



Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2022 – 10:32 AM EDT

PDB ID : 7MR6
Title : Crystal structure of the first bromodomain (BD1) of human BRD4 bound to GXH-II-082
Authors : Chan, A.; Schonbrunn, E.
Deposited on : 2021-05-07
Resolution : 1.85 Å(reported)

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

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

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 : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

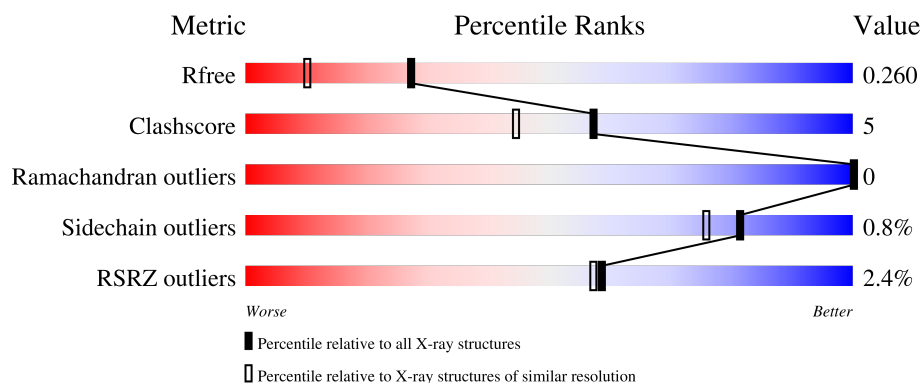
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

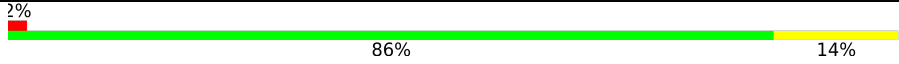
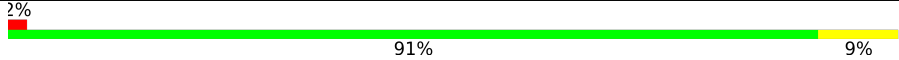
The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	127	
1	B	127	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2454 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.

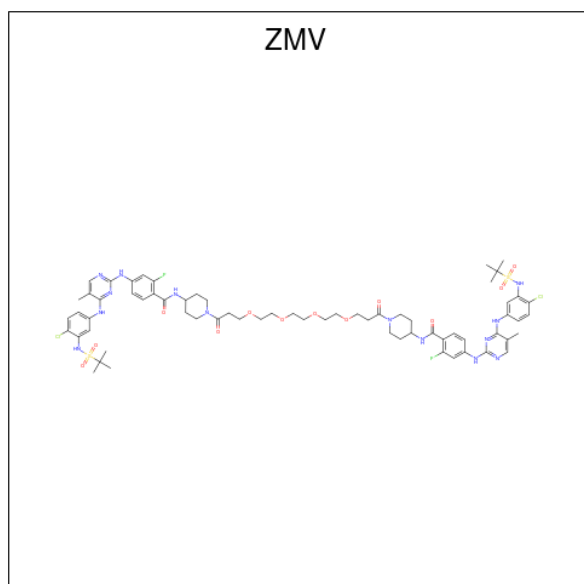
- Molecule 1 is a protein called Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1062	687	174	194	7			
1	B	127	Total	C	N	O	S	0	0	0
			1062	687	174	194	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	SER	-	expression tag	UNP O60885
A	43	MET	-	expression tag	UNP O60885
B	42	SER	-	expression tag	UNP O60885
B	43	MET	-	expression tag	UNP O60885

- Molecule 2 is N,N'-[(1,16-dioxo-4,7,10,13-tetraoxahexadecane-1,16-diyl)di(piperidine-1,4-diyl)]bis{4-[(4-{4-chloro-3-[(2-methylpropane-2-sulfonyl)amino]anilino}-5-methylpyrimidin-2-yl)amino]-2-fluorobenzamide} (three-letter code: ZMV) (formula: C₆₆H₈₄Cl₂F₂N₁₄O₁₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	B	1	Total	C	Cl	F	N	O	S	0	0
			98	66	2	2	14	12	2		

