



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:42 pm GMT

PDB ID : 1GSQ
Title : THREE-DIMENSIONAL STRUCTURE, CATALYTIC PROPERTIES AND EVOLUTION OF A SIGMA CLASS GLUTATHIONE TRANSFERASE FROM SQUID, A PROGENITOR OF THE LENS-CRYSTALLINS OF CEPHALOPODS
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Deposited on : 1995-01-09
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

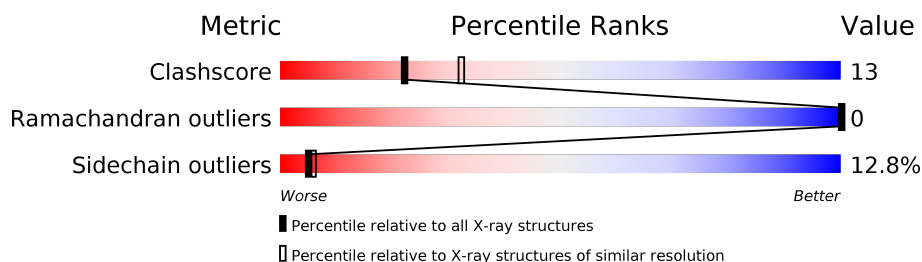
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	202	

2 Entry composition [i](#)

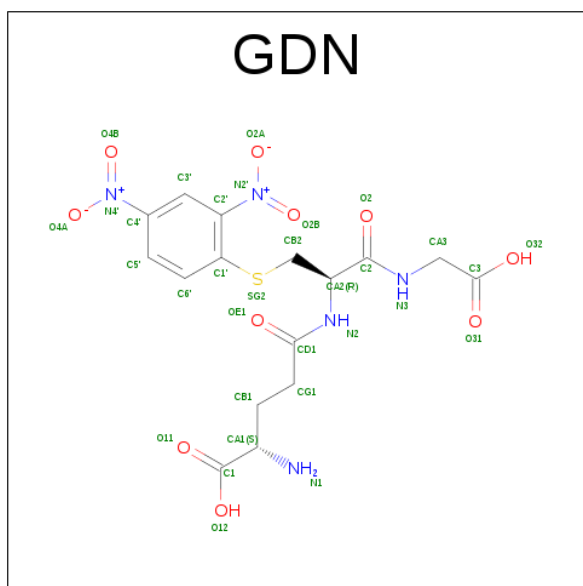
There are 3 unique types of molecules in this entry. The entry contains 1784 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 S-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1598	1022	273	290	13			

- Molecule 2 is GLUTATHIONE S-(2,4 DINITROBENZENE) (three-letter code: GDN) (formula: $C_{16}H_{19}N_5O_{10}S$).

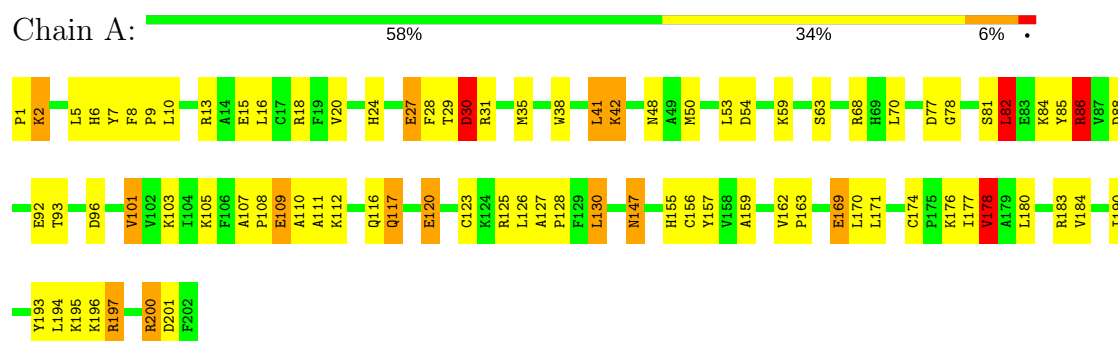


3 Residue-property plots [i](#)

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.

Note EDS was not executed.

