



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 09:40 PM BST

PDB ID : 5L8A
Title : Targeting the PEX14-PEX5 interaction by small molecules provides novel therapeutic routes to treat trypanosomiasis.
Authors : Dawidowski, M.; Emmanouilidis, L.; Sattler, M.; Popowicz, G.M.
Deposited on : 2016-06-07
Resolution : 1.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 2370 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 Peroxin 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	62	488	305	88	94	1	0	0	0
1	B	62	480	299	90	90	1	0	0	0
1	C	62	486	303	91	91	1	0	0	0
1	D	62	490	306	89	94	1	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8IEW2
A	-1	ALA	-	expression tag	UNP Q8IEW2
A	0	MET	-	expression tag	UNP Q8IEW2
A	1	TRP	-	expression tag	UNP Q8IEW2
B	-2	GLY	-	expression tag	UNP Q8IEW2
B	-1	ALA	-	expression tag	UNP Q8IEW2
B	0	MET	-	expression tag	UNP Q8IEW2
B	1	TRP	-	expression tag	UNP Q8IEW2
C	-2	GLY	-	expression tag	UNP Q8IEW2
C	-1	ALA	-	expression tag	UNP Q8IEW2
C	0	MET	-	expression tag	UNP Q8IEW2
C	1	TRP	-	expression tag	UNP Q8IEW2
D	-2	GLY	-	expression tag	UNP Q8IEW2
D	-1	ALA	-	expression tag	UNP Q8IEW2
D	0	MET	-	expression tag	UNP Q8IEW2
D	1	TRP	-	expression tag	UNP Q8IEW2

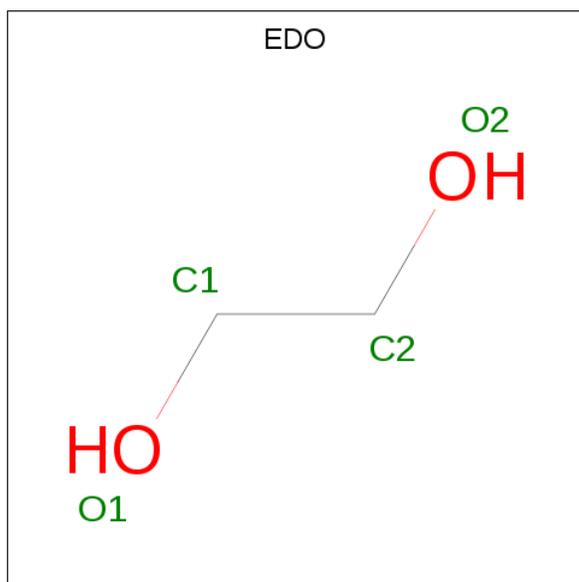
- Molecule 2 is 1-(2-hydroxyethyl)-5-[(4-methoxynaphthalen-1-yl)methyl]- {N}-(phenylmethyl)-6,7-dihydro-4 {H}-pyrazolo[4,3-c]pyridine-3-carboxamide (three-letter code: 6RB) (formula: C₂₈H₃₀N₄O₃).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	2	1	2		

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

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	84	Total	O	0	0
			84	84		
6	B	63	Total	O	0	0
			63	63		
6	C	68	Total	O	0	0
			68	68		
6	D	61	Total	O	0	0
			61	61		

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Peroxin 14

Chain A:  90% 10%



- Molecule 1: Peroxin 14

Chain B:  87% 10%



- Molecule 1: Peroxin 14

Chain C:  86% 10%



- Molecule 1: Peroxin 14

Chain D:  83% 6% 10%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	36.10Å 36.28Å 55.31Å 94.12° 105.87° 100.54°	Depositor
Resolution (Å)	27.79 – 1.57	Depositor
% Data completeness (in resolution range)	92.5 (27.79-1.57)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.57Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.191 , 0.252	Depositor
Wilson B-factor (Å ²)	15.3	Xtrriage
Anisotropy	0.069	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2370	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: 6RB, EDO, NA

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	0.85	0/493	0.79	0/658
1	B	0.74	0/485	0.76	0/648
1	C	0.83	0/491	0.77	0/655
1	D	0.84	0/495	0.95	5/660 (0.8%)
All	All	0.81	0/1964	0.82	5/2621 (0.2%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	VAL	CB-CA-C	6.95	124.60	111.40
1	D	25	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	D	23	VAL	CA-CB-CG1	5.79	119.59	110.90
1	D	25	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	D	22	ARG	NE-CZ-NH1	5.36	122.98	120.30

