



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:14 am BST

PDB ID : 4YBM  
Title : Crystal structure of TRIM24 PHD-bromodomain complexed with N-{6-[3-(benzyloxy)phenoxy]-1,3-dimethyl-2-oxo-2,3-dihydro-1H-1,3-benzodiazol-5-yl}-3,4-dimethoxybenzene-1-sulfonamide (7b)  
Authors : Poncet-Montange, G.; Palmer, W.; Jones, P.  
Deposited on : 2015-02-18  
Resolution : 1.46 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 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 : 2.11  
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) : 2.11

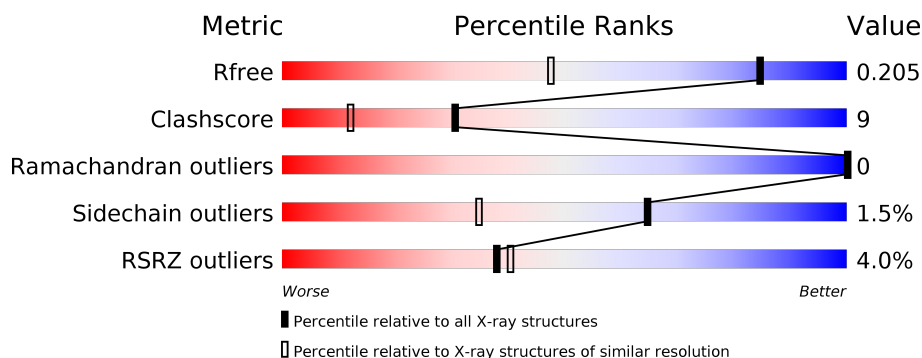
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.46 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 on 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	184	<div> <div>3%</div> <div>89%</div> <div>6%</div> <div>• •</div> </div>
1	B	184	<div> <div>5%</div> <div>76%</div> <div>15%</div> <div>• 8%</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
3	GOL	A	1104	-	-	X	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3565 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 Transcription intermediary factor 1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	3	0
			1461	936	233	277	15			
1	B	170	Total	C	N	O	S	0	3	0
			1408	901	224	267	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	823	SER	-	expression tag	UNP O15164
B	823	SER	-	expression tag	UNP O15164

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

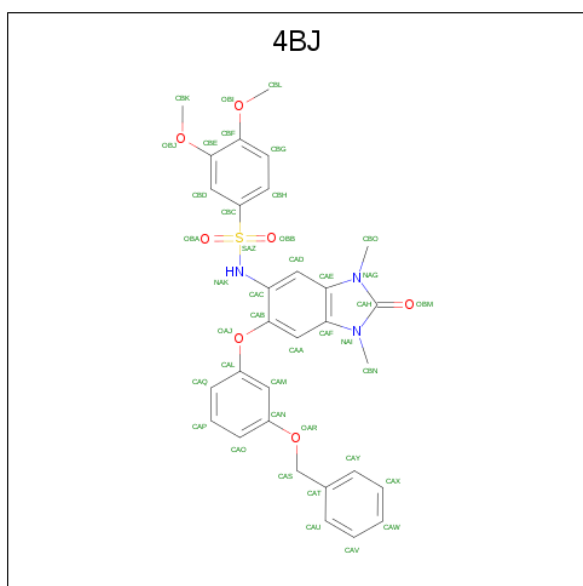
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is N-{6-[3-(benzyloxy)phenoxy]-1,3-dimethyl-2-oxo-2,3-dihydro-1H-benzimidazol-5-yl}-3,4-dimethoxybenzenesulfonamide (three-letter code: 4BJ) (formula: C<sub>30</sub>H<sub>29</sub>N<sub>3</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			41	30	3	7	1		
4	B	1	Total	C	N	O	S	0	0
			41	30	3	7	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