• Molecule 1: GLUTATHIONE S-TRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.76 Å 72.76 Å 94.63 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	75.0 (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA, PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1784	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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: GDN

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	1.07	1/1632 (0.1%)	1.80	31/2200 (1.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	GLU	CD-OE1	-5.11	1.20	1.25

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	CD-NE-CZ	21.06	153.08	123.60
1	A	77	ASP	CB-CG-OD1	11.68	128.81	118.30
1	A	125	ARG	NE-CZ-NH1	-11.02	114.79	120.30
1	A	125	ARG	NE-CZ-NH2	10.95	125.77	120.30
1	A	68	ARG	NE-CZ-NH2	-10.79	114.90	120.30
1	A	2	LYS	N-CA-CB	9.63	127.94	110.60
1	A	30	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	110	ALA	CB-CA-C	7.46	121.29	110.10
1	A	27	GLU	CA-CB-CG	7.27	129.40	113.40
1	A	117	GLN	CA-CB-CG	6.69	128.12	113.40
1	A	96	ASP	CB-CG-OD1	6.43	124.08	118.30
1	A	1	PRO	CA-N-CD	-6.39	102.55	111.50
1	A	13	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	18	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	68	ARG	NH1-CZ-NH2	6.17	126.19	119.40
1	A	41	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	86	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	183	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	109	GLU	N-CA-CB	5.83	121.09	110.60
1	A	13	ARG	NE-CZ-NH1	5.68	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	197	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	82	LEU	CB-CA-C	5.28	120.24	110.20
1	A	178	VAL	CA-CB-CG2	5.21	118.71	110.90
1	A	92	GLU	CA-CB-CG	5.09	124.60	113.40
1	A	201	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	53	LEU	N-CA-CB	5.07	120.55	110.40
1	A	183	ARG	CD-NE-CZ	5.07	130.70	123.60
1	A	2	LYS	N-CA-C	-5.05	97.36	111.00
1	A	15	GLU	N-CA-CB	5.03	119.64	110.60
1	A	24	HIS	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1598	0	1620	43	0
2	A	32	0	18	0	0
3	A	154	0	0	2	0
All	All	1784	0	1638	43	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 13.