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	488	0	504	0	0
1	B	480	0	493	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	486	0	504	5	0
1	D	490	0	511	2	1
2	A	35	0	0	0	0
2	B	35	0	0	1	0
2	C	35	0	0	0	0
2	D	35	0	0	0	0
3	A	5	0	2	0	0
4	C	1	0	0	0	0
5	D	4	0	6	0	0
6	A	84	0	0	0	0
6	B	63	0	0	1	0
6	C	68	0	0	5	1
6	D	61	0	0	2	1
All	All	2370	0	2020	9	2

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.

The worst 5 of 9 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:60:GLU:HG3	6:D:234:HOH:O	1.75	0.87
1:C:63:ARG:NH1	6:C:202:HOH:O	2.31	0.64
1:B:36:LYS:HE2	6:B:248:HOH:O	2.09	0.52
1:C:5:SER:CB	6:C:249:HOH:O	2.58	0.51
1:D:13:ASN:ND2	6:D:204:HOH:O	2.47	0.48

All (2) 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:C:266:HOH:O	6:D:261:HOH:O[1_656]	2.06	0.14
1:B:66:SER:OXT	1:D:25:ARG:NH2[1_656]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
2	6RB	C	101	-	38,39,39	2.31	11 (28%)	44,54,54	3.64	16 (36%)
2	6RB	D	101	-	38,39,39	1.87	10 (26%)	44,54,54	4.64	15 (34%)
2	6RB	A	101	-	38,39,39	2.39	9 (23%)	44,54,54	2.11	16 (36%)
3	GLY	A	102	-	1,4,4	0.25	0	0,4,4	0.00	-
5	EDO	D	102	-	3,3,3	0.35	0	2,2,2	0.35	0
2	6RB	B	101	-	38,39,39	2.18	11 (28%)	44,54,54	4.21	19 (43%)

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	6RB	C	101	-	-	4/14/27/27	0/5/5/5
2	6RB	D	101	-	-	4/14/27/27	0/5/5/5
2	6RB	A	101	-	-	1/14/27/27	0/5/5/5
3	GLY	A	102	-	-	0/0/2/2	-
5	EDO	D	102	-	-	0/1/1/1	-
2	6RB	B	101	-	-	3/14/27/27	0/5/5/5

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	6RB	CBC-CAY	-9.00	1.37	1.50
2	C	101	6RB	CBC-CAY	-7.55	1.39	1.50
2	B	101	6RB	CBC-CAY	-7.10	1.39	1.50
2	D	101	6RB	CBC-CAY	-5.70	1.42	1.50
2	A	101	6RB	CAU-CBD	-5.44	1.40	1.51

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	101	6RB	CBC-CAY-NAW	21.78	136.90	115.67
2	B	101	6RB	CBC-CAY-NAW	18.71	133.91	115.67
2	C	101	6RB	CBC-CAY-NAW	15.68	130.96	115.67
2	D	101	6RB	CAR-NBI-CBE	-11.47	113.89	128.48
2	D	101	6RB	OAB-CAY-NAW	-9.57	103.54	122.61