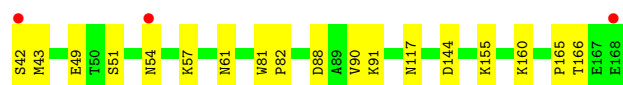
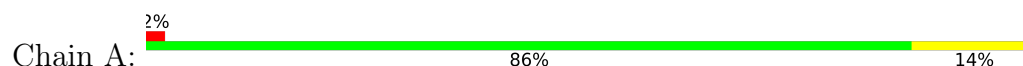
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total	O	0	0
			101	101		
3	B	131	Total	O	0	0
			131	131		

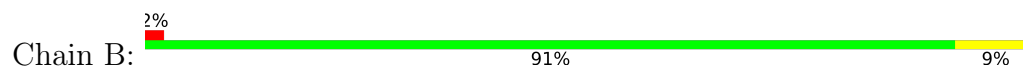
3 Residue-property plots [i](#)

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-containing protein 4



- Molecule 1: Bromodomain-containing protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	30.23Å 40.35Å 57.20Å 100.23° 104.69° 90.29°	Depositor
Resolution (Å)	29.54 – 1.85 54.38 – 1.85	Depositor EDS
% Data completeness (in resolution range)	90.3 (29.54-1.85) 90.3 (54.38-1.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_3260	Depositor
R, R_{free}	0.204 , 0.260 0.204 , 0.260	Depositor DCC
R_{free} test set	1100 reflections (5.55%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2454	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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: ZMV

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	0.42	0/1092	0.56	0/1484
1	B	0.42	0/1092	0.58	0/1484
All	All	0.42	0/2184	0.57	0/2968

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1062	0	1056	14	0
1	B	1062	0	1056	7	0
2	B	98	0	0	1	0
3	A	101	0	0	5	1
3	B	131	0	0	3	1
All	All	2454	0	2112	21	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 5.

All (21) 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:49:GLU:OE1	3:A:201:HOH:O	1.81	0.96
1:B:57:LYS:HG3	1:B:117:ASN:HB2	1.58	0.86
1:A:42:SER:OG	1:A:43:MET:N	2.24	0.67
1:A:61:ASN:HD22	1:A:165:PRO:HB2	1.67	0.58
1:A:91:LYS:NZ	3:A:206:HOH:O	2.36	0.58
1:A:155:LYS:NZ	3:A:208:HOH:O	2.38	0.57
1:B:127:GLN:NE2	3:B:305:HOH:O	2.35	0.55
1:B:66:LEU:HD23	1:B:70:VAL:HG21	1.91	0.52
1:B:78:GLN:HG2	3:B:388:HOH:O	2.09	0.51
1:B:168:GLU:O	3:B:302:HOH:O	2.18	0.51
1:A:57:LYS:HG2	1:A:117:ASN:HB2	1.95	0.47
1:A:42:SER:HG	1:A:43:MET:H	1.59	0.47
1:B:109:THR:O	1:B:113:ARG:HG3	2.15	0.46
1:A:88:ASP:OD1	1:A:90:VAL:HG22	2.17	0.45
1:A:160:LYS:HD3	1:A:160:LYS:HA	1.84	0.44
1:A:144:ASP:OD1	3:A:202:HOH:O	2.21	0.43
1:A:54:ASN:ND2	3:A:214:HOH:O	2.49	0.43
1:A:61:ASN:ND2	1:A:166:THR:O	2.44	0.43
1:A:61:ASN:ND2	1:A:165:PRO:HB2	2.33	0.43
1:B:94:LEU:HD11	2:B:201:ZMV:C78	2.50	0.41
1:A:81:TRP:CD2	1:A:82:PRO:HD3	2.56	0.41

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)
3:A:288:HOH:O	3:B:399:HOH:O[1_554]	2.14	0.06

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	125/127 (98%)	122 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	125/127 (98%)	124 (99%)	1 (1%)	0	100	100
All	All	250/254 (98%)	246 (98%)	4 (2%)	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	120/120 (100%)	119 (99%)	1 (1%)	81	76
1	B	120/120 (100%)	119 (99%)	1 (1%)	81	76
All	All	240/240 (100%)	238 (99%)	2 (1%)	81	76

