



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2019 – 02:05 AM EDT

PDB ID : 1GNE  
Title : THE THREE-DIMENSIONAL STRUCTURE OF GLUTATHIONE S-TRANSFERASE OF SCHISTOSOMA JAPONICUM FUSED WITH A CONSERVED NEUTRALIZING EPITOPE ON GP41 OF HUMAN IMMUNODEFICIENCY VIRUS TYPE 1  
Authors : Lim, K.; Ho, J.X.; Keeling, K.; Gilliland, G.L.; Ji, X.; Ruker, F.; Carter, D.C.  
Deposited on : 1994-06-16  
Resolution : 2.50 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  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

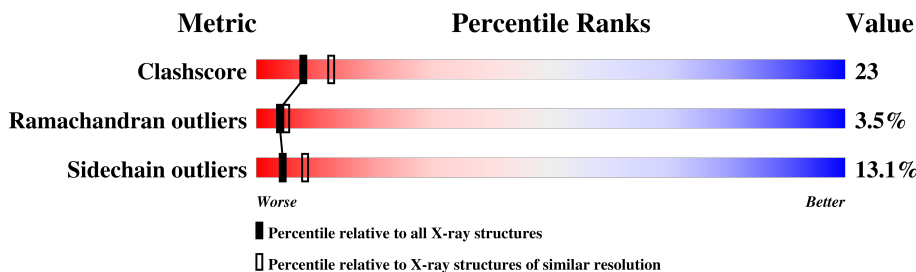
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)

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. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	232	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GSH	A	233	X	-	-	-

## 2 Entry composition [i](#)

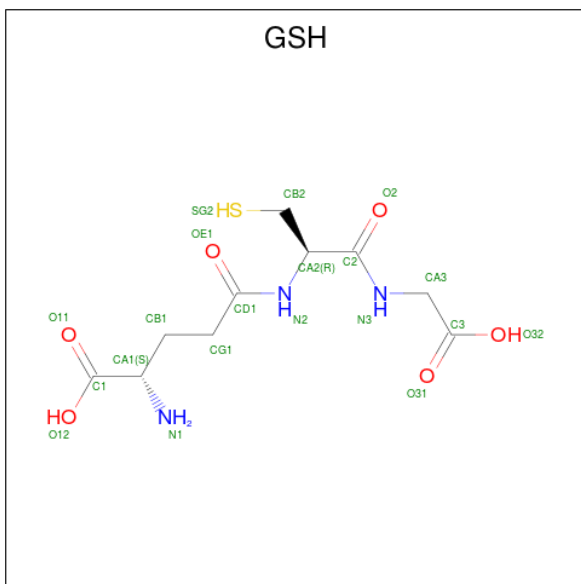
There are 3 unique types of molecules in this entry. The entry contains 2051 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	232	1905	1238	310	344	13	0	0	0

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	20	10	3	6	1	0	0

- Molecule 3 is water.

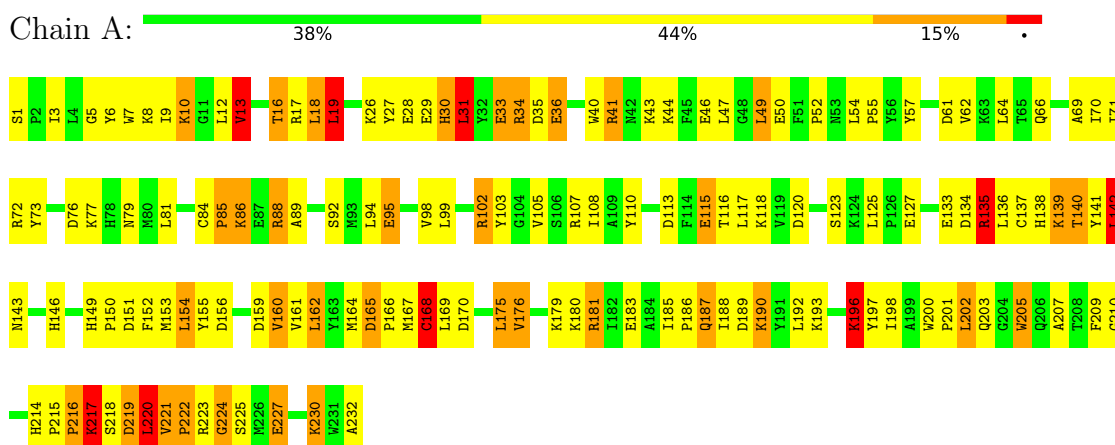
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	126	Total	O	0	0
			126	126		

