



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:53 am BST

PDB ID : 5OET  
Title : The structure of a glutathione synthetase like-effector (GSS30) from *Globodera pallida* in apoform.  
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Deposited on : 2017-07-10  
Resolution : 2.57 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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

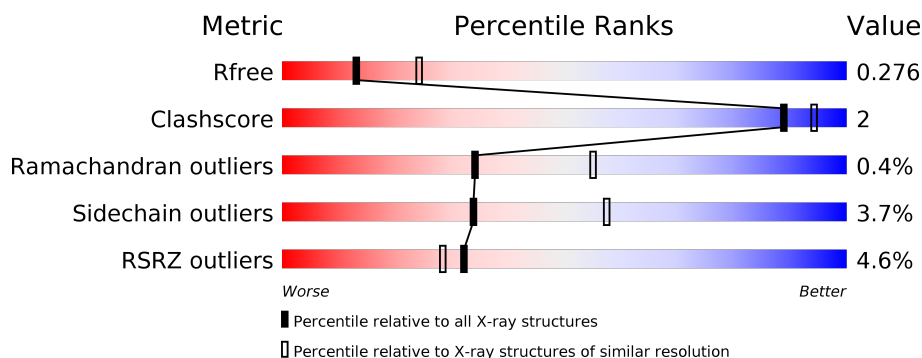
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	525	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>6%</div> <div>22%</div> </div> </div>
1	B	525	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>6%</div> <div>20%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6705 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 Glutathione synthetase-like effector 30 (Gpa-GSS30-apo).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	420	Total	C	N	O	S	0	0	0
			3377	2166	576	609	26			
1	A	411	Total	C	N	O	S	0	0	0
			3316	2131	566	594	25			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

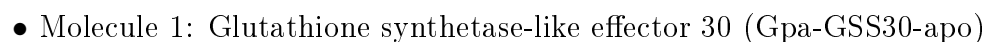
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	O	0	0
			2	2		
3	A	9	Total	O	0	0
			9	9		



- Molecule 1: Glutathione synthetase-like effector 30 (Gpa-GSS30-apo)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.75Å 81.62Å 93.84Å 90.00° 103.18° 90.00°	Depositor
Resolution (Å)	50.00 – 2.57 45.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.57) 99.7 (45.68-2.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.251 , 0.285 0.244 , 0.276	Depositor DCC
$R_{free}$ test set	1610 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1642e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 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	0.55	0/3385	0.75	1/4557 (0.0%)
1	B	0.55	0/3446	0.75	0/4640
All	All	0.55	0/6831	0.75	1/9197 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	NE-CZ-NH1	5.30	122.95	120.30

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	3316	0	3325	12	0
1	B	3377	0	3378	13	0
2	B	1	0	0	0	0
3	A	9	0	0	0	0
3	B	2	0	0	0	0
All	All	6705	0	6703	25	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 2.

All (25) 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:B:219:VAL:HG11	1:B:523:TYR:CE1	2.30	0.66
1:A:219:VAL:HG11	1:A:523:TYR:CE1	2.30	0.66
1:B:50:GLN:NE2	1:B:92:TYR:OH	2.37	0.57
1:A:50:GLN:NE2	1:A:92:TYR:OH	2.37	0.56
1:A:193:SER:N	1:A:261:GLU:OE1	2.39	0.53
1:A:107:VAL:HG22	1:A:376:ALA:HB1	1.91	0.52
1:B:193:SER:N	1:B:261:GLU:OE1	2.39	0.51
1:B:163:PHE:HD2	1:B:481:LEU:HD12	1.76	0.50
1:B:63:LEU:HD21	1:B:199:ARG:HB2	1.95	0.49
1:A:249:PHE:CE2	1:A:312:PHE:HD2	2.31	0.48
1:B:481:LEU:HD21	1:B:493:PHE:CE1	2.48	0.48
1:B:249:PHE:CE2	1:B:312:PHE:HD2	2.32	0.48
1:A:63:LEU:HD21	1:A:199:ARG:HB2	1.96	0.46
1:B:67:VAL:HG12	1:B:68:ASP:N	2.32	0.45
1:B:219:VAL:HG11	1:B:523:TYR:CZ	2.51	0.45
1:A:219:VAL:HG11	1:A:523:TYR:CZ	2.53	0.44
1:A:175:ASP:O	1:A:176:ASP:HB2	2.17	0.43
1:A:188:THR:HA	1:A:191:ILE:HD11	2.01	0.42
1:A:219:VAL:CG1	1:A:523:TYR:CE1	3.01	0.42
1:B:188:THR:HA	1:B:191:ILE:HD11	2.03	0.41
1:B:219:VAL:CG1	1:B:523:TYR:CE1	3.02	0.41
1:A:38:PRO:O	1:A:42:GLN:NE2	2.53	0.41
1:B:34:GLN:CD	1:B:525:VAL:HG13	2.41	0.41
1:B:162:MET:HA	1:B:482:LEU:HD12	2.02	0.40
1:A:162:MET:HA	1:A:482:LEU:HD12	2.03	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	391/525 (74%)	381 (97%)	9 (2%)	1 (0%)	41	62
1	B	400/525 (76%)	388 (97%)	10 (2%)	2 (0%)	29	50
All	All	791/1050 (75%)	769 (97%)	19 (2%)	3 (0%)	34	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	276	ARG
1	A	176	ASP
1	B	403	GLU