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	B	51	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	ASN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	ZMV	B	201	-	105,105,105	2.20	23 (21%)	144,150,150	2.23	37 (25%)

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	ZMV	B	201	-	-	16/85/105/105	0/8/8/8

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	ZMV	S63-N62	8.43	1.71	1.59
2	B	201	ZMV	S88-N87	8.35	1.71	1.59
2	B	201	ZMV	C45-N44	5.92	1.47	1.34
2	B	201	ZMV	C20-N17	5.78	1.46	1.35
2	B	201	ZMV	C54-N55	5.24	1.45	1.36
2	B	201	ZMV	C82-N83	5.18	1.45	1.36
2	B	201	ZMV	C36-N38	5.03	1.45	1.35
2	B	201	ZMV	C11-N13	4.86	1.44	1.34
2	B	201	ZMV	C52-N51	4.48	1.45	1.36
2	B	201	ZMV	C05-N06	4.19	1.45	1.36
2	B	201	ZMV	C91-S88	3.28	1.84	1.81
2	B	201	ZMV	C02-C82	-3.16	1.36	1.41
2	B	201	ZMV	C05-N04	-2.68	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	ZMV	C18-N17	2.60	1.51	1.47
2	B	201	ZMV	C16-N17	2.53	1.51	1.47
2	B	201	ZMV	C50-N51	2.43	1.46	1.40
2	B	201	ZMV	C56-N55	2.35	1.46	1.40
2	B	201	ZMV	C86-N87	2.31	1.46	1.42
2	B	201	ZMV	C07-N06	2.25	1.45	1.40
2	B	201	ZMV	C95-CL96	2.22	1.78	1.73
2	B	201	ZMV	O46-C45	-2.20	1.18	1.23
2	B	201	ZMV	C84-N83	2.12	1.45	1.40
2	B	201	ZMV	C59-CL60	2.07	1.78	1.73

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	ZMV	O65-S63-O64	-8.82	102.67	120.57
2	B	201	ZMV	O90-S88-O89	-8.48	103.35	120.57
2	B	201	ZMV	C71-C73-N74	-7.53	117.41	125.11
2	B	201	ZMV	O89-S88-C91	6.14	112.53	107.60
2	B	201	ZMV	C14-N13-C11	-5.77	114.56	122.55
2	B	201	ZMV	C02-C03-N04	-5.51	119.48	125.11
2	B	201	ZMV	C19-C18-N17	4.95	118.35	110.82
2	B	201	ZMV	N74-C52-N53	-4.86	121.94	126.55
2	B	201	ZMV	N04-C05-N81	-4.80	122.00	126.55
2	B	201	ZMV	C09-C10-C78	4.48	121.76	116.67
2	B	201	ZMV	C73-N74-C52	4.20	122.22	115.88
2	B	201	ZMV	C71-C54-N53	-3.86	118.97	123.37
2	B	201	ZMV	N83-C82-N81	3.74	124.69	119.12
2	B	201	ZMV	C01-C02-C82	-3.60	118.84	121.97
2	B	201	ZMV	C48-C47-C76	3.51	120.66	116.67
2	B	201	ZMV	C75-C76-C47	-3.49	119.81	123.53
2	B	201	ZMV	C59-C61-N62	-3.43	117.56	120.74
2	B	201	ZMV	C03-N04-C05	3.12	120.58	115.88
2	B	201	ZMV	C80-C78-C10	-2.96	120.37	123.53
2	B	201	ZMV	C02-C82-N83	-2.91	114.83	119.22
2	B	201	ZMV	C93-C91-S88	2.88	112.08	107.86
2	B	201	ZMV	O90-S88-N87	2.80	114.49	109.42
2	B	201	ZMV	O65-S63-N62	2.76	114.42	109.42
2	B	201	ZMV	C15-C16-N17	2.61	114.79	110.82
2	B	201	ZMV	O65-S63-C66	2.60	109.69	107.60
2	B	201	ZMV	C02-C82-N81	-2.53	120.48	123.37
2	B	201	ZMV	N55-C54-N53	2.50	122.84	119.12
2	B	201	ZMV	C76-C47-C45	-2.44	119.44	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	ZMV	C84-N83-C82	-2.31	123.59	129.39
2	B	201	ZMV	C69-C66-S63	2.25	111.16	107.86
2	B	201	ZMV	C10-C11-N13	2.25	120.97	116.80
2	B	201	ZMV	C98-C84-C85	2.18	122.23	119.65
2	B	201	ZMV	C01-C02-C03	2.17	123.67	120.01
2	B	201	ZMV	C42-C41-C40	2.14	114.52	110.82
2	B	201	ZMV	C86-C95-CL96	-2.12	117.13	119.54
2	B	201	ZMV	C40-C41-N44	-2.07	106.28	110.56
2	B	201	ZMV	C08-C07-C80	2.04	122.08	119.65