### 3 Residue-property plots

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. 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. 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 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.74Å 94.74Å 58.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR, GPRLSA	Depositor
R, $R_{free}$	0.219 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2051	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GSH

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	1.10	0/1957	2.01	66/2641 (2.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	CD-NE-CZ	13.48	142.48	123.60
1	A	181	ARG	NE-CZ-NH1	12.94	126.77	120.30
1	A	223	ARG	CD-NE-CZ	11.02	139.03	123.60
1	A	34	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	A	72	ARG	CD-NE-CZ	10.61	138.46	123.60
1	A	54	LEU	CA-CB-CG	10.09	138.51	115.30
1	A	134	ASP	CB-CG-OD1	9.94	127.24	118.30
1	A	220	LEU	CA-CB-CG	9.26	136.60	115.30
1	A	223	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	31	LEU	CA-CB-CG	8.94	135.85	115.30
1	A	135	ARG	CD-NE-CZ	8.41	135.38	123.60
1	A	142	LEU	CA-CB-CG	8.22	134.20	115.30
1	A	181	ARG	CD-NE-CZ	7.88	134.64	123.60
1	A	95	GLU	CA-CB-CG	7.86	130.69	113.40
1	A	196	LYS	CA-CB-CG	7.64	130.21	113.40
1	A	102	ARG	NE-CZ-NH1	7.25	123.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	A	41	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	A	160	VAL	CA-CB-CG1	6.97	121.36	110.90
1	A	103	TYR	CA-CB-CG	6.94	126.58	113.40
1	A	133	GLU	CA-CB-CG	6.89	128.56	113.40
1	A	170	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	220	LEU	C-N-CA	6.82	138.75	121.70
1	A	17	ARG	CD-NE-CZ	6.63	132.88	123.60
1	A	162	LEU	CA-CB-CG	6.53	130.31	115.30
1	A	50	GLU	CA-CB-CG	6.52	127.75	113.40
1	A	137	CYS	N-CA-CB	6.45	122.21	110.60
1	A	19	LEU	CA-CB-CG	6.45	130.14	115.30
1	A	72	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	217	LYS	CB-CA-C	6.38	123.17	110.40
1	A	30	HIS	CA-CB-CG	6.37	124.43	113.60
1	A	34	ARG	CA-CB-CG	6.34	127.36	113.40
1	A	35	ASP	CB-CG-OD2	6.22	123.89	118.30
1	A	107	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	140	THR	CA-CB-CG2	6.14	121.00	112.40
1	A	181	ARG	CG-CD-NE	6.14	124.70	111.80
1	A	88	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	175	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	13	VAL	CA-CB-CG1	5.97	119.86	110.90
1	A	137	CYS	CA-CB-SG	-5.97	103.26	114.00
1	A	216	PRO	N-CA-C	5.96	127.60	112.10
1	A	209	PHE	CB-CG-CD2	-5.94	116.64	120.80
1	A	181	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	127	GLU	CA-CB-CG	5.88	126.34	113.40
1	A	99	LEU	CA-CB-CG	5.84	128.73	115.30
1	A	43	LYS	CB-CG-CD	5.81	126.70	111.60
1	A	136	LEU	CA-CB-CG	5.80	128.63	115.30
1	A	139	LYS	CB-CG-CD	5.79	126.67	111.60
1	A	176	VAL	CA-CB-CG2	5.75	119.52	110.90
1	A	102	ARG	CD-NE-CZ	5.75	131.65	123.60
1	A	165	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	221	VAL	CA-CB-CG2	5.61	119.32	110.90
1	A	230	LYS	N-CA-CB	5.57	120.62	110.60
1	A	12	LEU	CA-CB-CG	5.49	127.93	115.30
1	A	220	LEU	O-C-N	-5.38	114.08	122.70
1	A	113	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	232	ALA	CB-CA-C	5.26	117.99	110.10
1	A	99	LEU	CB-CA-C	5.20	120.08	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ARG	CD-NE-CZ	5.19	130.87	123.60
1	A	159	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	A	202	LEU	CB-CA-C	5.09	119.87	110.20
1	A	49	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	156	ASP	N-CA-CB	5.07	119.72	110.60
1	A	40	TRP	N-CA-CB	5.06	119.70	110.60
1	A	18	LEU	CA-CB-CG	5.02	126.84	115.30
1	A	180	LYS	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LYS	Mainchain
1	A	115	GLU	Mainchain
1	A	168	CYS	Mainchain

## 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	1905	0	1902	88	0
2	A	20	0	15	1	0
3	A	126	0	0	7	0
All	All	2051	0	1917	88	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 23.

