



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:54 PM UTC

PDB ID : 1JS9 / pdb\_00001js9  
Title : Brome Mosaic Virus  
Authors : Lucas, R.W.; Larson, S.B.; McPherson, A.  
Deposited on : 2001-08-16  
Resolution : 3.40 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](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 ⓘ](#)) 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

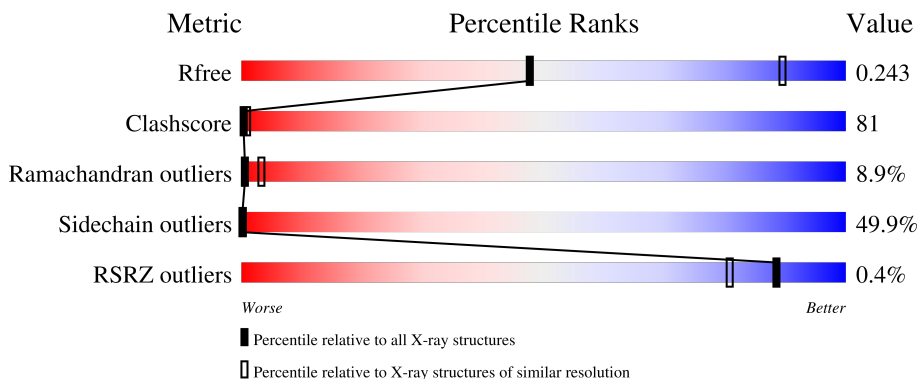
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	189	
1	B	189	
1	C	189	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3762 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.

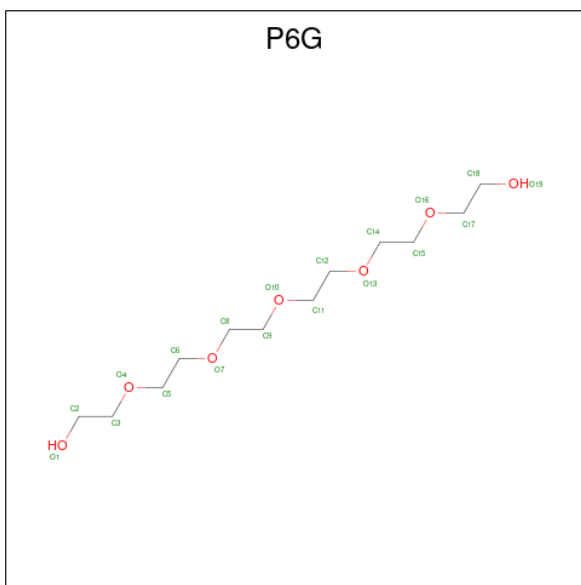
- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	149	Total 1133	C 728	N 190	O 212	S 3	8	0	0
1	B	165	Total 1245	C 799	N 211	O 232	S 3	4	0	0
1	C	189	Total 1363	C 869	N 235	O 256	S 3	4	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).

