



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:05 PM UTC

PDB ID : 1GNE / pdb_00001gne
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

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
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

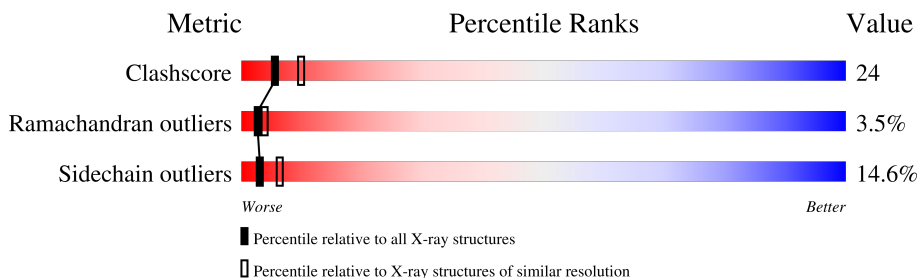
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	232	29% 43% 22% 6%

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	X	-	-

2 Entry composition [i](#)

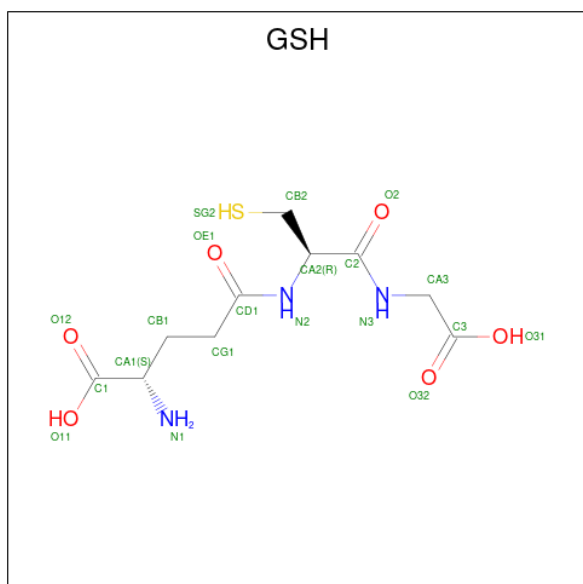
There are 3 unique types of molecules in this entry. The entry contains 2051 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



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

- Molecule 3 is water.

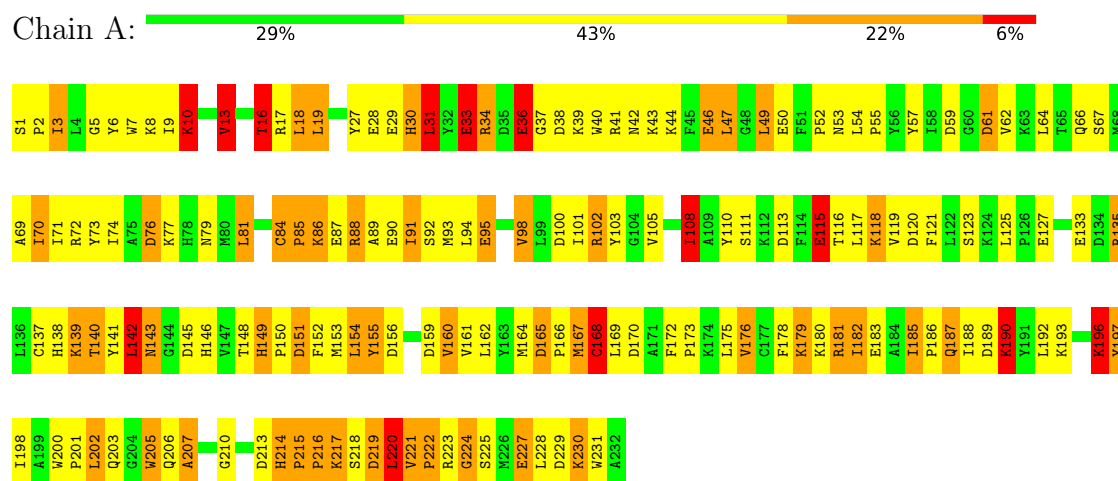
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	126	Total	O	0	0
			126	126		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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, α , β , γ	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	GPRLSA, X-PLOR	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 ²)	9.0	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: 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	1.36	5/1957 (0.3%)	2.49	145/2641 (5.5%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	VAL	CA-C	5.74	1.58	1.52
1	A	221	VAL	N-CA	-5.48	1.39	1.46
1	A	31	LEU	CA-CB	-5.36	1.46	1.53
1	A	91	ILE	CA-CB	5.16	1.60	1.54
1	A	216	PRO	CA-C	-5.04	1.48	1.52