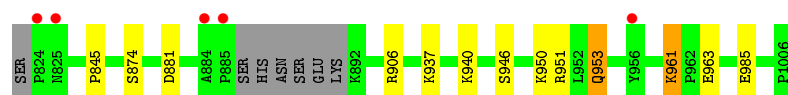
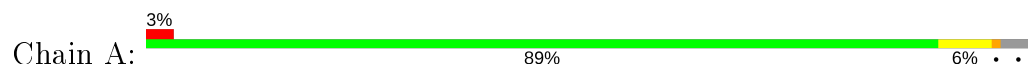
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	305	Total	O	0	0
			305	305		
6	B	271	Total	O	0	0
			271	271		

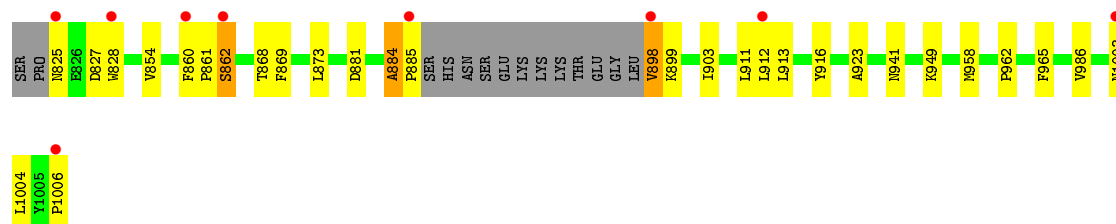
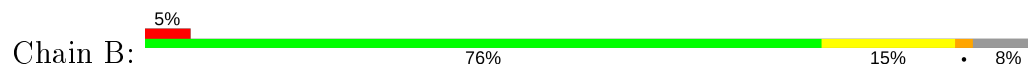
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Transcription intermediary factor 1-alpha



- Molecule 1: Transcription intermediary factor 1-alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.40 Å 79.82 Å 131.69 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.87 – 1.46 33.87 – 1.46	Depositor EDS
% Data completeness (in resolution range)	98.9 (33.87-1.46) 98.9 (33.87-1.46)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.46 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.163 , 0.196 0.172 , 0.205	Depositor DCC
$R_{free}$ test set	3461 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, 4BJ, SO4

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	1.07	3/1498 (0.2%)	1.15	5/2026 (0.2%)
1	B	1.00	0/1444	1.02	1/1957 (0.1%)
All	All	1.04	3/2942 (0.1%)	1.09	6/3983 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	874	SER	CB-OG	-6.91	1.33	1.42
1	A	946	SER	CB-OG	-6.17	1.34	1.42
1	A	963	GLU	CD-OE2	5.29	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	951	ARG	NE-CZ-NH1	10.09	125.35	120.30
1	A	881	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	A	881	ASP	CB-CG-OD1	7.88	125.39	118.30
1	A	951	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	906	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	881	ASP	CB-CG-OD1	5.43	123.19	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	884	ALA	Peptide

## 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	1461	0	1416	22	1
1	B	1408	0	1351	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	12	0	16	11	0
3	B	12	0	16	0	0
4	B	82	0	58	6	0
5	B	10	0	0	0	0
6	A	305	0	0	7	3
6	B	271	0	0	9	1
All	All	3565	0	2857	54	3

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 9.