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

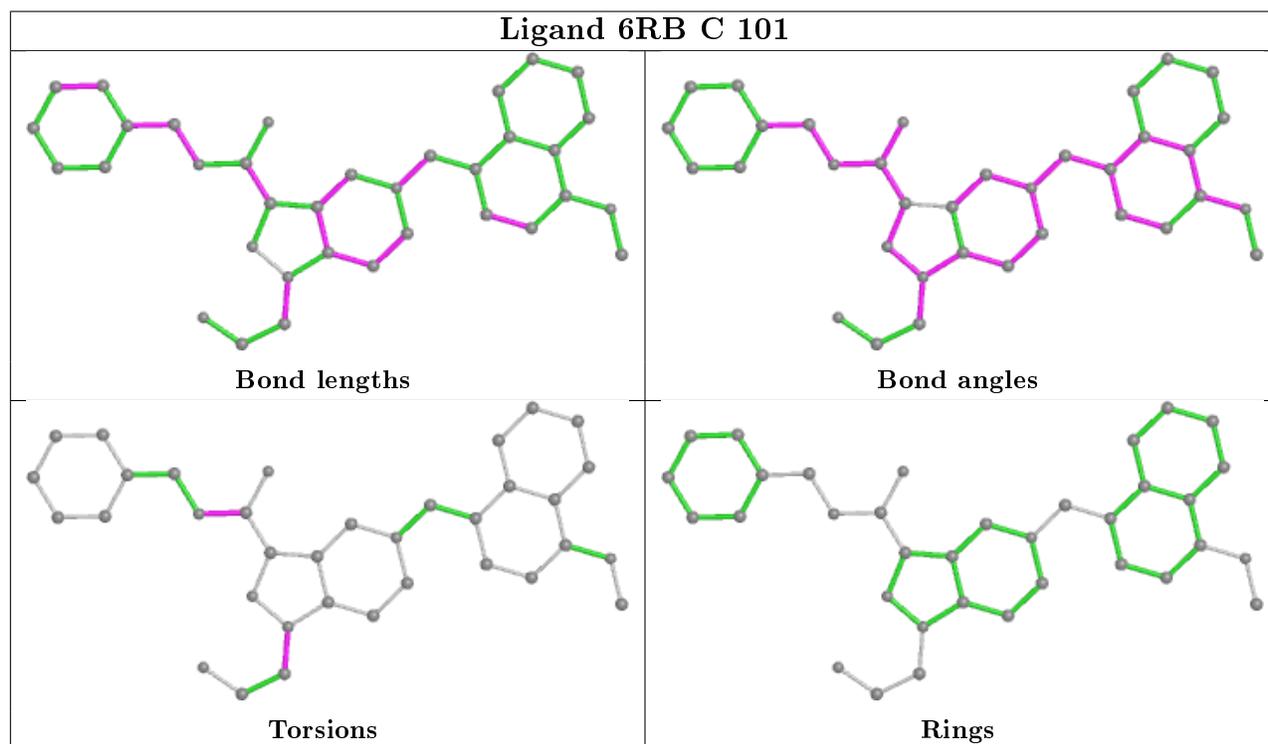
Mol	Chain	Res	Type	Atoms
2	D	101	6RB	CAO-CAR-NBI-CBE
2	D	101	6RB	CAO-CAR-NBI-NAV
2	D	101	6RB	CBC-CAY-NAW-CAS
2	B	101	6RB	OAC-CAO-CAR-NBI
2	B	101	6RB	CBC-CAY-NAW-CAS