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	CD-NE-CZ	12.91	142.48	124.40
1	A	213	ASP	CA-CB-CG	11.00	123.60	112.60
1	A	30	HIS	CA-CB-CG	10.63	124.43	113.80
1	A	216	PRO	N-CA-C	10.60	127.60	110.21
1	A	223	ARG	CD-NE-CZ	10.45	139.03	124.40
1	A	72	ARG	CD-NE-CZ	10.04	138.46	124.40
1	A	76	ASP	CA-CB-CG	9.53	122.12	112.60
1	A	220	LEU	CA-C-N	8.98	138.75	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	LEU	C-N-CA	8.98	138.75	122.13
1	A	46	GLU	CB-CG-CD	8.52	127.09	112.60
1	A	95	GLU	CA-CB-CG	8.30	130.69	114.10
1	A	37	GLY	CA-C-N	8.28	131.20	120.44
1	A	37	GLY	C-N-CA	8.28	131.20	120.44
1	A	137	CYS	N-CA-CB	8.26	122.21	110.24
1	A	170	ASP	CA-CB-CG	8.15	120.75	112.60
1	A	113	ASP	CA-CB-CG	8.15	120.75	112.60
1	A	133	GLU	CB-CG-CD	8.15	126.45	112.60
1	A	196	LYS	CA-CB-CG	8.05	130.21	114.10
1	A	121	PHE	CA-CB-CG	8.03	121.83	113.80
1	A	108	ILE	CB-CA-C	7.99	118.97	111.30
1	A	135	ARG	CD-NE-CZ	7.84	135.38	124.40
1	A	155	TYR	CA-C-O	-7.83	112.77	121.00
1	A	172	PHE	CA-CB-CG	7.69	121.49	113.80
1	A	228	LEU	N-CA-C	7.56	121.85	112.47
1	A	178	PHE	CA-CB-CG	7.40	121.20	113.80
1	A	165	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	181	ARG	CD-NE-CZ	7.31	134.64	124.40
1	A	229	ASP	CA-CB-CG	7.25	119.85	112.60
1	A	133	GLU	CA-CB-CG	7.23	128.56	114.10
1	A	118	LYS	CA-C-N	7.21	130.22	120.77
1	A	118	LYS	C-N-CA	7.21	130.22	120.77
1	A	33	GLU	CB-CG-CD	7.21	124.86	112.60
1	A	38	ASP	CA-C-N	7.12	130.54	120.28
1	A	38	ASP	C-N-CA	7.12	130.54	120.28
1	A	103	TYR	CA-CB-CG	7.04	126.58	113.90
1	A	53	ASN	CA-CB-CG	7.00	119.59	112.60
1	A	42	ASN	CA-CB-CG	6.89	119.50	112.60
1	A	202	LEU	N-CA-CB	-6.87	100.44	110.47
1	A	50	GLU	CA-CB-CG	6.83	127.75	114.10
1	A	100	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	61	ASP	CA-CB-CG	6.73	119.33	112.60
1	A	40	TRP	N-CA-CB	6.70	119.70	109.98
1	A	43	LYS	CB-CG-CD	6.70	126.70	111.30
1	A	139	LYS	CB-CG-CD	6.68	126.67	111.30
1	A	34	ARG	CA-CB-CG	6.63	127.36	114.10
1	A	220	LEU	CA-C-O	6.47	129.77	120.51
1	A	160	VAL	CA-CB-CG1	6.45	121.36	110.40
1	A	115	GLU	CA-C-N	6.44	130.10	120.31
1	A	115	GLU	C-N-CA	6.44	130.10	120.31
1	A	47	LEU	CB-CA-C	6.41	119.17	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	LEU	O-C-N	-6.39	114.08	122.59
1	A	50	GLU	N-CA-CB	6.39	119.09	110.59
1	A	54	LEU	CA-CB-CG	6.35	138.51	116.30
1	A	151	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	87	GLU	CB-CG-CD	6.32	123.35	112.60
1	A	149	HIS	CA-C-N	6.29	125.92	119.56
1	A	149	HIS	C-N-CA	6.29	125.92	119.56
1	A	145	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	87	GLU	N-CA-CB	6.27	119.10	110.01
1	A	140	THR	CA-CB-CG2	6.18	121.00	110.50
1	A	156	ASP	N-CA-CB	6.17	119.72	110.22
1	A	42	ASN	CA-C-O	-6.17	114.53	121.00
1	A	127	GLU	CA-CB-CG	6.12	126.34	114.10
1	A	190	LYS	CG-CD-CE	6.12	125.37	111.30
1	A	98	VAL	O-C-N	6.10	128.22	121.94
1	A	101	ILE	N-CA-CB	6.08	117.52	110.65
1	A	202	LEU	CB-CA-C	6.08	119.87	109.24
1	A	17	ARG	CD-NE-CZ	6.05	132.88	124.40
1	A	185	ILE	CB-CG1-CD1	6.03	126.46	113.80
1	A	230	LYS	N-CA-CB	5.99	120.62	110.49
1	A	42	ASN	N-CA-CB	5.95	118.60	109.91