All (54) 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)
4:B:1101:4BJ:NAK	4:B:1101:4BJ:SAZ	2.03	1.31
1:A:940:LYS:HB2	3:A:1104:GOL:O3	1.27	1.26
1:A:950[B]:LYS:NZ	6:A:1201:HOH:O	1.75	1.13
1:A:940:LYS:CB	3:A:1104:GOL:O3	2.06	1.03
1:B:854:VAL:HG11	1:B:912:LEU:HD23	1.44	0.98
1:B:854:VAL:CG1	1:B:912:LEU:HD23	2.14	0.78
1:A:985:GLU:HG3	6:A:1463:HOH:O	1.92	0.69
1:B:986:VAL:HG23	4:B:1102:4BJ:H6	1.75	0.68
1:B:898:VAL:N	6:B:1201:HOH:O	2.27	0.66
1:A:961:LYS:NZ	1:A:961:LYS:HB3	2.11	0.64
1:B:873:LEU:HB3	1:B:903:ILE:CD1	2.28	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:LYS:HA	3:A:1104:GOL:H32	1.80	0.63
1:A:961:LYS:HZ1	1:A:961:LYS:HB3	1.62	0.63
1:A:985:GLU:HG2	6:B:1367:HOH:O	1.98	0.62
1:A:953[B]:GLN:HG3	1:A:953[B]:GLN:O	1.99	0.62
1:A:940:LYS:HG3	3:A:1104:GOL:H32	1.81	0.61
1:B:899:LYS:HE3	6:B:1242:HOH:O	2.00	0.61
1:A:940:LYS:CB	3:A:1104:GOL:C3	2.79	0.60
1:A:953[A]:GLN:CD	6:A:1449:HOH:O	2.41	0.59
1:A:961:LYS:NZ	6:A:1203:HOH:O	2.33	0.58
1:B:873:LEU:HB3	1:B:903:ILE:HD11	1.86	0.57
1:B:825:ASN:N	6:B:1203:HOH:O	2.38	0.57
1:B:941[A]:ASN:ND2	6:B:1467:HOH:O	2.12	0.57
1:B:862:SER:HB2	6:B:1457:HOH:O	2.06	0.56
1:B:958[B]:MET:HE1	6:B:1255:HOH:O	2.06	0.56
1:A:940:LYS:CG	3:A:1104:GOL:C3	2.85	0.54
4:B:1102:4BJ:CBK	4:B:1102:4BJ:H13	2.39	0.53
1:B:898:VAL:HG23	6:B:1201:HOH:O	2.09	0.53
1:A:940:LYS:HG3	3:A:1104:GOL:C3	2.38	0.52
1:B:860:PHE:CD2	1:B:861:PRO:HD2	2.46	0.51
1:B:962:PRO:HA	1:B:965:PHE:CE2	2.45	0.50
1:B:911:LEU:HG	1:B:1004:LEU:CD1	2.43	0.49
1:B:884:ALA:HB1	1:B:885:PRO:CD	2.43	0.48
1:A:940:LYS:HB2	3:A:1104:GOL:HO3	1.66	0.48
1:B:986:VAL:CG2	4:B:1102:4BJ:H6	2.44	0.47
1:B:912:LEU:HD11	1:B:916:TYR:HE1	1.78	0.47
1:B:884:ALA:CB	1:B:885:PRO:HD2	2.45	0.47
1:A:953[A]:GLN:HG2	6:A:1449:HOH:O	2.15	0.46
1:A:953[A]:GLN:CG	6:A:1449:HOH:O	2.64	0.46
1:B:912:LEU:HD11	1:B:916:TYR:CE1	2.49	0.46
4:B:1102:4BJ:H2	4:B:1102:4BJ:H13	1.99	0.45
1:B:923:ALA:O	4:B:1102:4BJ:H15	2.17	0.45
1:A:937:LYS:HG3	6:A:1294:HOH:O	2.18	0.44
1:B:869:PHE:CZ	1:B:913:LEU:HG	2.53	0.44
1:A:940:LYS:HA	3:A:1104:GOL:C3	2.48	0.43
1:B:1003[B]:ASN:OD1	1:B:1003[B]:ASN:O	2.36	0.43
1:B:1004:LEU:C	1:B:1006:PRO:HD3	2.38	0.43
1:A:940:LYS:CA	3:A:1104:GOL:H32	2.47	0.43
1:B:884:ALA:CB	1:B:885:PRO:CD	2.97	0.42
1:A:940:LYS:CA	3:A:1104:GOL:O3	2.66	0.42
1:B:827:ASP:HB2	1:B:828:TRP:CE3	2.54	0.42
1:B:912:LEU:HD21	1:B:949:LYS:HB2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:941[B]:ASN:HB3	6:B:1320:HOH:O	2.21	0.41
1:B:868:THR:HB	1:B:913:LEU:HD22	2.03	0.40

All (3) 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)
1:A:961:LYS:CE	6:A:1237:HOH:O[4_445]	1.88	0.32
6:A:1301:HOH:O	6:A:1303:HOH:O[1_655]	1.99	0.21
6:A:1204:HOH:O	6:B:1225:HOH:O[3_654]	2.14	0.06