All (88) 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:98:VAL:HG11	1:A:153:MET:HB3	1.43	0.97
1:A:64:LEU:HD11	1:A:69:ALA:HB1	1.65	0.78
1:A:19:LEU:HD12	1:A:71:ILE:HG13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:HB2	1:A:81:LEU:HD22	1.68	0.74
1:A:49:LEU:HD23	1:A:52:PRO:HA	1.77	0.66
1:A:27:TYR:HE2	1:A:29:GLU:HG3	1.63	0.64
1:A:217:LYS:HA	1:A:217:LYS:NZ	2.13	0.64
1:A:92:SER:HA	1:A:95:GLU:HB3	1.80	0.63
1:A:108:ILE:HD11	1:A:117:LEU:HD12	1.79	0.62
1:A:219:ASP:H	1:A:220:LEU:HD22	1.65	0.62
1:A:62:VAL:HG11	1:A:73:TYR:CE2	2.34	0.61
1:A:125:LEU:HD23	1:A:168:CYS:SG	2.40	0.61
1:A:7:TRP:HB2	1:A:9:ILE:HG12	1.82	0.61
1:A:179:LYS:O	1:A:183:GLU:HG3	2.01	0.60
1:A:200:TRP:CZ3	1:A:216:PRO:HD3	2.37	0.59
1:A:217:LYS:HZ2	1:A:217:LYS:HA	1.69	0.58
1:A:186:PRO:HG2	1:A:187:GLN:NE2	2.19	0.57
1:A:57:TYR:HB3	1:A:70:ILE:HD12	1.87	0.57
1:A:5:GLY:HA2	1:A:30:HIS:O	2.05	0.57
1:A:64:LEU:HG	1:A:70:ILE:HD13	1.87	0.56
1:A:227:GLU:HG3	3:A:307:HOH:O	2.06	0.55
1:A:186:PRO:O	1:A:190:LYS:HG2	2.07	0.55
1:A:186:PRO:HG2	1:A:187:GLN:HE21	1.71	0.55
1:A:142:LEU:HD21	1:A:154:LEU:HD12	1.89	0.54
1:A:155:TYR:HE1	1:A:179:LYS:HG3	1.72	0.54
1:A:215:PRO:HD2	3:A:356:HOH:O	2.06	0.54
1:A:76:ASP:HA	3:A:318:HOH:O	2.06	0.54
1:A:224:GLY:HA3	1:A:230:LYS:HB3	1.90	0.54
1:A:13:VAL:HG23	1:A:55:PRO:HG3	1.91	0.53
1:A:27:TYR:CE2	1:A:29:GLU:HG3	2.42	0.53
1:A:105:VAL:HG13	1:A:164:MET:HE3	1.91	0.53
1:A:120:ASP:O	1:A:123:SER:HB2	2.09	0.52
1:A:196:LYS:O	1:A:198:ILE:HD12	2.10	0.52
1:A:169:LEU:HD11	1:A:175:LEU:HB3	1.90	0.52
1:A:150:PRO:HA	1:A:153:MET:HB2	1.91	0.52
1:A:138:HIS:O	1:A:139:LYS:HG3	2.09	0.52
1:A:142:LEU:HD11	1:A:154:LEU:HD12	1.93	0.50
1:A:149:HIS:N	1:A:150:PRO:HD2	2.27	0.50
1:A:33:GLU:O	1:A:36:GLU:HB2	2.12	0.50
1:A:214:HIS:HB3	3:A:356:HOH:O	2.10	0.50
1:A:185:ILE:HG22	1:A:187:GLN:H	1.75	0.50
1:A:140:THR:HG22	1:A:141:TYR:CD2	2.46	0.50
1:A:7:TRP:HB3	1:A:205:TRP:CH2	2.47	0.49
1:A:217:LYS:HG3	3:A:309:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:CZ	1:A:160:VAL:HG21	2.41	0.49