1	A	228	LEU	N-CA-CB	-5.91	103.47	112.28
1	A	231	TRP	N-CA-CB	-5.90	102.20	111.23
1	A	59	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	84	CYS	CA-C-N	5.83	127.13	119.84
1	A	84	CYS	C-N-CA	5.83	127.13	119.84
1	A	220	LEU	CA-CB-CG	5.80	136.60	116.30
1	A	181	ARG	CG-CD-NE	5.77	124.70	112.00
1	A	88	ARG	CA-C-N	5.72	129.00	120.31
1	A	88	ARG	C-N-CA	5.72	129.00	120.31
1	A	36	GLU	N-CA-C	5.71	122.97	110.80
1	A	3	ILE	CB-CA-C	5.70	119.02	110.98
1	A	185	ILE	O-C-N	5.69	127.86	120.75
1	A	143	ASN	OD1-CG-ND2	5.68	128.28	122.60
1	A	16	THR	CA-C-O	-5.68	114.40	120.42
1	A	173	PRO	CA-C-N	5.67	128.44	120.28
1	A	173	PRO	C-N-CA	5.67	128.44	120.28
1	A	190	LYS	CB-CG-CD	5.66	124.33	111.30
1	A	103	TYR	CA-C-N	5.61	126.21	119.98
1	A	103	TYR	C-N-CA	5.61	126.21	119.98
1	A	215	PRO	CB-CA-C	5.60	117.75	110.92
1	A	31	LEU	CA-CB-CG	5.59	135.85	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	LEU	CA-C-N	5.58	128.22	120.29
1	A	18	LEU	C-N-CA	5.58	128.22	120.29
1	A	207	ALA	CA-C-N	5.58	128.79	120.31
1	A	207	ALA	C-N-CA	5.58	128.79	120.31
1	A	13	VAL	CA-CB-CG1	5.57	119.86	110.40
1	A	185	ILE	N-CA-C	-5.57	102.89	108.96
1	A	16	THR	N-CA-CB	5.55	118.38	110.16
1	A	10	LYS	CA-C-N	5.46	128.86	120.07
1	A	10	LYS	C-N-CA	5.46	128.86	120.07
1	A	74	ILE	N-CA-CB	5.46	116.82	110.65
1	A	197	TYR	N-CA-C	5.41	118.02	109.96
1	A	229	ASP	CA-C-N	5.39	131.84	121.54
1	A	229	ASP	C-N-CA	5.39	131.84	121.54
1	A	176	VAL	CA-CB-CG2	5.37	119.52	110.40
1	A	206	GLN	OE1-CD-NE2	5.34	127.94	122.60
1	A	182	ILE	CA-CB-CG2	5.30	119.51	110.50
1	A	159	ASP	O-C-N	5.29	127.73	122.12
1	A	39	LYS	CG-CD-CE	5.28	123.45	111.30
1	A	42	ASN	O-C-N	5.28	127.52	122.03
1	A	181	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	A	165	ASP	CA-C-N	5.26	125.58	119.47
1	A	165	ASP	C-N-CA	5.26	125.58	119.47
1	A	111	SER	N-CA-CB	5.25	117.61	109.48
1	A	221	VAL	CA-CB-CG2	5.25	119.32	110.40
1	A	180	LYS	N-CA-CB	5.24	117.82	110.12
1	A	127	GLU	N-CA-CB	5.22	117.86	110.13
1	A	17	ARG	CA-C-N	5.21	127.52	120.38
1	A	17	ARG	C-N-CA	5.21	127.52	120.38
1	A	214	HIS	CA-C-N	5.21	125.75	120.38
1	A	214	HIS	C-N-CA	5.21	125.75	120.38
1	A	2	PRO	N-CA-C	-5.20	103.03	111.19
1	A	102	ARG	CD-NE-CZ	5.18	131.65	124.40
1	A	140	THR	N-CA-C	-5.18	105.32	111.69
1	A	180	LYS	CA-CB-CG	5.16	124.42	114.10
1	A	13	VAL	CA-C-O	-5.15	114.69	120.25
1	A	102	ARG	CA-C-O	-5.14	115.10	120.55
1	A	70	ILE	N-CA-CB	5.13	117.14	110.57
1	A	67	SER	CA-C-O	-5.12	115.42	120.90
1	A	142	LEU	CA-CB-CG	5.11	134.20	116.30
1	A	108	ILE	CA-CB-CG2	5.10	119.18	110.50
1	A	142	LEU	CA-C-O	5.09	126.49	120.58
1	A	119	VAL	CA-C-N	5.08	127.05	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	VAL	C-N-CA	5.08	127.05	120.44
1	A	127	GLU	CA-C-N	5.06	127.31	120.38
1	A	127	GLU	C-N-CA	5.06	127.31	120.38
1	A	160	VAL	CB-CA-C	5.06	118.44	111.97
1	A	142	LEU	CA-C-N	5.05	131.19	121.54
1	A	142	LEU	C-N-CA	5.05	131.19	121.54
1	A	179	LYS	CA-C-O	-5.04	115.20	120.55
1	A	113	ASP	CB-CA-C	5.03	118.98	111.88
1	A	167	MET	CA-C-N	5.01	127.25	120.38
1	A	167	MET	C-N-CA	5.01	127.25	120.38
1	A	229	ASP	CB-CA-C	5.00	119.26	109.35