## 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	176/184 (96%)	175 (99%)	1 (1%)	0	100	100
1	B	169/184 (92%)	166 (98%)	3 (2%)	0	100	100
All	All	345/368 (94%)	341 (99%)	4 (1%)	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	168/172 (98%)	164 (98%)	4 (2%)	49	16
1	B	162/172 (94%)	160 (99%)	2 (1%)	71	43
All	All	330/344 (96%)	324 (98%)	6 (2%)	65	26

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

Mol	Chain	Res	Type
1	A	845	PRO
1	A	953[A]	GLN
1	A	953[B]	GLN
1	A	961	LYS
1	B	862	SER
1	B	898	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	4BJ	B	1102	-	42,45,45	2.43	6 (14%)	54,65,65	1.85	7 (12%)
3	GOL	B	1106	-	5,5,5	0.23	0	5,5,5	0.46	0
5	SO4	B	1108	-	4,4,4	0.44	0	6,6,6	0.97	0
3	GOL	B	1107	-	5,5,5	0.26	0	5,5,5	0.50	0
5	SO4	B	1103	-	4,4,4	0.40	0	6,6,6	0.12	0
3	GOL	A	1104	-	5,5,5	0.13	0	5,5,5	0.36	0
3	GOL	A	1103	-	5,5,5	0.43	0	5,5,5	0.54	0
4	4BJ	B	1101	-	42,45,45	4.52	12 (28%)	54,65,65	2.10	15 (27%)

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
4	4BJ	B	1102	-	-	5/24/24/24	0/5/5/5
3	GOL	B	1106	-	-	2/4/4/4	-
3	GOL	B	1107	-	-	2/4/4/4	-
3	GOL	A	1104	-	-	1/4/4/4	-
3	GOL	A	1103	-	-	4/4/4/4	-
4	4BJ	B	1101	-	-	0/24/24/24	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101	4BJ	SAZ-NAK	23.86	2.03	1.63
4	B	1101	4BJ	OBA-SAZ	11.62	1.56	1.43
4	B	1102	4BJ	OBB-SAZ	8.76	1.53	1.43
4	B	1102	4BJ	OBA-SAZ	8.70	1.53	1.43
4	B	1101	4BJ	OBB-SAZ	5.69	1.50	1.43
4	B	1101	4BJ	CBC-SAZ	5.67	1.85	1.76
4	B	1102	4BJ	CAC-NAK	-5.58	1.33	1.42
4	B	1102	4BJ	CAS-CAT	-4.74	1.39	1.50
4	B	1101	4BJ	OBJ-CBE	-4.04	1.30	1.37
4	B	1102	4BJ	CAA-CAF	-3.45	1.33	1.40
4	B	1102	4BJ	CAD-CAE	-3.44	1.33	1.40
4	B	1101	4BJ	CAS-CAT	-3.16	1.43	1.50
4	B	1101	4BJ	CAH-NAI	-2.88	1.28	1.35
4	B	1101	4BJ	CAD-CAE	-2.87	1.35	1.40
4	B	1101	4BJ	OBI-CBL	2.41	1.50	1.42
4	B	1101	4BJ	CAC-NAK	-2.18	1.39	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101	4BJ	CAM-CAL	-2.06	1.35	1.38
4	B	1101	4BJ	OBI-CBF	-2.01	1.34	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1102	4BJ	OBB-SAZ-OBA	-8.20	109.47	119.55
4	B	1101	4BJ	CBD-CBC-SAZ	-6.91	111.34	119.08
4	B	1102	4BJ	CBK-OBJ-CBE	-5.31	109.52	117.53
4	B	1102	4BJ	CBL-OBI-CBF	-5.30	109.53	117.53
4	B	1101	4BJ	CAD-CAC-CAB	-4.72	112.92	118.94
4	B	1101	4BJ	CAA-CAB-CAC	4.64	126.12	120.53
4	B	1101	4BJ	CBH-CBC-SAZ	4.46	124.62	119.77
4	B	1101	4BJ	OBA-SAZ-CBC	-3.90	103.16	107.97
4	B	1101	4BJ	CAN-CAM-CAL	3.79	124.18	118.48
4	B	1102	4BJ	CAB-OAJ-CAL	-3.38	109.57	118.00
4	B	1102	4BJ	CAS-OAR-CAN	-3.29	109.53	117.65
4	B	1101	4BJ	CBL-OBI-CBF	-2.96	113.07	117.53
4	B	1101	4BJ	CAC-CAD-CAE	2.65	123.61	121.32
4	B	1101	4BJ	CAD-CAC-NAK	2.63	126.51	120.74
4	B	1101	4BJ	CAA-CAF-CAE	-2.49	115.66	121.48
4	B	1101	4BJ	OAJ-CAL-CAM	2.48	126.87	119.10
4	B	1101	4BJ	CBH-CBC-CBD	2.45	123.63	120.62
4	B	1101	4BJ	CAS-OAR-CAN	2.33	123.39	117.65
4	B	1102	4BJ	CAC-CAD-CAE	-2.27	119.36	121.32
4	B	1101	4BJ	CBG-CBH-CBC	-2.17	117.20	119.45
4	B	1102	4BJ	CBC-SAZ-NAK	2.11	109.48	106.83
4	B	1101	4BJ	CAY-CAT-CAU	2.10	121.47	118.17

