



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 10:44 AM UTC

PDB ID : 1AQV / pdb_00001aqv
Title : GLUTATHIONE S-TRANSFERASE IN COMPLEX WITH P-BROMOBENZYLGLUTATHIONE
Authors : Prade, L.; Huber, R.; Manoharan, T.H.; Fahl, W.E.; Reuter, W.
Deposited on : 1997-08-01
Resolution : 1.94 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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 1.94 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

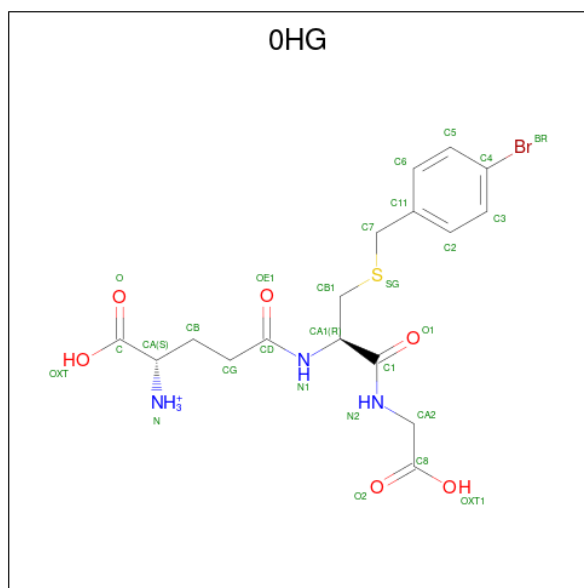
There are 4 unique types of molecules in this entry. The entry contains 4817 atoms, of which 1214 are hydrogens and 0 are deuteriums.

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 GLUTATHIONE S-TRANSFERASE.

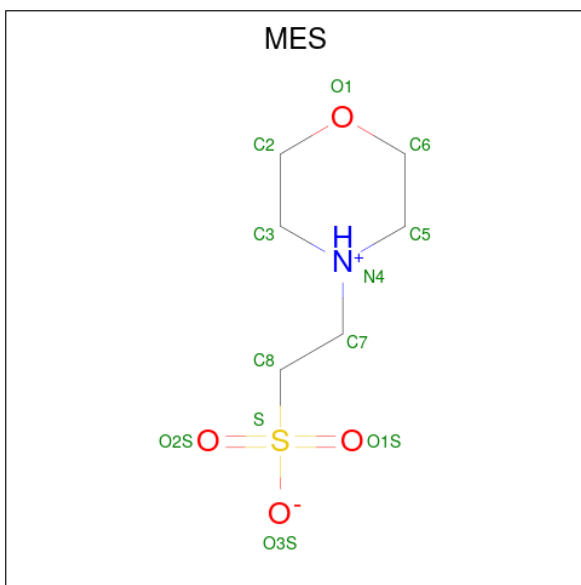
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	209	Total	C	H	N	O	S	0	0	0
			1993	1052	355	272	308	6			
1	B	209	Total	C	H	N	O	S	0	0	0
			1993	1052	355	272	308	6			

- Molecule 2 is N-[(4S)-4-ammonio-4-carboxybutanoyl]-S-(4-bromobenzyl)-L-cysteinylglycine (CCD ID: 0HG) (formula: $C_{17}H_{23}BrN_3O_6S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	H	N	O	S	0
			33	1	17	5	3	6	1	
2	B	1	Total	Br	C	H	N	O	S	0
			33	1	17	5	3	6	1	

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	113	Total	H	O	0	0
			339	226	113		
4	B	134	Total	H	O	0	0
			402	268	134		

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.66 Å 90.07 Å 69.57 Å 90.00° 99.19° 90.00°	Depositor
Resolution (Å)	7.00 – 1.94	Depositor
% Data completeness (in resolution range)	93.0 (7.00-1.94)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.5	Depositor
R, R_{free}	0.194 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4817	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

4 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MES	B	2400	-	12,12,12	2.73	3 (25%)	15,16,16	1.56	4 (26%)
2	OHG	B	2101	-	27,28,28	1.28	2 (7%)	33,36,36	0.90	2 (6%)
2	OHG	A	2201	-	27,28,28	1.29	3 (11%)	33,36,36	0.98	3 (9%)
3	MES	A	2300	-	12,12,12	2.73	3 (25%)	15,16,16	1.55	4 (26%)

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	MES	B	2400	-	-	5/6/14/14	0/1/1/1
2	OHG	B	2101	-	-	0/28/28/28	0/1/1/1
2	OHG	A	2201	-	-	0/28/28/28	0/1/1/1
3	MES	A	2300	-	-	4/6/14/14	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2300	MES	O3S-S	5.47	1.67	1.47
3	B	2400	MES	O3S-S	5.46	1.67	1.47
3	A	2300	MES	O2S-S	4.93	1.59	1.45
3	B	2400	MES	O2S-S	4.90	1.58	1.45
3	B	2400	MES	O1S-S	4.83	1.58	1.45
3	A	2300	MES	O1S-S	4.81	1.58	1.45
2	A	2201	OHG	C7-C11	-4.26	1.41	1.51
2	B	2101	OHG	C7-C11	-3.97	1.42	1.51
2	B	2101	OHG	C7-SG	-3.05	1.76	1.82
2	A	2201	OHG	CB1-CA1	2.18	1.58	1.53
2	A	2201	OHG	C7-SG	-2.16	1.78	1.82

