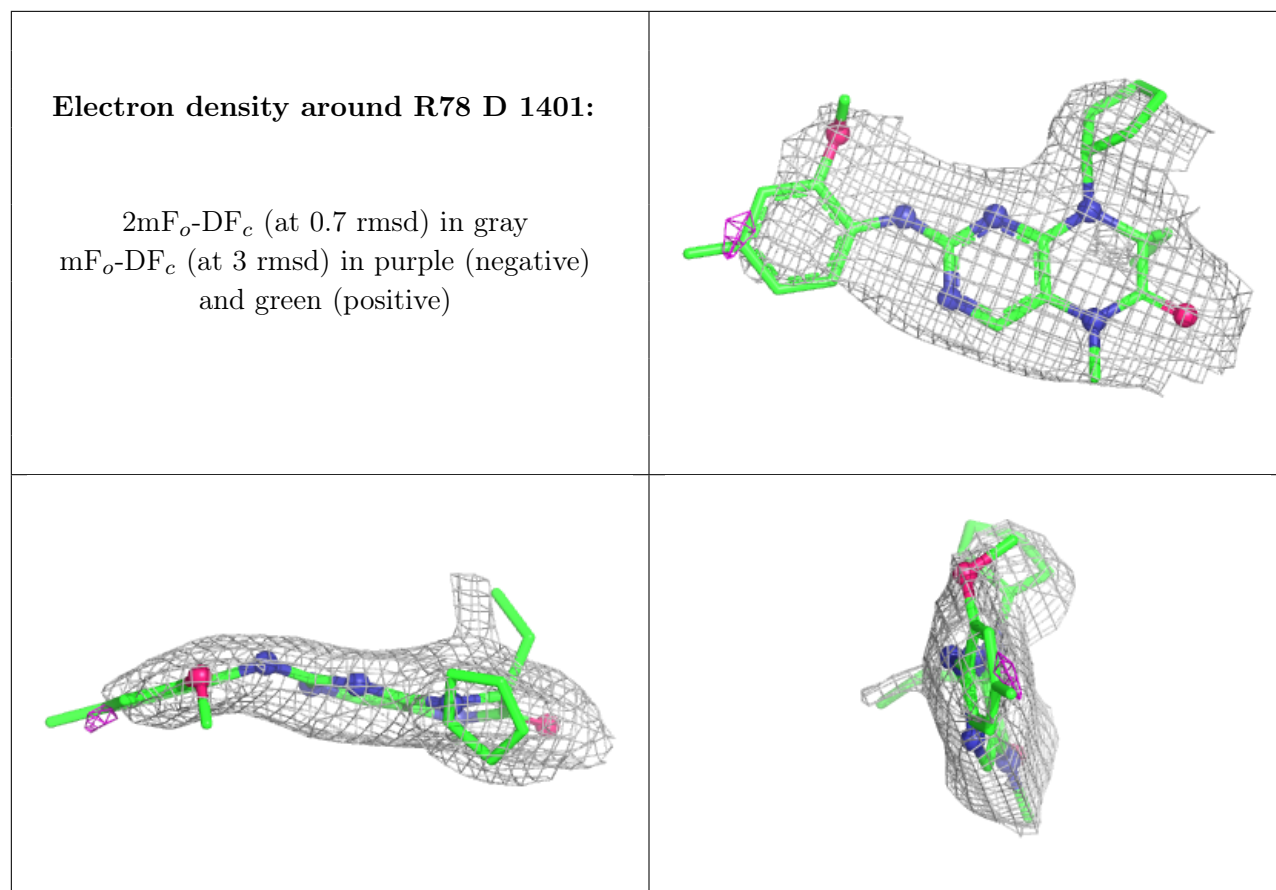
**Electron density around R78 C 1401:**

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

**Electron density around R78 B 1401:**

$2mF_o-DF_c$  (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.