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1107	GOL	O1-C1-C2-C3
3	A	1103	GOL	C1-C2-C3-O3
4	B	1102	4BJ	CBE-CBF-OBI-CBL
4	B	1102	4BJ	CBG-CBF-OBI-CBL
4	B	1102	4BJ	CAO-CAN-OAR-CAS
4	B	1102	4BJ	CAM-CAN-OAR-CAS
3	B	1106	GOL	C1-C2-C3-O3
3	A	1104	GOL	C1-C2-C3-O3
3	A	1103	GOL	O1-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	1107	GOL	O1-C1-C2-O2
3	A	1103	GOL	O2-C2-C3-O3
4	B	1102	4BJ	CBF-CBE-OBJ-CBK
3	B	1106	GOL	O2-C2-C3-O3
3	A	1103	GOL	O1-C1-C2-O2

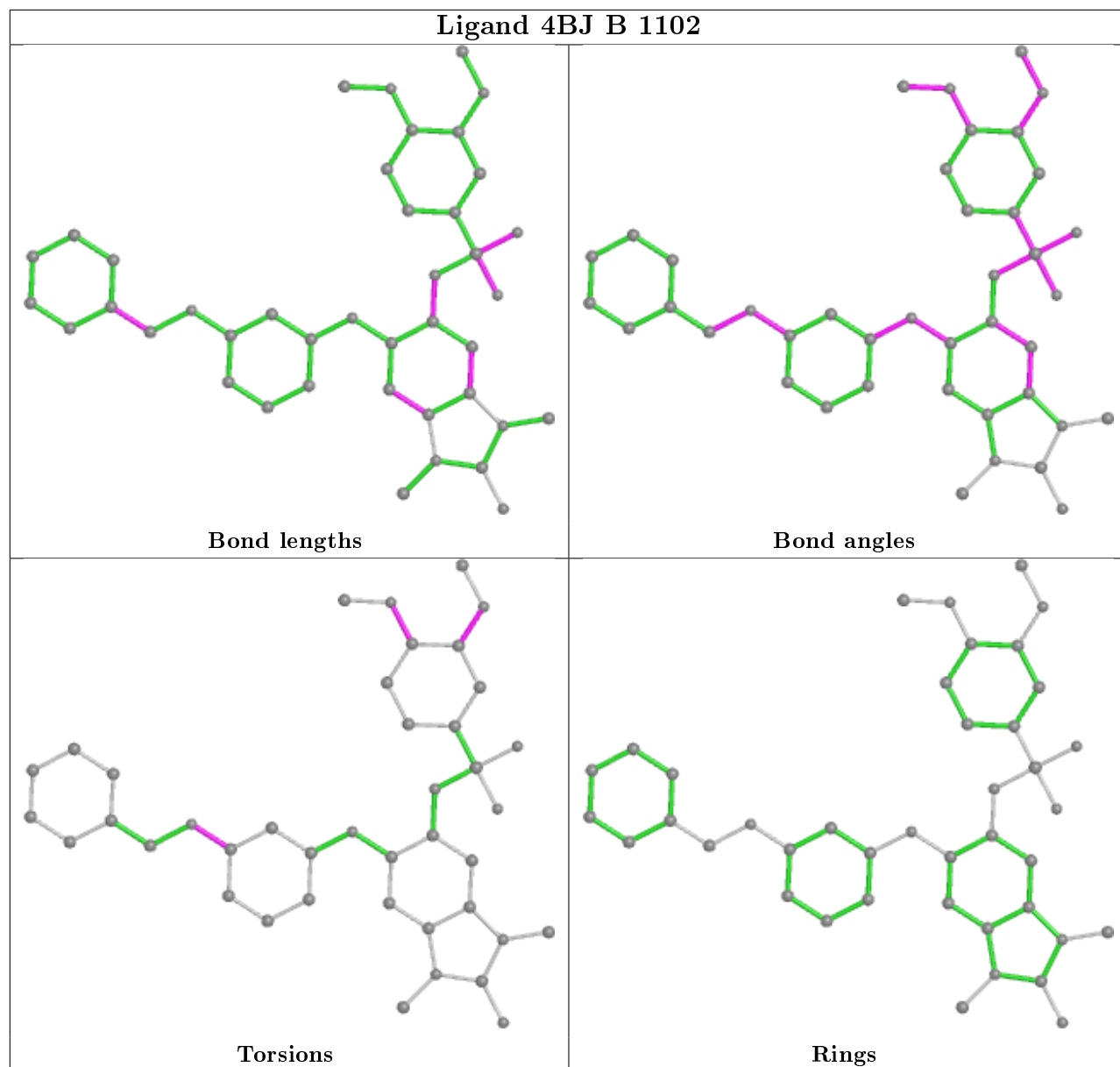
There are no ring outliers.