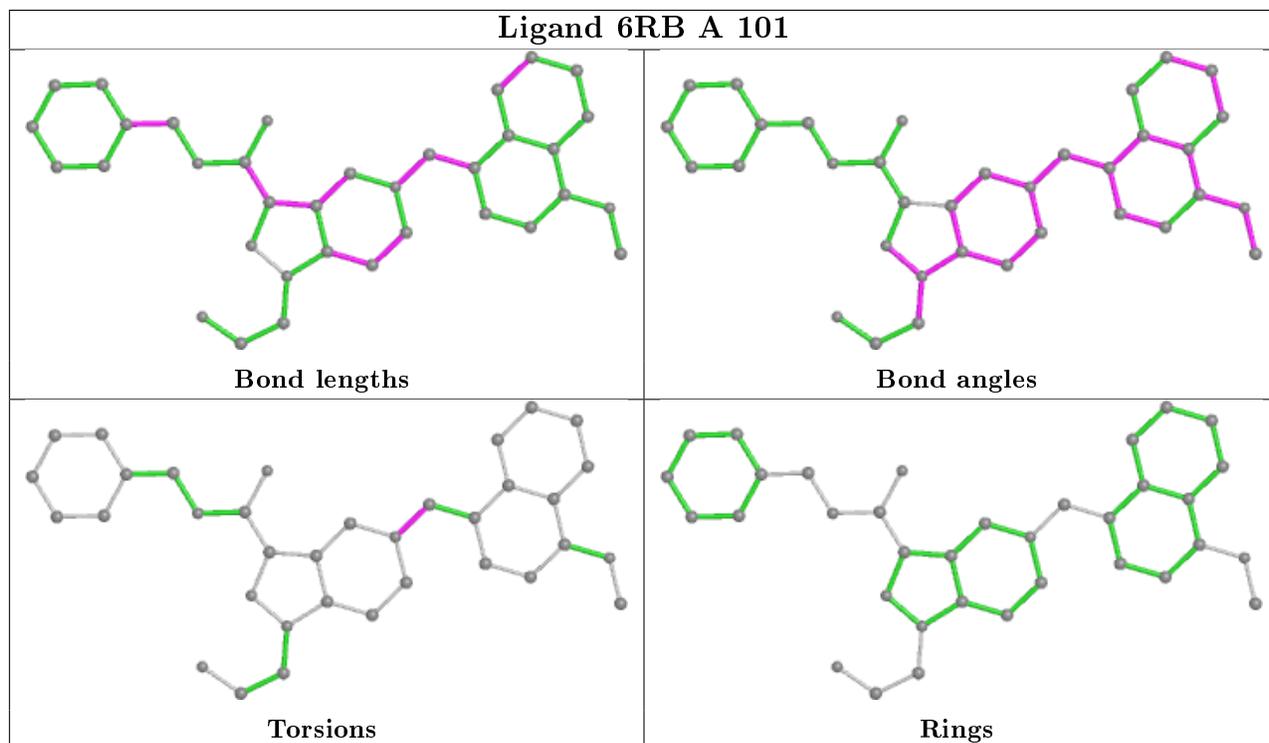
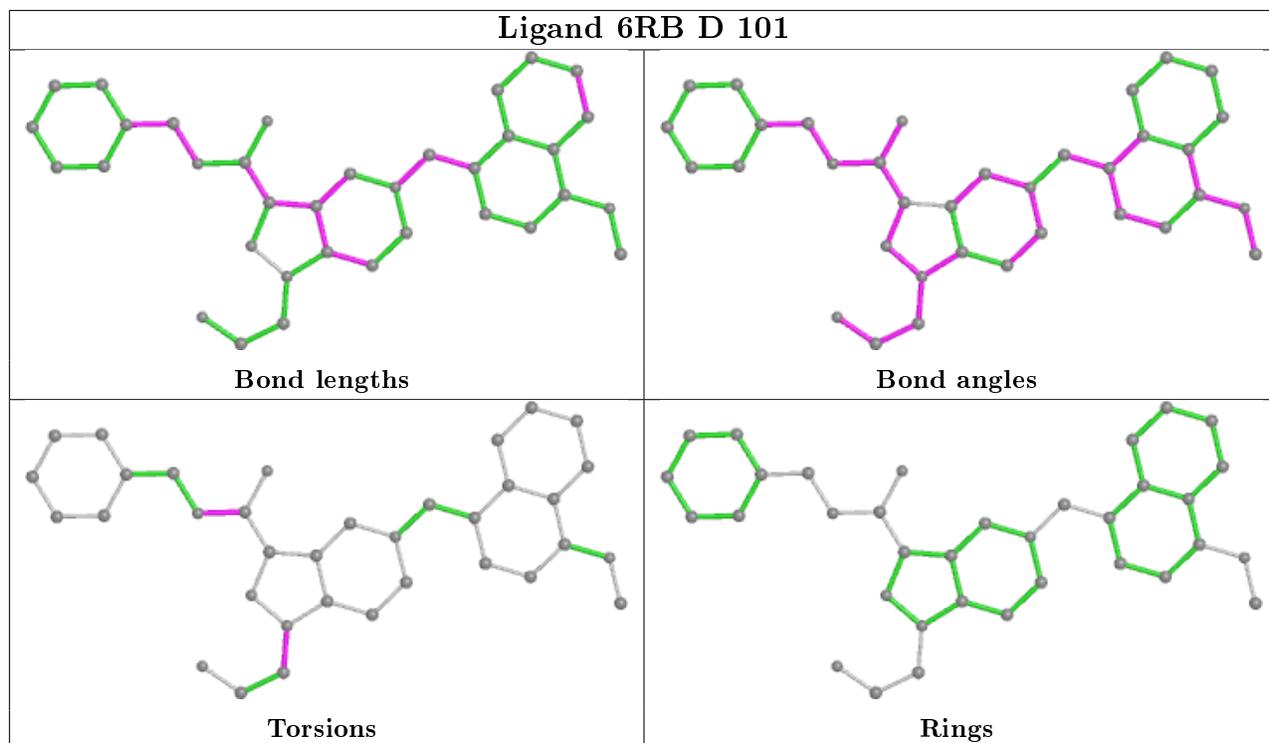
There are no ring outliers.