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	ZMV	C20-C22-C23-O24
2	B	201	ZMV	C86-N87-S88-O89
2	B	201	ZMV	C22-C23-O24-C25
2	B	201	ZMV	O24-C25-C26-O27
2	B	201	ZMV	N04-C05-N06-C07
2	B	201	ZMV	N81-C05-N06-C07
2	B	201	ZMV	C28-C29-O30-C31
2	B	201	ZMV	N44-C45-C47-C76
2	B	201	ZMV	O46-C45-C47-C76
2	B	201	ZMV	C26-C25-O24-C23
2	B	201	ZMV	C35-C34-O33-C32
2	B	201	ZMV	C25-C26-O27-C28
2	B	201	ZMV	C32-C31-O30-C29
2	B	201	ZMV	C34-C35-C36-N38
2	B	201	ZMV	C92-C91-S88-O89
2	B	201	ZMV	C34-C35-C36-O37

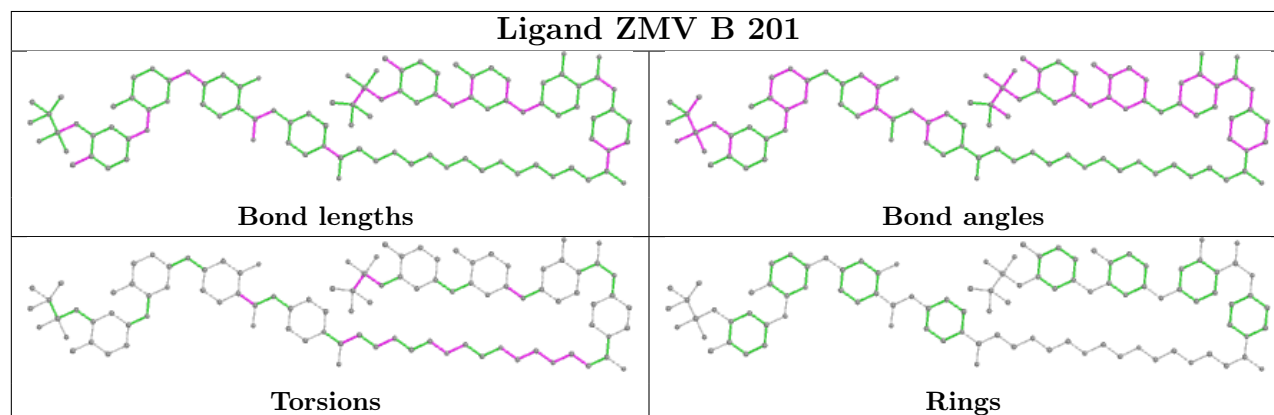
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	ZMV	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	127/127 (100%)	0.11	3 (2%) 59 57	14, 21, 34, 48	0
1	B	127/127 (100%)	0.07	3 (2%) 59 57	14, 21, 34, 48	0
All	All	254/254 (100%)	0.09	6 (2%) 59 57	14, 21, 34, 48	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	GLU	4.4
1	B	42	SER	4.1
1	A	54	ASN	3.1
1	B	54	ASN	2.9
1	A	42	SER	2.1
1	A	168	GLU	2.1