1:A:221:VAL:HG12	1:A:222:PRO:O	2.13	0.49
1:A:8:LYS:O	1:A:201:PRO:HD2	2.13	0.48
1:A:1:SER:HB3	1:A:27:TYR:HA	1.95	0.48
1:A:155:TYR:CE1	1:A:179:LYS:HG3	2.48	0.48
1:A:189:ASP:O	1:A:193:LYS:HG2	2.13	0.48
1:A:16:THR:HG21	1:A:70:ILE:HG22	1.97	0.47
1:A:219:ASP:HB3	1:A:220:LEU:HD13	1.96	0.46
1:A:192:LEU:HA	1:A:197:TYR:CD1	2.50	0.46
1:A:6:TYR:CD2	1:A:13:VAL:HB	2.50	0.46
1:A:94:LEU:O	1:A:98:VAL:HG23	2.16	0.46
1:A:84:CYS:HA	1:A:85:PRO:HD2	1.68	0.46
1:A:218:SER:HB2	1:A:220:LEU:HD22	1.97	0.46
1:A:33:GLU:H	1:A:36:GLU:HB2	1.81	0.46
1:A:85:PRO:HD3	1:A:88:ARG:HH12	1.81	0.46
1:A:3:ILE:HA	1:A:28:GLU:O	2.16	0.45
1:A:146:HIS:HB3	3:A:302:HOH:O	2.14	0.45
1:A:219:ASP:C	1:A:220:LEU:HD13	2.36	0.45
1:A:57:TYR:CB	1:A:70:ILE:HD12	2.46	0.45
1:A:105:VAL:HG13	1:A:164:MET:CE	2.47	0.45
1:A:18:LEU:HD21	1:A:155:TYR:HD2	1.81	0.45
1:A:165:ASP:OD1	1:A:167:MET:HB2	2.16	0.45
1:A:34:ARG:NH1	1:A:205:TRP:HB3	2.32	0.45
1:A:10:LYS:HG2	1:A:198:ILE:O	2.18	0.44
1:A:7:TRP:HB3	1:A:205:TRP:HH2	1.82	0.44
1:A:165:ASP:HA	1:A:166:PRO:HD2	1.69	0.44
1:A:6:TYR:HE1	2:A:233:GSH:HB22	1.83	0.44
1:A:41:ARG:O	1:A:44:LYS:HB3	2.18	0.43
1:A:142:LEU:HB2	1:A:151:ASP:OD1	2.18	0.43
1:A:3:ILE:HG12	1:A:28:GLU:CG	2.48	0.43
1:A:110:TYR:CE2	1:A:207:ALA:HB2	2.54	0.42
1:A:79:ASN:HB3	3:A:330:HOH:O	2.20	0.42
1:A:16:THR:HA	1:A:71:ILE:HD12	2.01	0.42
1:A:201:PRO:HB2	1:A:203:GLN:O	2.19	0.42
1:A:86:LYS:O	1:A:89:ALA:HB3	2.18	0.42
1:A:81:LEU:O	1:A:88:ARG:HG3	2.20	0.41
1:A:3:ILE:HG12	1:A:28:GLU:HG2	2.01	0.41
1:A:152:PHE:CE1	1:A:188:ILE:HD11	2.56	0.41
1:A:135:ARG:O	1:A:139:LYS:HD3	2.20	0.41
1:A:202:LEU:HD22	1:A:210:GLY:HA3	2.01	0.41
1:A:115:GLU:O	1:A:118:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PRO:HA	1:A:216:PRO:HD3	1.82	0.40
1:A:8:LYS:HG3	1:A:31:LEU:HB2	2.04	0.40
1:A:9:ILE:HG22	1:A:201:PRO:CG	2.52	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	230/232 (99%)	195 (85%)	27 (12%)	8 (4%)	<b>4</b> <b>5</b>