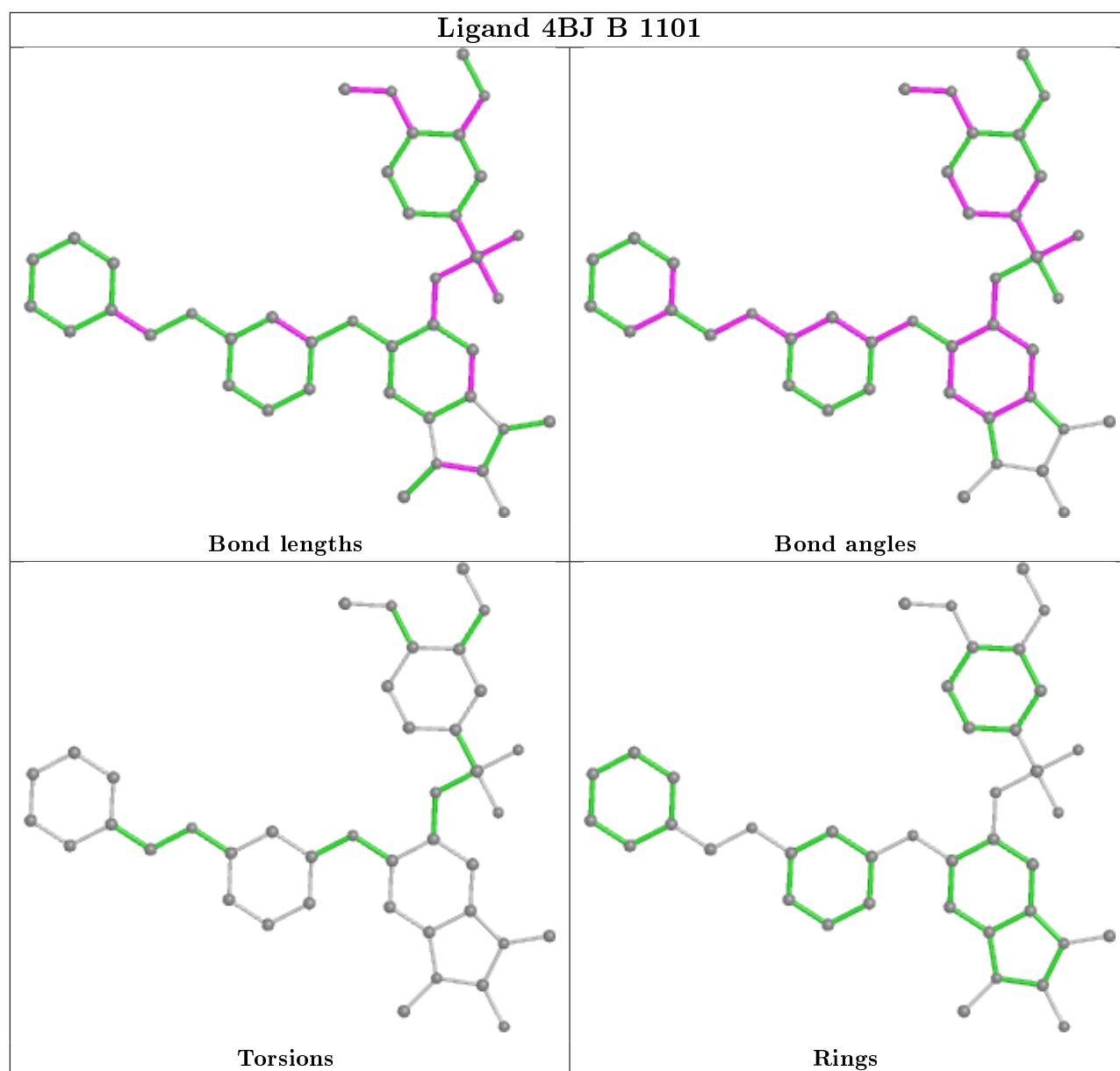
3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1102	4BJ	5	0
3	A	1104	GOL	11	0
4	B	1101	4BJ	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, 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	177/184 (96%)	-0.04	5 (2%) 53 55	14, 21, 38, 74	0
1	B	170/184 (92%)	0.06	9 (5%) 26 29	15, 24, 48, 79	0
All	All	347/368 (94%)	0.01	14 (4%) 38 40	14, 23, 45, 79	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	885	PRO	5.8
1	B	1006	PRO	4.2
1	B	862	SER	4.1
1	B	825	ASN	4.0
1	A	824	PRO	3.3
1	A	884	ALA	3.2
1	B	828	TRP	3.0
1	B	898	VAL	2.8
1	B	912	LEU	2.7
1	B	885	PRO	2.5
1	B	1003[A]	ASN	2.4
1	A	956	TYR	2.4
1	B	860	PHE	2.1
1	A	825	ASN	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