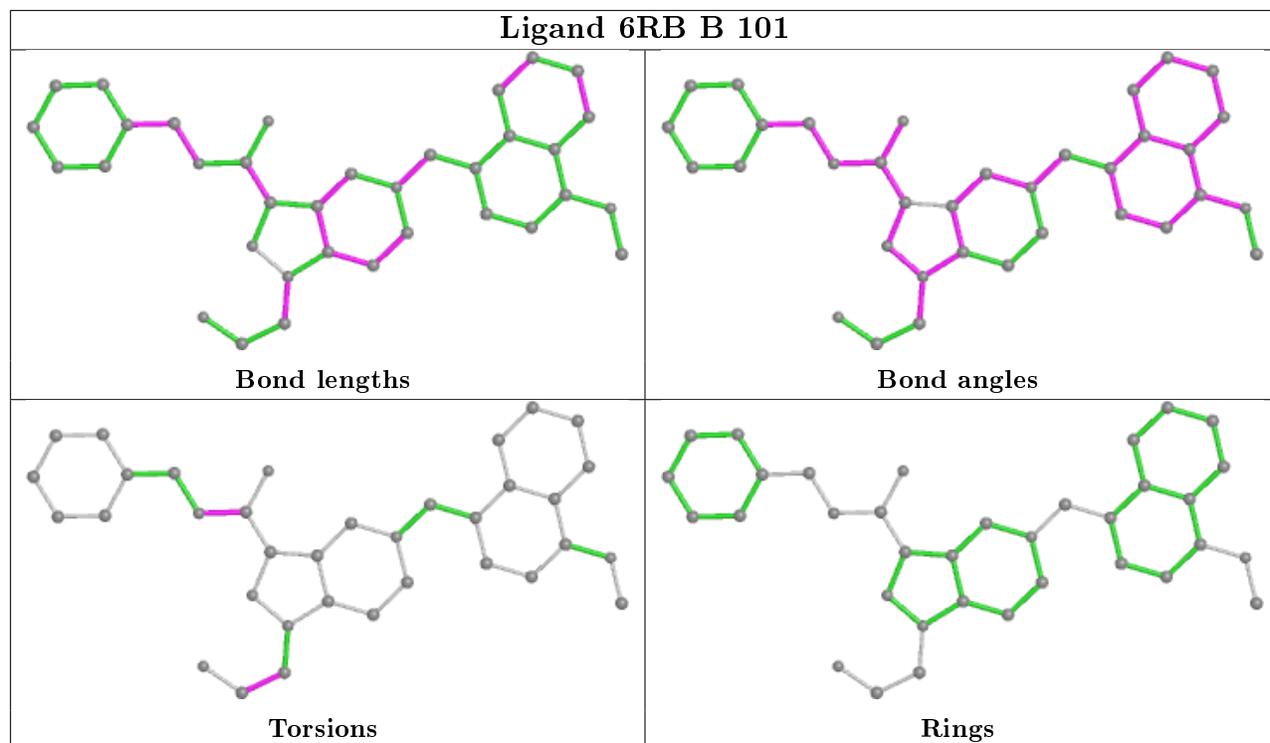
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	101	6RB	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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

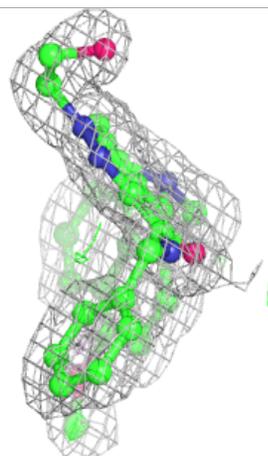
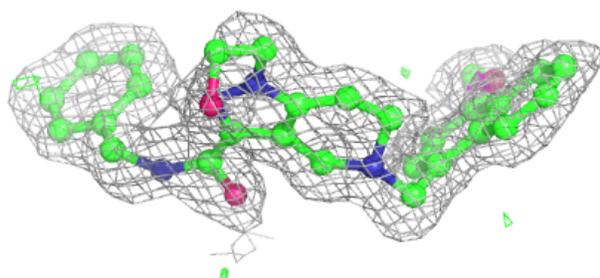
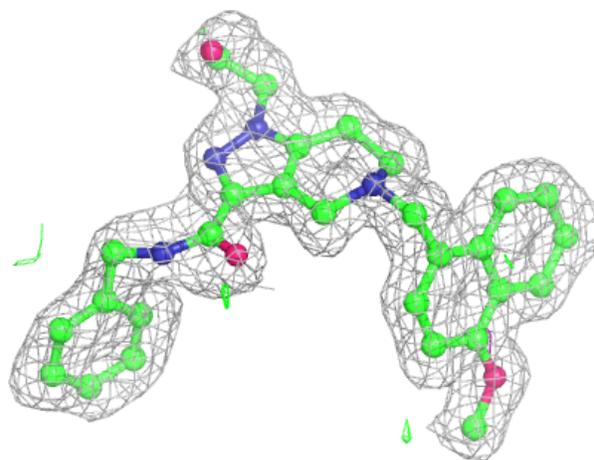
6.4 Ligands

