



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:33 PM UTC

PDB ID : 5OET / pdb_00005oet
Title : The structure of a glutathione synthetase like-effector (GSS30) from *Globodera pallida* in apoform.
Authors : Lilley, C.J.; Maqbool, A.; Wu, D.; Yusup, H.B.; Jones, L.M.; Birch, P.R.J.; Banfield, M.J.; Urwin, P.E.; Eves-van den Akker, S.
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

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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

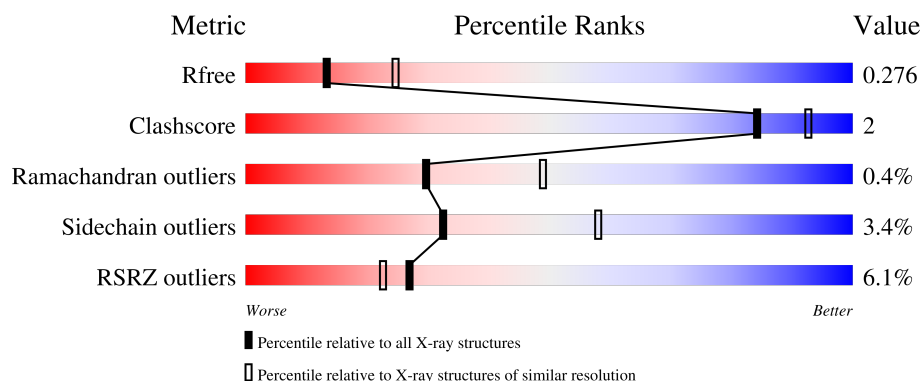
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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 of 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 $\leq 5\%$. 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	 4% 72% 6% 22%
1	B	525	 6% 72% 8% 20%

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			

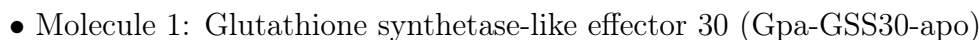
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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, α , β , γ	72.75Å 81.62Å 93.84Å 90.00° 103.18° 90.00°	Depositor
Resolution (Å)	50.00 – 2.57 50.00 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.57) 99.6 (50.00-2.57)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.73	0/3385	0.93	1/4557 (0.0%)
1	B	0.74	0/3446	0.94	1/4640 (0.0%)
All	All	0.74	0/6831	0.93	2/9197 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ASP	N-CA-C	6.71	118.68	111.36
1	A	275	GLU	N-CA-C	6.50	120.81	113.01

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	14	0
1	B	3377	0	3378	17	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	31	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 (31) 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:351:MET:HE3	1:B:354:VAL:HB	1.86	0.57
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:351:MET:HE3	1:A:354:VAL:HB	1.87	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:82:MET:HE3	1:B:255:ASN:HD22	1.76	0.49
1:B:63:LEU:HD21	1:B:199:ARG:HB2	1.95	0.49
1:B:481:LEU:HD21	1:B:493:PHE:CE1	2.48	0.48
1:A:249:PHE:CE2	1:A:312:PHE:HD2	2.31	0.48
1:B:82:MET:HE3	1:B:255:ASN:ND2	2.28	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:34:GLN:CD	1:B:525:VAL:HG13	2.41	0.45
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:162:MET:HE1	1:B:233:LEU:HG	2.02	0.41
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:A:162:MET:HE1	1:A:233:LEU:HG	2.03	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

5.3.1 Protein backbone

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%)	36	56
1	B	400/525 (76%)	388 (97%)	10 (2%)	2 (0%)	24	44
All	All	791/1050 (75%)	769 (97%)	19 (2%)	3 (0%)	30	49

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%)	352 (96%)	14 (4%)	29	54
1	B	372/463 (80%)	361 (97%)	11 (3%)	36	62
All	All	738/926 (80%)	713 (97%)	25 (3%)	32	58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	GLN
1	B	55	LYS
1	B	126	LYS

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Mol	Chain	Res	Type
1	B	170	MET
1	B	178	GLN
1	B	280	ARG
1	B	292	LYS
1	B	349	LYS
1	B	387	ILE
1	B	412	ASN
1	B	518	VAL
1	A	42	GLN
1	A	55	LYS
1	A	126	LYS
1	A	127	GLU
1	A	170	MET
1	A	175	ASP
1	A	176	ASP
1	A	178	GLN
1	A	280	ARG
1	A	292	LYS
1	A	349	LYS
1	A	372	HIS
1	A	409	VAL
1	A	518	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	ASN
1	B	45	GLN
1	B	50	GLN
1	B	102	GLN
1	B	173	GLN
1	B	251	HIS
1	B	255	ASN
1	B	264	GLN
1	B	352	GLN
1	B	462	ASN
1	A	39	ASN
1	A	50	GLN
1	A	102	GLN
1	A	108	GLN
1	A	165	GLN
1	A	187	ASN

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Mol	Chain	Res	Type
1	A	210	ASN
1	A	412	ASN
1	A	498	HIS

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 oligosaccharides 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, 95th 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 ²)	Q < 0.9
1	A	411/525 (78%)	0.44	19 (4%)	37 33	35, 57, 78, 90	0
1	B	420/525 (80%)	0.49	32 (7%)	20 16	36, 54, 86, 107	0
All	All	831/1050 (79%)	0.47	51 (6%)	27 22	35, 56, 82, 107	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	ASP	3.8
1	A	315	LEU	3.8
1	B	516	PHE	3.5
1	A	188	THR	3.5
1	A	189	GLY	3.5
1	B	402	THR	3.5
1	B	414	GLY	3.4
1	B	218	SER	3.4
1	B	315	LEU	3.2
1	B	324	MET	3.1
1	A	313	ASP	3.1
1	A	414	GLY	3.0
1	B	286	GLU	2.9
1	B	429	LEU	2.9
1	A	279	CYS	2.8
1	B	436	ALA	2.8
1	A	191	ILE	2.7
1	A	372	HIS	2.6
1	B	41	GLU	2.5
1	A	145	VAL	2.5
1	A	218	SER	2.5
1	B	191	ILE	2.5
1	A	516	PHE	2.5
1	B	82	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	155	GLY	2.5
1	B	401	ALA	2.5
1	A	129	HIS	2.4
1	B	151	MET	2.4
1	B	282	ILE	2.3
1	B	430	LYS	2.3
1	B	434	THR	2.3
1	B	449	LEU	2.3
1	A	324	MET	2.3
1	B	432	LEU	2.2
1	A	442	PHE	2.2
1	B	433	LYS	2.2
1	B	141	ILE	2.2
1	B	276	ARG	2.2
1	B	505	ALA	2.2
1	A	122	TYR	2.2
1	B	504	LEU	2.2
1	B	439	ASP	2.2
1	B	298	PHE	2.2
1	B	155	GLY	2.1
1	A	190	ALA	2.1
1	B	129	HIS	2.1
1	B	435	MET	2.1
1	A	274	THR	2.1
1	B	422	MET	2.0
1	A	505	ALA	2.0
1	B	421	ASP	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 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, 95th 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	0.99	0.20	15,15,15,15	1

6.5 Other polymers [i](#)

There are no such residues in this entry.