

Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 02:05 am BST

PDB ID : 5LHB

Title : POLYADPRIBOSYL GLYCOSIDASE IN COMPLEX WITH PDD00017262

Authors : Tucker, J.; Barkauskaite, E.

Deposited on : 2016-07-10

Resolution : 2.23 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

Mol Probity : 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)

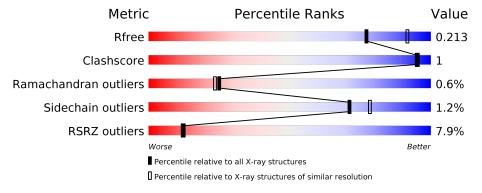
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.23 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar resolution} \\ (\#{\rm Entries, resolution range(\AA)}) \end{array}$
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 >=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 <=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	
			8%	
1	A	531	91%	5% •



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4486 atoms, of which 24 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 Poly(ADP-ribose) glycohydrolase.

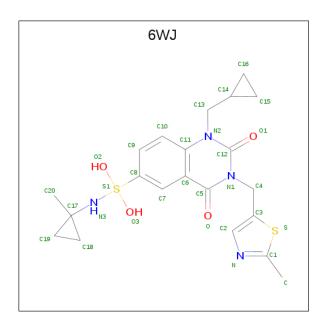
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	508	Total 4104	C 2624	N 706	O 748	S 26	0	8	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	GLY	-	expression tag	UNP Q86W56
A	447	SER	-	expression tag	UNP Q86W56
A	616	ALA	LYS	engineered mutation	UNP Q86W56
A	617	ALA	GLN	engineered mutation	UNP Q86W56
A	618	ALA	LYS	engineered mutation	UNP Q86W56
A	681	6WK	CYS	modified residue	UNP Q86W56
A	688	ALA	GLU	engineered mutation	UNP Q86W56
A	689	ALA	LYS	engineered mutation	UNP Q86W56
A	690	ALA	LYS	engineered mutation	UNP Q86W56

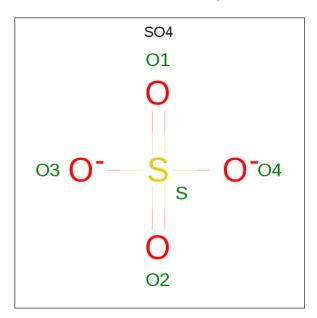
• Molecule 2 is 1-(cyclopropylmethyl)-6-[[(1-methylcyclopropyl)amino]-bis(oxidanyl)-\$l^{4}-s ulfanyl]-3-[(2-methyl-1,3-thiazol-5-yl)methyl]quinazoline-2,4-dione (three-letter code: 6WJ) (formula: $C_{21}H_{26}N_4O_4S_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
9	Λ	1	Total	С	Н	N	О	S	24	0
	A	1	55	21	24	4	4	2	24	0

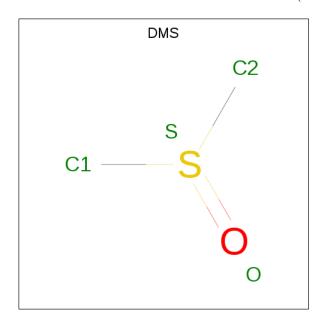
 \bullet Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



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



 \bullet Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: $\mathrm{C_2H_6OS}).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total C C 4 2 1		0	0
4	A	1	Total C C 4 2 1		0	0
4	A	1	Total C C 4 2 1) S 1	0	0

• Molecule 5 is water.

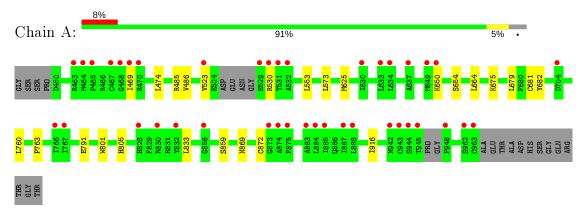
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	300	Total O 300 300	0	1



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: Poly(ADP-ribose) glycohydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	67.01Å 89.73Å 95.44Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.61 - 2.23	Depositor
Resolution (A)	27.42 - 2.23	EDS
% Data completeness	99.4 (27.61-2.23)	Depositor
(in resolution range)	99.4 (27.42-2.23)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.90 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
P. P.	0.162 , 0.211	Depositor
R, R_{free}	0.161 , 0.213	DCC
R_{free} test set	1444 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 56.1	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4486	wwPDB-VP
Average B, all atoms $(Å^2)$	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: DMS, SO4, 6WJ, 6WK

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).