EDS failed to run properly - this section is therefore empty.

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.

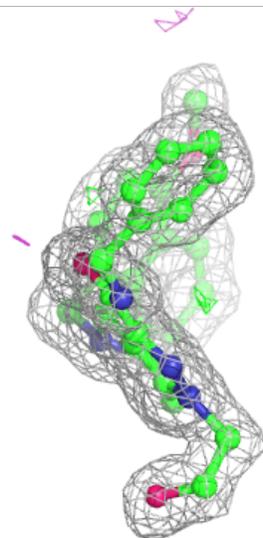
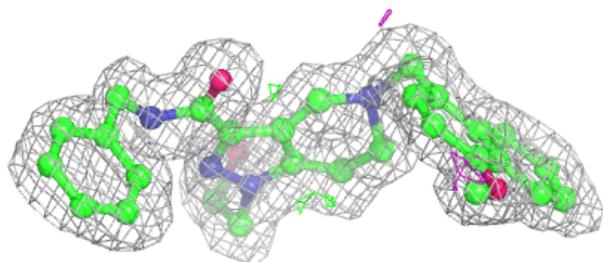
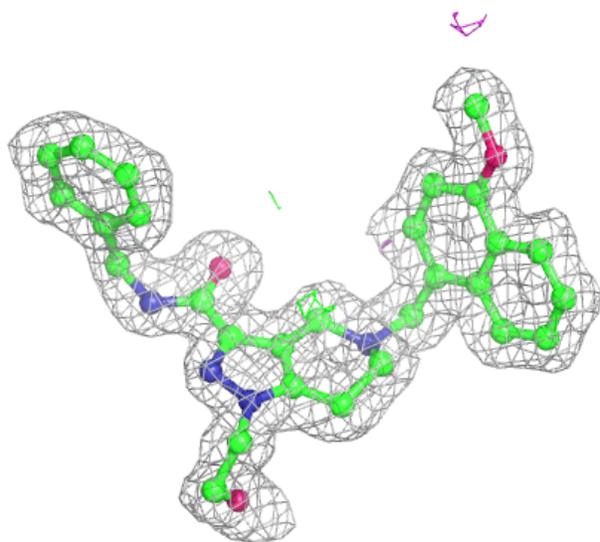
Electron density around 6RB D 101:

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



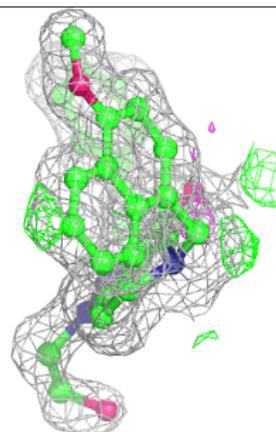
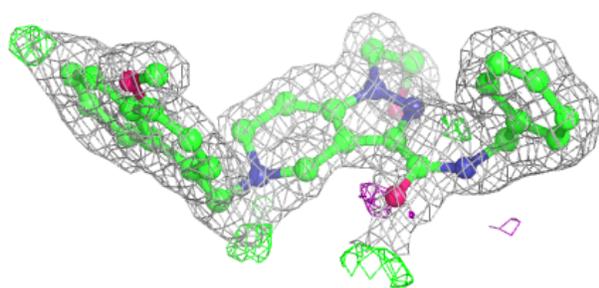
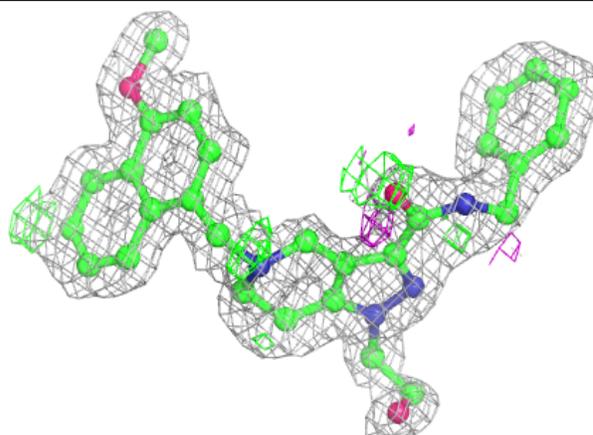
Electron density around 6RB A 101:

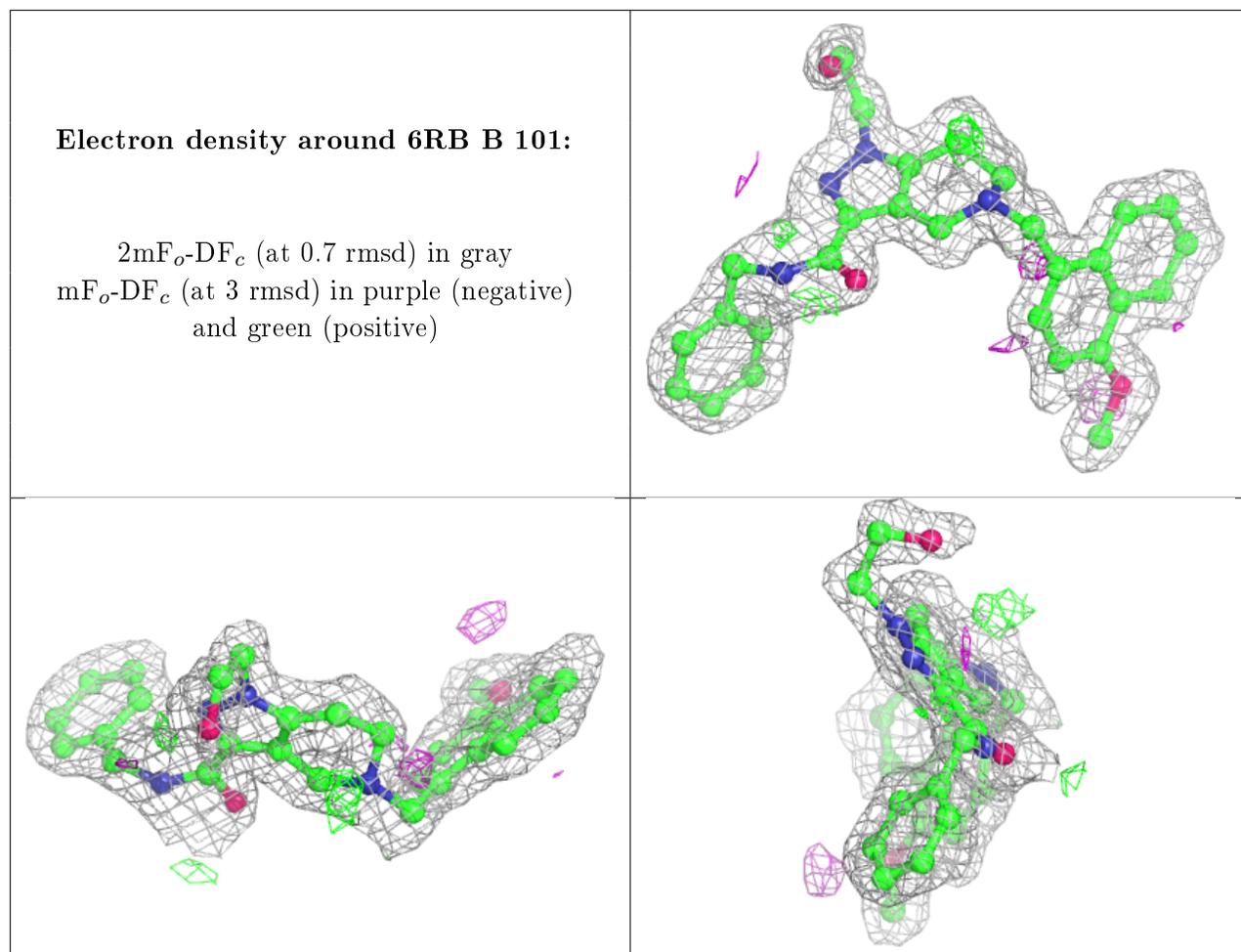
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 6RB 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)





6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.