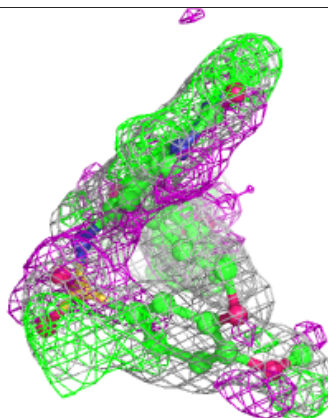
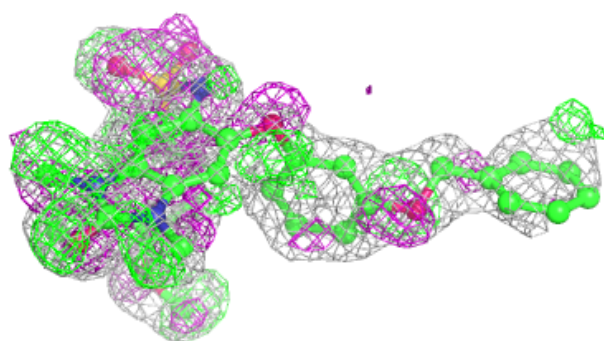
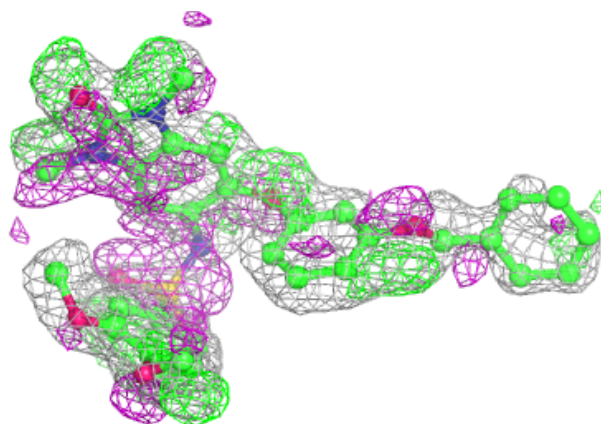
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	GOL	A	1104	6/6	0.55	0.59	20,20,20,20	0
3	GOL	B	1107	6/6	0.67	0.20	54,55,65,65	0
4	4BJ	B	1102	41/41	0.76	0.19	14,21,46,55	0
3	GOL	A	1103	6/6	0.78	0.21	46,50,56,59	0
3	GOL	B	1106	6/6	0.82	0.19	68,72,77,89	0
5	SO4	B	1103	5/5	0.83	0.35	99,102,107,117	0
5	SO4	B	1108	5/5	0.95	0.17	46,50,56,59	0
4	4BJ	B	1101	41/41	0.95	0.10	12,17,27,40	0
2	ZN	B	1105	1/1	0.97	0.04	25,25,25,25	0
2	ZN	A	1102	1/1	0.99	0.04	20,20,20,20	0
2	ZN	A	1101	1/1	1.00	0.04	17,17,17,17	0
2	ZN	B	1104	1/1	1.00	0.04	19,19,19,19	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.