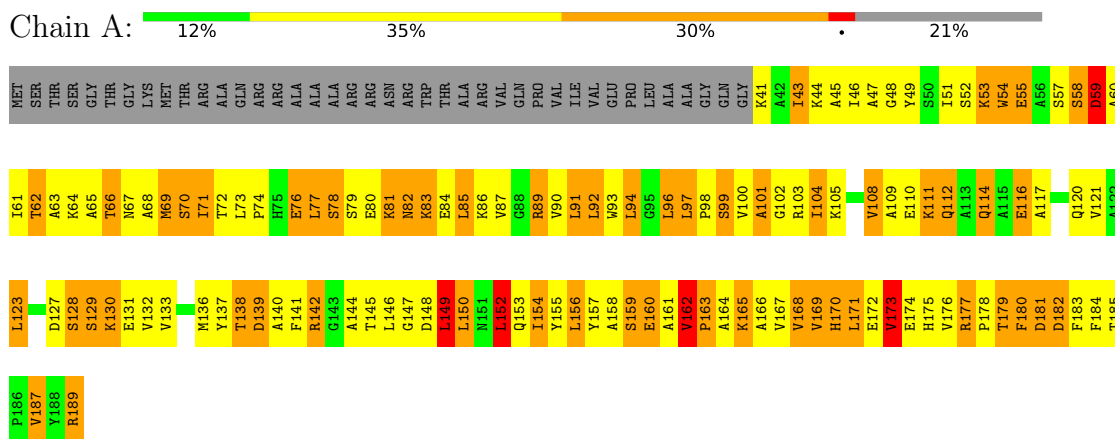


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	19	12	7	0	0

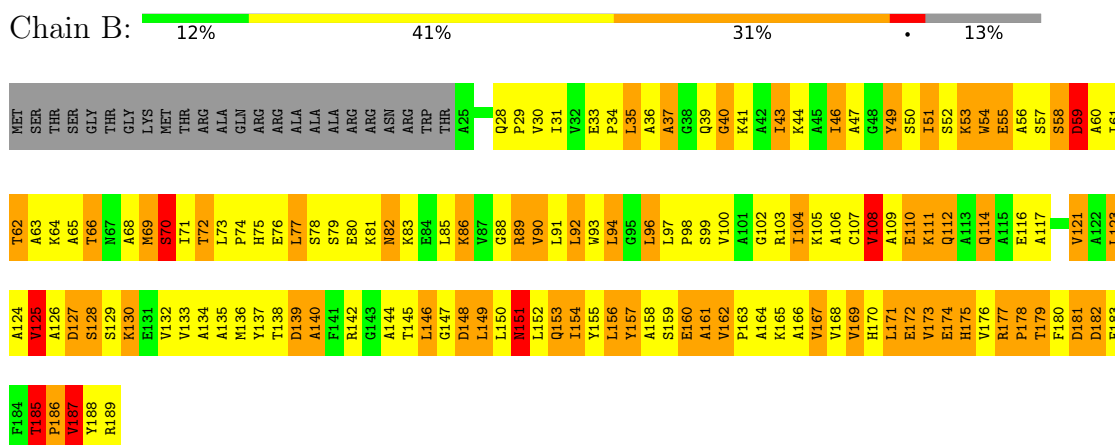
### 3 Residue-property plots [i](#)

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.

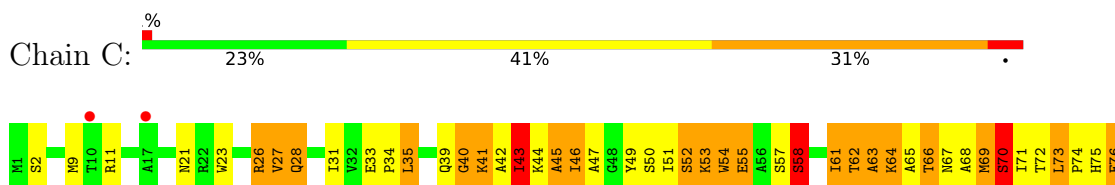
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



L77	A140
S78	F141
S79	R142
E80	G143
K81	A144
N82	T145
K83	L146
E84	G147
L85	D148
K86	L149
V87	L150
G88	M151
R89	L152
V90	Q153
L91	I154
L92	Y155
W93	L156
L94	Y157
G95	A158
L96	S159
L97	E160
P98	A161
S99	V162
V100	P163
	A164
R103	K165
I104	A166
K105	V167
A106	V168
C107	V169
V108	H170
A109	L171
E110	E172
K111	V173
Q112	E174
A113	H175
Q114	V176
A115	R177
E116	P178
A117	T179
	F180
Q120	D181
V121	D182
A122	F183
L123	F184
A124	T185
V125	P186
A126	V187
D127	Y188
S128	R189
S129	
K130	
	V133
	A134
	A135
	M136
	Y137
	T138
	D139

## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	269.24Å 269.24Å 638.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.70 – 3.40 39.70 – 3.40	Depositor EDS
% Data completeness (in resolution range)	50.3 (39.70-3.40) 69.2 (39.70-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.59 (at 3.40Å)	Xtriage
Refinement program	X-PLOR 3.851, CNS 1.1	Depositor
R, $R_{free}$	0.238 , 0.250 0.231 , 0.243	Depositor DCC
$R_{free}$ test set	5118 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 535.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.007 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.009 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l 0.005 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3* k-1/3*l 0.008 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k- 1/3*l,4/3*h-4/3*k-1/3*l 0.006 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3 *k-1/3*l 0.019 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.42	EDS
Total number of atoms	3762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: P6G, MG