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	91	0
2	A	20	0	15	1	0
3	A	126	0	0	7	0
All	All	2051	0	1917	91	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 24.

All (91) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PRO:HA	1:A:153:MET:HE3	1.58	0.85
1:A:64:LEU:HD11	1:A:69:ALA:HB1	1.65	0.78
1:A:105:VAL:HG13	1:A:164:MET:HE3	1.66	0.76
1:A:19:LEU:HD12	1:A:71:ILE:HG13	1.69	0.74
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:NZ	1:A:217:LYS:HA	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:217:LYS:HA	1:A:217:LYS:HZ2	1.67	0.60
1:A:200:TRP:CZ3	1:A:216:PRO:HD3	2.37	0.59
1:A:186:PRO:HG2	1:A:187:GLN:NE2	2.19	0.57
1:A:5:GLY:HA2	1:A:30:HIS:O	2.05	0.57
1:A:57:TYR:HB3	1:A:70:ILE:HD12	1.87	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:HG2	1:A:187:GLN:HE21	1.71	0.55
1:A:186:PRO:O	1:A:190:LYS:HG2	2.07	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:150:PRO:CA	1:A:153:MET:HE3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:102:ARG:CZ	1:A:160:VAL:HG21	2.41	0.49
1:A:219:ASP:C	1:A:220:LEU:HD13	2.36	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:57:TYR:CB	1:A:70:ILE:HD12	2.46	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:3:ILE:HG12	1:A:28:GLU:CG	2.48	0.43
1:A:142:LEU:HB2	1:A:151:ASP:OD1	2.18	0.43
1:A:90:GLU:HG3	1:A:93:MET:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:148:THR:C	1:A:150:PRO:HD2	2.46	0.41
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%)	3 4

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 ⓘ

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%)	176 (85%)	30 (15%)	3 6

All (30) 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	31	LEU
1	A	33	GLU
1	A	46	GLU
1	A	47	LEU
1	A	49	LEU
1	A	61	ASP
1	A	66	GLN
1	A	77	LYS
1	A	81	LEU
1	A	86	LYS
1	A	91	ILE
1	A	108	ILE
1	A	116	THR
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	182	ILE
1	A	187	GLN
1	A	190	LYS
1	A	196	LYS
1	A	217	LYS
1	A	220	LEU
1	A	225	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	146	HIS
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 oligosaccharides 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	-	18,19,19	2.00	7 (38%)	21,24,24	3.04	12 (57%)