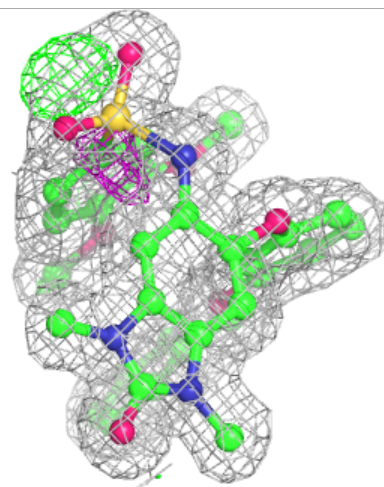
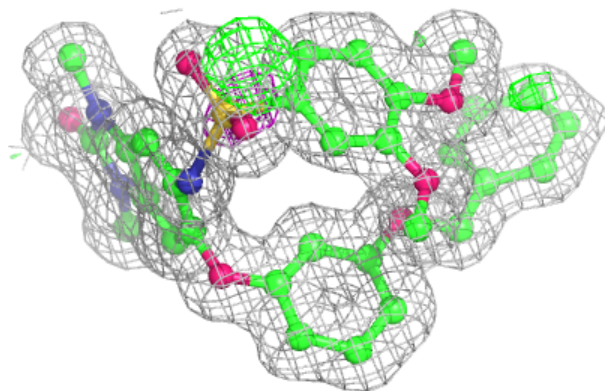
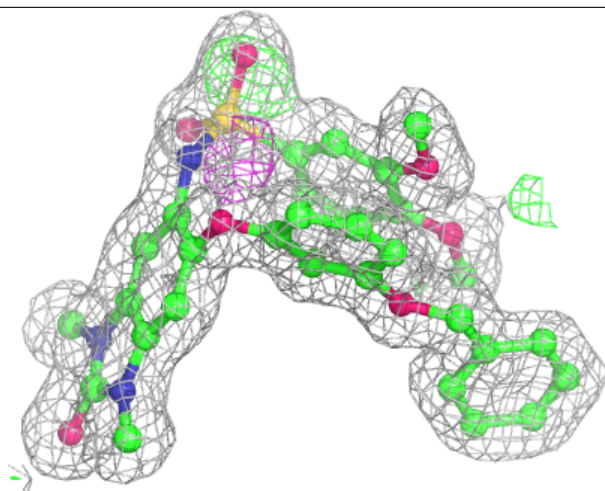
**Electron density around 4BJ B 1102:**

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



**Electron density around 4BJ B 1101:**

$2mF_o-DF_c$  (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.