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	0.53	0/1154	1.06	9/1566 (0.6%)
1	B	0.49	0/1268	1.02	8/1723 (0.5%)
1	C	0.49	0/1386	1.06	9/1887 (0.5%)
All	All	0.50	0/3808	1.04	26/5176 (0.5%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	27	VAL	N-CA-C	11.42	123.11	110.21
1	A	71	ILE	N-CA-C	8.04	119.51	108.89
1	A	162	VAL	CA-C-N	7.61	129.36	119.84
1	A	162	VAL	C-N-CA	7.61	129.36	119.84
1	B	59	ASP	N-CA-C	-7.36	98.25	109.95

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	1133	0	1159	189	0
1	B	1245	0	1278	222	0
1	C	1363	0	1343	207	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	B	19	0	26	0	0
All	All	3762	0	3806	609	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 81.

The worst 5 of 609 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:123:LEU:HD22	1:A:123:LEU:H	1.16	1.05
1:B:85:LEU:HB3	1:B:86:LYS:HZ1	1.23	1.03
1:B:53:LYS:HG2	1:B:172:GLU:HG3	1.38	1.01
1:B:35:LEU:HD12	1:B:35:LEU:H	1.22	1.00
1:C:69:MET:HG3	1:C:154:ILE:HD11	1.43	1.00

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	147/189 (78%)	108 (74%)	28 (19%)	11 (8%)	<b>1</b> <b>5</b>
1	B	163/189 (86%)	117 (72%)	30 (18%)	16 (10%)	<b>0</b> <b>3</b>
1	C	187/189 (99%)	126 (67%)	44 (24%)	17 (9%)	<b>0</b> <b>3</b>
All	All	497/567 (88%)	351 (71%)	102 (20%)	44 (9%)	<b>0</b> <b>3</b>

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ALA
1	A	111	LYS
1	A	139	ASP
1	A	181	ASP
1	B	111	LYS

### 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	117/146 (80%)	58 (50%)	59 (50%)	0	0
1	B	128/146 (88%)	66 (52%)	62 (48%)	0	0
1	C	128/146 (88%)	63 (49%)	65 (51%)	0	0
All	All	373/438 (85%)	187 (50%)	186 (50%)	0	0

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	177	ARG
1	C	90	VAL
1	B	185	THR
1	C	58	SER
1	C	103	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	67	ASN
1	C	82	ASN
1	C	153	GLN
1	A	153	GLN
1	B	28	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
3	P6G	B	2001	-	18,18,18	0.73	0	17,17,17	0.78	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
3	P6G	B	2001	-	-	4/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

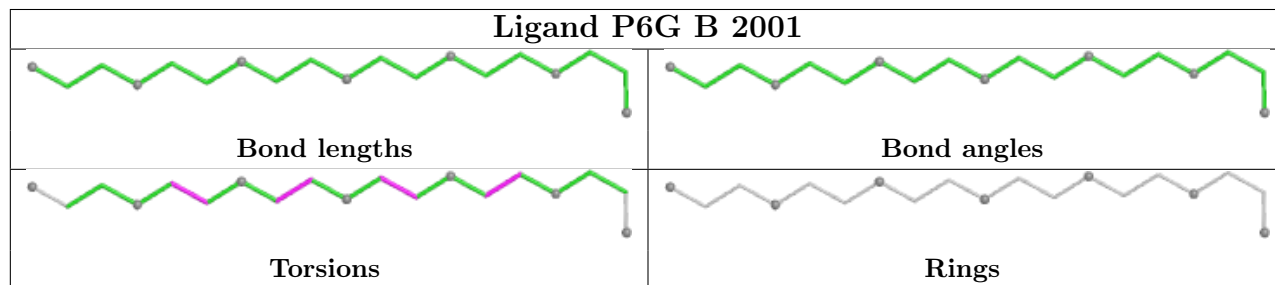
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	P6G	O7-C8-C9-O10
3	B	2001	P6G	O10-C11-C12-O13
3	B	2001	P6G	O4-C5-C6-O7
3	B	2001	P6G	O13-C14-C15-O16

There are no ring outliers.

No monomer is involved in short contacts.