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2201	OHG	CB1-CA1-C1	-3.15	102.34	109.46
3	A	2300	MES	O2S-S-C8	2.78	110.93	106.73
3	B	2400	MES	O2S-S-C8	2.75	110.89	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2101	0HG	CB1-CA1-C1	-2.69	103.39	109.46
2	A	2201	0HG	BR-C4-C3	2.48	122.68	119.30
3	B	2400	MES	O3S-S-C8	2.44	110.79	106.00
3	A	2300	MES	O3S-S-C8	2.41	110.71	106.00
3	B	2400	MES	O1S-S-C8	2.38	110.33	106.73
3	A	2300	MES	O1S-S-C8	2.37	110.30	106.73
3	A	2300	MES	C5-N4-C3	2.06	113.28	108.84
2	B	2101	0HG	BR-C4-C3	2.03	122.07	119.30
3	B	2400	MES	C5-N4-C3	2.03	113.22	108.84
2	A	2201	0HG	C5-C4-C3	-2.03	118.26	121.33

There are no chirality outliers.

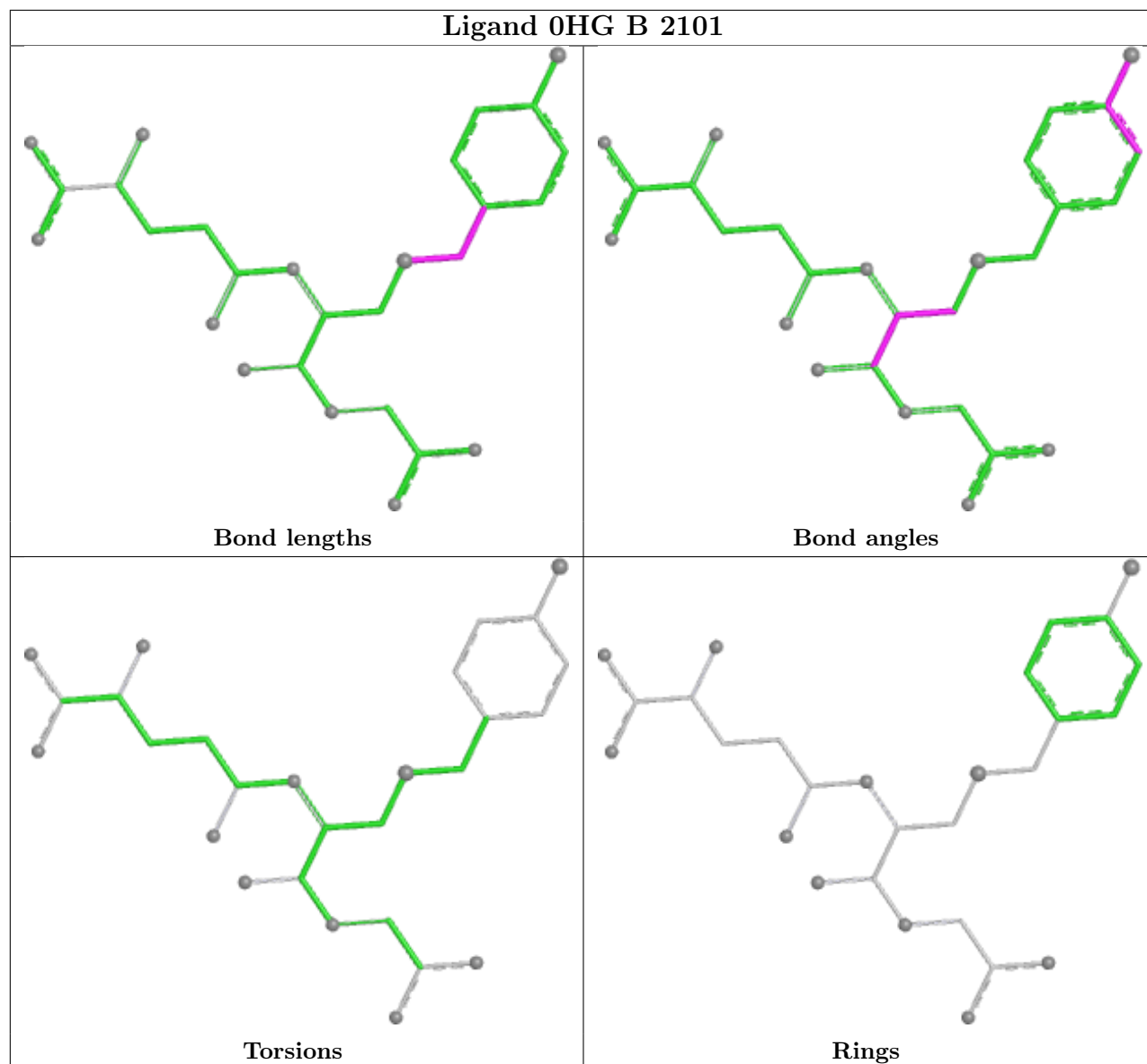
All (9) torsion outliers are listed below:

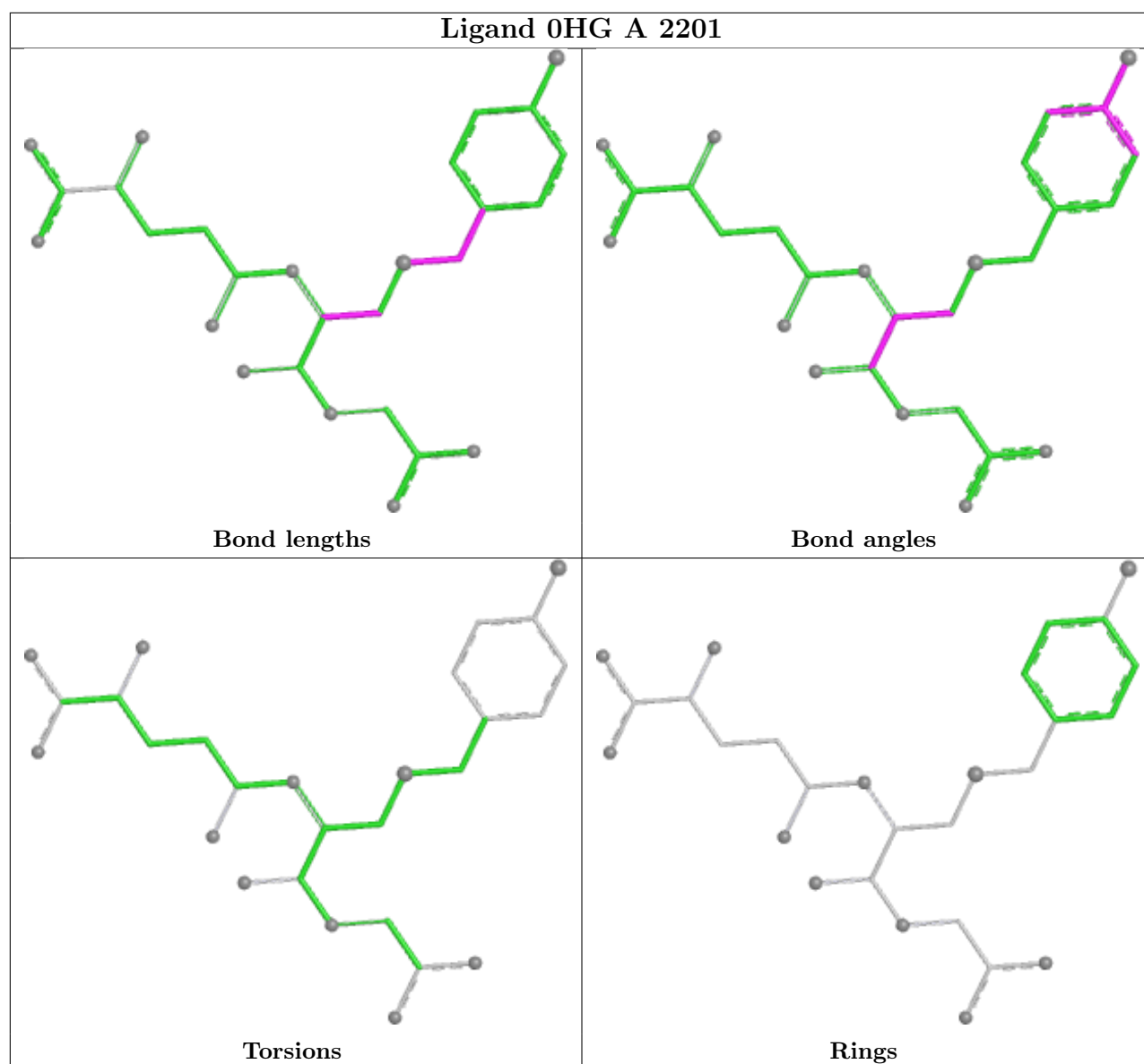
Mol	Chain	Res	Type	Atoms
3	A	2300	MES	C7-C8-S-O2S
3	B	2400	MES	C7-C8-S-O2S
3	B	2400	MES	C7-C8-S-O3S
3	A	2300	MES	C7-C8-S-O3S
3	A	2300	MES	C8-C7-N4-C5
3	B	2400	MES	C8-C7-N4-C5
3	A	2300	MES	C7-C8-S-O1S
3	B	2400	MES	C7-C8-S-O1S
3	B	2400	MES	C8-C7-N4-C3

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.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.