Mal	Chain	Bond	lengths	Bond angles		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.51	0/4189	0.63	0/5686	

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 (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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	4104	0	3935	10	0
2	A	31	24	0	0	0
3	A	15	0	0	0	0
4	A	12	0	18	1	0
5	A	300	0	0	0	0
All	All	4462	24	3953	10	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 1.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance} ({ m \AA})$	$ \text{overlap } (\text{\AA})$
1:A:553:LEU:HD23	1:A:573:LEU:HD21	1.88	0.55
1:A:681:6WK:SD	1:A:801:TRP:HZ2	2.29	0.54
1:A:474:LEU:O	1:A:486:VAL:HG11	2.08	0.53
1:A:485:ARG:HA	4:A:1005:DMS:O	2.11	0.51
1:A:791:GLU:HG3	1:A:805:HIS:HB2	1.93	0.51
1:A:682:TYR:HB2	1:A:763:PRO:HG2	1.95	0.49
1:A:625:MET:HB2	1:A:625:MET:HE2	1.84	0.45
1:A:650:LYS:O	1:A:654:SER:HB3	2.18	0.43
1:A:664[A]:LEU:HD21	1:A:679:LEU:HD12	2.03	0.40
1:A:675:LYS:HG2	1:A:760:LEU:HD11	2.04	0.40

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	509/531 (96%)	493 (97%)	13 (3%)	3 (1%)	25 23	3

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	869	ASN
1	A	530	ARG
1	A	469	ILE

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	Analysed Rotameric		Percentiles	
1	A	423/461 (92%)	418 (99%)	5 (1%)	71 78	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	523	VAL
1	A	833	LEU
1	A	859	SER
1	A	872	CYS
1	A	916	ILE

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	Dog	s Link	Bond lengths			\mid B	ond ang	gles
MIOI	Туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	6WK	A	681	1	11,13,14	0.35	0	7,15,17	1.05	1 (14%)

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
1	6WK	A	681	1	-	6/12/15/17	_



There are no bond length outliers.

All (1) bond angle outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	A	681	6WK	C2-C1-S3	2.06	120.45	114.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	681	6WK	S3-C1-C2-O4
1	A	681	6WK	S3-C1-C2-C3
1	A	681	6WK	C2-C3-C4-SD
1	A	681	6WK	O3-C3-C4-SD
1	A	681	6WK	C4-SD-SG-CB
1	A	681	6WK	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	${f Res}$	Type	Clashes	Symm-Clashes
1	A	681	6WK	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 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	Туре	Chain	Chain	Chain	Chain	Res	T in le	Bo	ond leng	$ ag{ths}$	В	ond ang	les
MIOI	туре		nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2			
4	DMS	A	1007	-	3,3,3	0.53	0	3,3,3	0.27	0			
4	DMS	A	1006	-	3,3,3	0.27	0	3,3,3	0.52	0			



Mol	Mol Type		${ m Res}$	Link	Bo	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	1004	_	4,4,4	0.19	0	6,6,6	0.11	0
4	DMS	A	1005	-	3,3,3	0.71	0	3,3,3	0.58	0
3	SO4	A	1003	-	4,4,4	0.38	0	6,6,6	0.53	0
2	6WJ	A	1001	-	26,35,35	1.54	4 (15%)	28,55,55	1.11	3 (10%)
3	SO4	A	1002	-	4,4,4	0.19	0	6,6,6	0.16	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	6WJ	A	1001	-	=	1/10/26/26	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	A	1001	6WJ	C13-N2	4.95	1.53	1.48
2	A	1001	6WJ	C5-C6	3.27	1.47	1.41
2	A	1001	6WJ	C11-N2	2.46	1.43	1.40
2	A	1001	6WJ	C2-N	2.23	1.39	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
2	A	1001	6WJ	C2-C3-S	-3.11	108.90	112.00
2	A	1001	6WJ	C10-C11-N2	2.11	123.43	121.36
2	A	1001	6WJ	C-C1-N	2.06	127.27	121.87