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	149/189 (78%)	-1.25	0 <a href="#">100</a> <a href="#">100</a>	35, 95, 153, 221	2 (1%)
1	B	165/189 (87%)	-1.25	0 <a href="#">100</a> <a href="#">100</a>	31, 93, 172, 274	1 (0%)
1	C	189/189 (100%)	-1.05	2 (1%) <a href="#">78</a> <a href="#">65</a>	32, 88, 156, 234	26 (13%)
All	All	503/567 (88%)	-1.17	2 (0%) <a href="#">88</a> <a href="#">81</a>	31, 92, 163, 274	29 (5%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	10	THR	4.4
1	C	17	ALA	2.7

### 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.

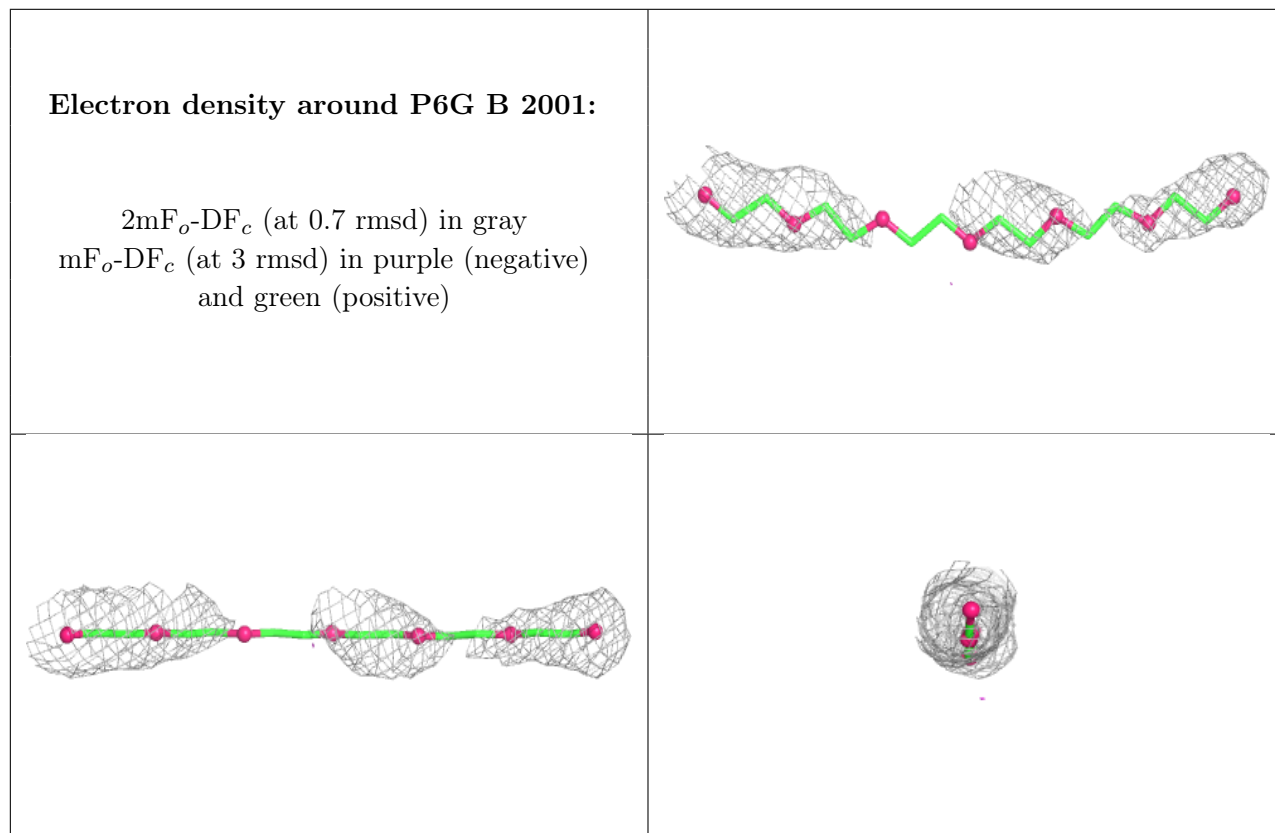
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	1002	1/1	0.96	0.12	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	P6G	B	2001	19/19	0.98	0.10	19,55,101,114	19
2	MG	C	1001	1/1	0.99	0.11	58,58,58,58	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 [i](#)

There are no such residues in this entry.