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	224	GLY
1	A	227	GLU
1	A	85	PRO
1	A	143	ASN
1	A	205	TRP
1	A	219	ASP
1	A	222	PRO

### 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	Rotameric	Outliers	Percentiles
1	A	206/206 (100%)	179 (87%)	27 (13%)	4 8

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

Mol	Chain	Res	Type
1	A	13	VAL
1	A	16	THR
1	A	19	LEU
1	A	26	LYS
1	A	31	LEU
1	A	33	GLU
1	A	46	GLU
1	A	47	LEU
1	A	61	ASP
1	A	66	GLN
1	A	77	LYS
1	A	86	LYS
1	A	116	THR
1	A	135	ARG
1	A	142	LEU
1	A	154	LEU
1	A	161	VAL
1	A	162	LEU
1	A	168	CYS
1	A	176	VAL
1	A	181	ARG
1	A	187	GLN
1	A	190	LYS
1	A	196	LYS
1	A	217	LYS
1	A	220	LEU
1	A	225	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	203	GLN

### 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	GSH	A	233	-	12,19,19	1.80	4 (33%)	15,24,24	3.33	11 (73%)

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	GSH	A	233	-	1/1/6/8	7/18/24/24	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	233	GSH	CG1-CD1	-3.01	1.45	1.51
2	A	233	GSH	CB1-CG1	-2.86	1.43	1.52
2	A	233	GSH	CA2-C2	2.28	1.58	1.52

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	233	GSH	CA1-N1	2.14	1.52	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	233	GSH	CB1-CG1-CD1	7.36	129.61	113.15
2	A	233	GSH	CB2-CA2-N2	4.75	118.28	111.39
2	A	233	GSH	CA2-N2-CD1	4.71	133.66	121.64
2	A	233	GSH	O2-C2-CA2	-3.78	112.48	120.45
2	A	233	GSH	OE1-CD1-N2	3.43	128.83	122.97
2	A	233	GSH	CG1-CD1-N2	-2.93	110.78	115.81
2	A	233	GSH	CA3-N3-C2	2.90	126.58	122.34
2	A	233	GSH	OE1-CD1-CG1	-2.80	116.89	122.02
2	A	233	GSH	CG1-CB1-CA1	-2.43	108.16	113.84
2	A	233	GSH	CB2-CA2-C2	2.35	114.73	109.69
2	A	233	GSH	C3-CA3-N3	2.11	114.29	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	233	GSH	CA1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	233	GSH	N1-CA1-CB1-CG1
2	A	233	GSH	C1-CA1-CB1-CG1
2	A	233	GSH	CG1-CD1-N2-CA2
2	A	233	GSH	OE1-CD1-N2-CA2
2	A	233	GSH	CA1-CB1-CG1-CD1
2	A	233	GSH	O2-C2-N3-CA3
2	A	233	GSH	N2-CA2-CB2-SG2

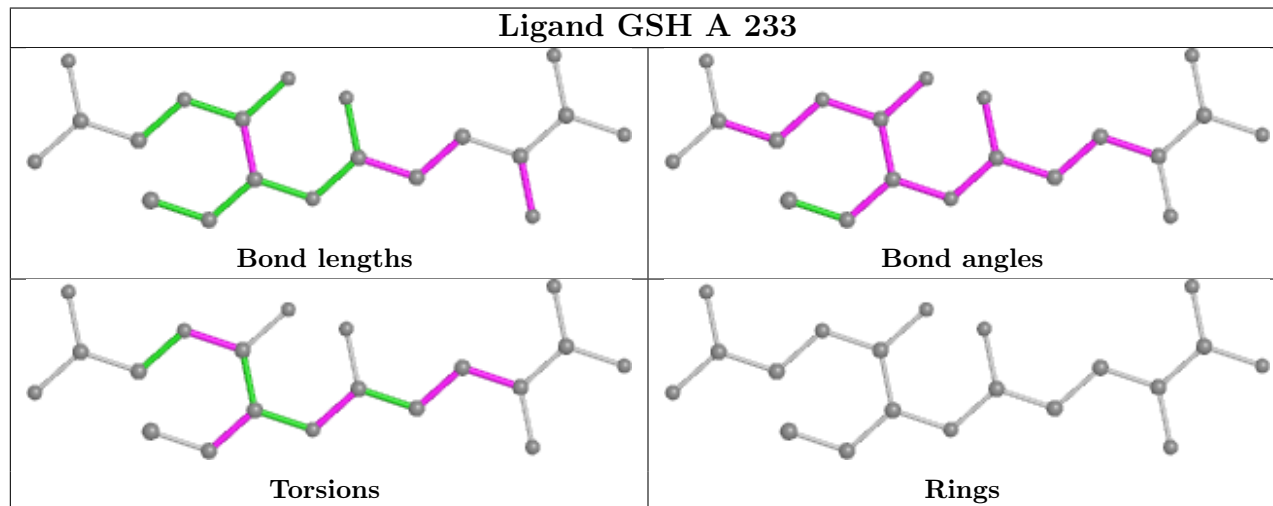
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	233	GSH	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 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.



## 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

### 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.