All (43) 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:170:LEU:HD23	1:A:171:LEU:HD13	1.72	0.72
1:A:6:HIS:HB3	1:A:50:MET:CE	2.20	0.72
1:A:147:ASN:C	1:A:147:ASN:HD22	1.96	0.69
1:A:109:GLU:HA	1:A:112:LYS:HD2	1.75	0.67
1:A:190:ILE:HG22	1:A:194:LEU:HD12	1.77	0.65
1:A:38:TRP:CZ2	1:A:42:LYS:HG2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:O	1:A:86:ARG:HB2	1.99	0.61
1:A:16:LEU:O	1:A:20:VAL:HG23	2.01	0.60
1:A:171:LEU:HD23	1:A:178:VAL:HG12	1.84	0.60
1:A:29:THR:HG21	1:A:31:ARG:HH21	1.68	0.59
1:A:127:ALA:HB3	1:A:128:PRO:HD3	1.86	0.57
1:A:93:THR:HG23	1:A:126:LEU:HD22	1.87	0.56
1:A:174:CYS:O	1:A:178:VAL:HG13	2.05	0.56
1:A:101:VAL:O	1:A:105:LYS:HG2	2.06	0.55
1:A:123:CYS:SG	1:A:170:LEU:HD11	2.49	0.53
1:A:193:TYR:O	1:A:196:LYS:HG2	2.09	0.52
1:A:162:VAL:HB	1:A:163:PRO:HD3	1.93	0.51
1:A:59:LYS:HD2	3:A:402:HOH:O	2.10	0.51
1:A:156:CYS:SG	1:A:177:ILE:HG23	2.52	0.50
1:A:42:LYS:HE3	1:A:48:ASN:O	2.12	0.49
1:A:54:ASP:OD2	1:A:59:LYS:HE2	2.13	0.49
1:A:155:HIS:CE1	1:A:159:ALA:HB2	2.48	0.49
1:A:156:CYS:SG	1:A:180:LEU:HD23	2.54	0.48
1:A:93:THR:HG22	1:A:130:LEU:HD21	1.96	0.47
1:A:85:TYR:O	1:A:88:ASP:HB3	2.15	0.47
1:A:107:ALA:O	1:A:112:LYS:NZ	2.48	0.46
1:A:7:TYR:N	1:A:50:MET:HE1	2.31	0.46
1:A:190:ILE:O	1:A:194:LEU:HB2	2.17	0.45
1:A:8:PHE:HB3	1:A:9:PRO:HD2	1.98	0.45
1:A:28:PHE:HE2	1:A:30:ASP:OD2	2.00	0.45
1:A:108:PRO:O	1:A:111:ALA:N	2.50	0.45
1:A:147:ASN:HA	3:A:325:HOH:O	2.17	0.44
1:A:169:GLU:O	1:A:170:LEU:C	2.57	0.43
1:A:147:ASN:C	1:A:147:ASN:ND2	2.68	0.43
1:A:107:ALA:H	1:A:112:LYS:HZ1	1.66	0.43
1:A:78:GLY:O	1:A:84:LYS:NZ	2.52	0.42
1:A:200:ARG:HE	1:A:200:ARG:HB2	1.67	0.42
1:A:2:LYS:HA	1:A:2:LYS:HD2	1.66	0.42
1:A:195:LYS:HD2	1:A:195:LYS:HA	1.66	0.42
1:A:103:LYS:O	1:A:107:ALA:HB2	2.20	0.41
1:A:130:LEU:HB3	1:A:177:ILE:HD11	2.03	0.40
1:A:116:GLN:O	1:A:120:GLU:HG2	2.21	0.40
1:A:157:TYR:HB2	1:A:184:VAL:HG11	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	200/202 (99%)	180 (90%)	20 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	172/172 (100%)	150 (87%)	22 (13%)	5	6

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	10	LEU
1	A	27	GLU
1	A	30	ASP
1	A	35	MET
1	A	41	LEU
1	A	42	LYS
1	A	63	SER
1	A	70	LEU
1	A	81	SER
1	A	82	LEU
1	A	86	ARG
1	A	101	VAL

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Mol	Chain	Res	Type
1	A	117	GLN
1	A	120	GLU
1	A	130	LEU
1	A	147	ASN
1	A	169	GLU
1	A	176	LYS
1	A	178	VAL
1	A	197	ARG
1	A	200	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDN	A	203	-	21,32,32	1.71	6 (28%)	25,43,43	2.62	12 (48%)

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	GDN	A	203	-	-	0/25/35/35	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	203	GDN	C1'-SG2	-3.56	1.72	1.77
2	A	203	GDN	CB2-SG2	-2.79	1.75	1.81
2	A	203	GDN	C4'-N4'	-2.62	1.40	1.45
2	A	203	GDN	C6'-C1'	2.14	1.43	1.39
2	A	203	GDN	C3'-C4'	2.58	1.43	1.39
2	A	203	GDN	O4B-N4'	2.71	1.27	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	203	GDN	CB1-CG1-CD1	-4.23	103.60	113.18
2	A	203	GDN	CG1-CB1-CA1	-3.97	104.58	113.84
2	A	203	GDN	C3'-C2'-C1'	-3.41	119.53	122.93
2	A	203	GDN	CG1-CD1-N2	-3.12	110.33	115.82
2	A	203	GDN	C6'-C1'-SG2	-3.06	113.72	121.40
2	A	203	GDN	C2-CA2-N2	-2.66	103.90	111.20
2	A	203	GDN	O2-C2-CA2	-2.34	115.38	120.43
2	A	203	GDN	CA2-C2-N3	2.49	121.59	116.51
2	A	203	GDN	C5'-C4'-N4'	3.11	121.78	119.41
2	A	203	GDN	CB2-CA2-C2	3.93	118.61	109.55
2	A	203	GDN	OE1-CD1-N2	4.32	130.43	122.97
2	A	203	GDN	CB2-SG2-C1'	5.88	115.69	102.27

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.