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](#)

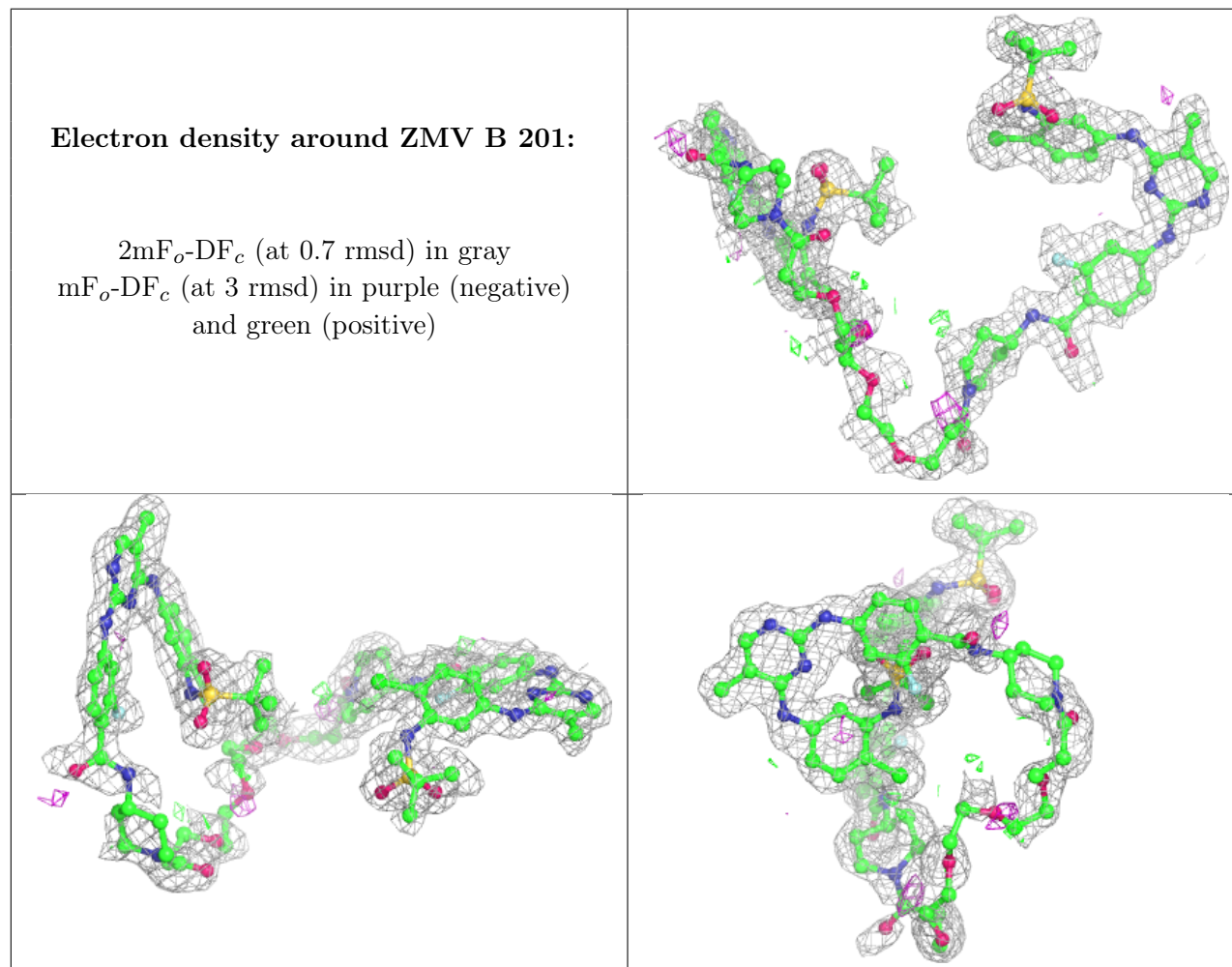
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
2	ZMV	B	201	98/98	0.91	0.15	13,27,50,53	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.