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	6WJ	N2-C13-C14-C16

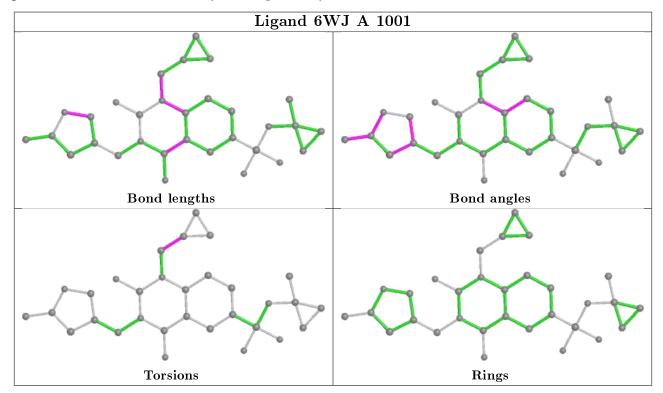
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	${f Res}$	Type	Clashes	Symm-Clashes
4	A	1005	DMS	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 then 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^{th} 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	$\langle { m RSRZ} \rangle$	#RSR	$Z{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	507/531 (95%)	0.03	40 (7%) 1	2 12	24, 40, 73, 125	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	874	ALA	6.9
1	A	468	GLY	6.5
1	A	530	ARG	6.1
1	A	943	CYS	4.8
1	A	464	MET	4.7
1	A	529	GLU	4.4
1	A	873	GLY	4.3
1	A	875	PHE	4.3
1	A	856	GLY	4.2
1	A	944	SER	4.2
1	A	467	CYS	4.1
1	A	469	ILE	3.9
1	A	704	ASP	3.7
1	A	945	THR	3.6
1	A	884	LEU	3.5
1	A	465	PRO	3.4
1	A	885	ILE	3.2
1	A	649	MET	3.1
1	A	887	ILE	3.1
1	A	634	LEU	3.1
1	A	963	CYS	3.0
1	A	531	THR	3.0
1	A	828	HIS	3.0
1	A	948	PRO	2.9
1	A	830	ARG	2.9
1	A	942	ASN	2.8
1	A	637	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	962	SER	2.6
1	A	470	ARG	2.5
1	A	832	TYR	2.5
1	A	463	ARG	2.5
1	A	883	ALA	2.4
1	A	767	ILE	2.4
1	A	633	LEU	2.2
1	A	630	ILE	2.2
1	A	532	ALA	2.2
1	A	650	LYS	2.1
1	A	888	LEU	2.1
1	A	766	ILE	2.0
1	A	523	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
1	6WK	A	681	14/15	0.87	0.19	26,66,81,85	0

6.3 Carbohydrates (i)

There are no carbohydrates 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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	SO4	A	1004	5/5	0.77	0.29	109,109,109,111	0
3	SO4	A	1002	5/5	0.79	0.31	128,128,128,128	0
4	DMS	A	1005	4/4	0.90	0.26	66,69,69,71	0
4	DMS	A	1006	4/4	0.94	0.21	72,74,75,77	0

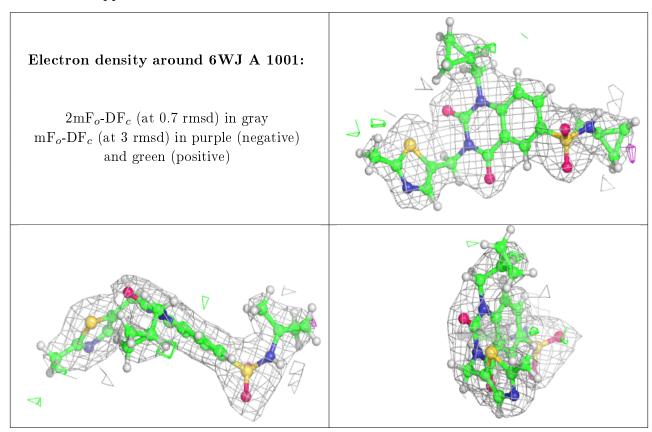
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$ extbf{B-factors}(extbf{A}^2)$	Q < 0.9
4	DMS	A	1007	4/4	0.95	0.31	$75,\!76,\!76,\!76$	0
3	SO4	A	1003	5/5	0.96	0.12	53,56,59,63	0
2	6WJ	A	1001	31/31	0.97	0.09	28,34,45,45	24

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.