### 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	366/463 (79%)	350 (96%)	16 (4%)	28	51
1	B	372/463 (80%)	361 (97%)	11 (3%)	41	65
All	All	738/926 (80%)	711 (96%)	27 (4%)	34	57

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	CYS
1	B	42	GLN
1	B	55	LYS
1	B	170	MET
1	B	178	GLN
1	B	218	SER
1	B	292	LYS
1	B	313	ASP
1	B	349	LYS
1	B	412	ASN
1	B	518	VAL
1	A	36	CYS
1	A	42	GLN

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Mol	Chain	Res	Type
1	A	53	ASP
1	A	55	LYS
1	A	99	LYS
1	A	127	GLU
1	A	170	MET
1	A	175	ASP
1	A	176	ASP
1	A	178	GLN
1	A	218	SER
1	A	292	LYS
1	A	313	ASP
1	A	349	LYS
1	A	372	HIS
1	A	518	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	ASN
1	B	50	GLN
1	B	108	GLN
1	B	173	GLN
1	B	251	HIS
1	B	255	ASN
1	B	264	GLN
1	B	352	GLN
1	A	50	GLN
1	A	210	ASN
1	A	352	GLN

### 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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	411/525 (78%)	0.51	17 (4%)	37 33	35, 57, 79, 90	0
1	B	420/525 (80%)	0.60	21 (5%)	28 25	36, 54, 86, 107	0
All	All	831/1050 (79%)	0.56	38 (4%)	32 28	35, 56, 82, 107	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	ASP	4.9
1	B	177	GLY	4.7
1	A	442	PHE	4.1
1	A	145	VAL	3.7
1	B	436	ALA	3.4
1	A	188	THR	3.3
1	B	298	PHE	3.2
1	B	174	GLU	3.2
1	A	174	GLU	3.1
1	A	177	GLY	3.1
1	A	122	TYR	3.0
1	B	404	ASN	3.0
1	B	328	PHE	2.9
1	A	123	GLU	2.8
1	B	40	ILE	2.8
1	B	295	PRO	2.7
1	B	122	TYR	2.5
1	B	41	GLU	2.5
1	A	178	GLN	2.5
1	B	525	VAL	2.5
1	B	286	GLU	2.5
1	B	145	VAL	2.4
1	B	141	ILE	2.4
1	A	525	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	408	TYR	2.4
1	A	384	GLY	2.3
1	A	468	ASN	2.3
1	B	450	ARG	2.3
1	A	460	ARG	2.2
1	B	466	THR	2.2
1	A	146	LYS	2.2
1	B	213	ILE	2.2
1	B	324	MET	2.1
1	B	449	LEU	2.1
1	B	276	ARG	2.1
1	A	173	GLN	2.1
1	A	298	PHE	2.0
1	A	328	PHE	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 [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( $\text{\AA}^2$ )	Q<0.9
2	MG	B	601	1/1	0.98	0.29	15,15,15,15	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.