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	9/24/24/24	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	233	GSH	O32-C3	3.52	1.33	1.22
2	A	233	GSH	CB1-CG1	-3.05	1.43	1.52
2	A	233	GSH	O12-C1	3.05	1.31	1.22
2	A	233	GSH	CG1-CD1	-2.89	1.45	1.51
2	A	233	GSH	O11-C1	-2.55	1.22	1.30
2	A	233	GSH	CA2-C2	2.36	1.58	1.52
2	A	233	GSH	OE1-CD1	2.02	1.27	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	233	GSH	CB1-CG1-CD1	7.42	129.61	113.06
2	A	233	GSH	CB2-CA2-N2	4.90	118.28	111.28
2	A	233	GSH	CA2-N2-CD1	4.78	133.66	121.68
2	A	233	GSH	O31-C3-O32	-3.96	113.15	123.33
2	A	233	GSH	O2-C2-CA2	-3.82	112.48	120.48
2	A	233	GSH	OE1-CD1-N2	3.47	128.83	122.95
2	A	233	GSH	O31-C3-CA3	3.30	125.34	112.81
2	A	233	GSH	CG1-CD1-N2	-2.89	110.78	115.86
2	A	233	GSH	OE1-CD1-CG1	-2.83	116.89	122.02
2	A	233	GSH	CG1-CB1-CA1	-2.48	108.16	113.86
2	A	233	GSH	CB2-CA2-C2	2.41	114.73	109.50
2	A	233	GSH	CA3-N3-C2	2.06	126.58	121.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	233	GSH	CA1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	233	GSH	N1-CA1-CB1-CG1
2	A	233	GSH	CG1-CD1-N2-CA2
2	A	233	GSH	OE1-CD1-N2-CA2
2	A	233	GSH	O31-C3-CA3-N3
2	A	233	GSH	O2-C2-N3-CA3

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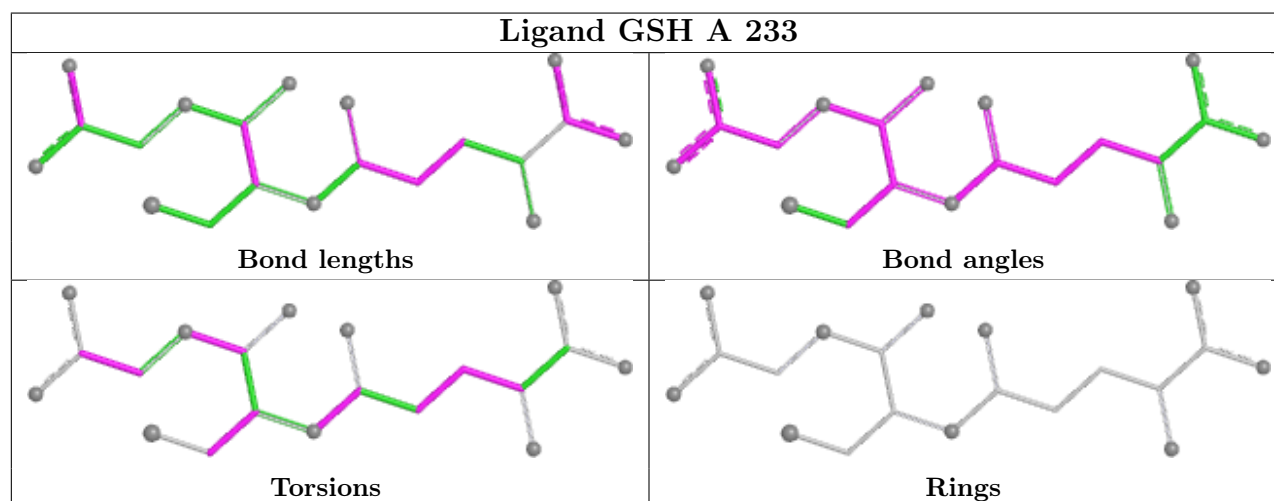
Mol	Chain	Res	Type	Atoms
2	A	233	GSH	CA1-CB1-CG1-CD1
2	A	233	GSH	O32-C3-CA3-N3
2	A	233	GSH	N2-CA2-CB2-SG2
2	A	233	GSH	C1-CA1-CB1-CG1

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 ⓘ

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.