



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:22 AM UTC

PDB ID : 6GST / pdb_00006gst
Title : FIRST-SPHERE AND SECOND-SPHERE ELECTROSTATIC EFFECTS IN
THE ACTIVE SITE OF A CLASS MU GLUTATHIONE TRANSFERASE
Authors : Xiao, G.; Ji, X.; Armstrong, R.N.; Gilliland, G.L.
Deposited on : 1996-01-26
Resolution : 2.20 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

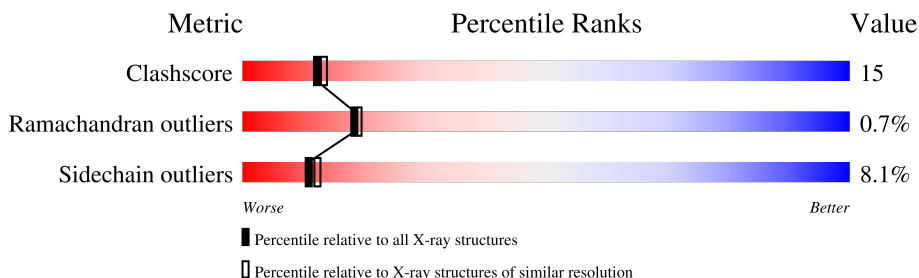
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	217	 43% 44% 10% .
1	B	217	 41% 41% 17% .

2 Entry composition [i](#)

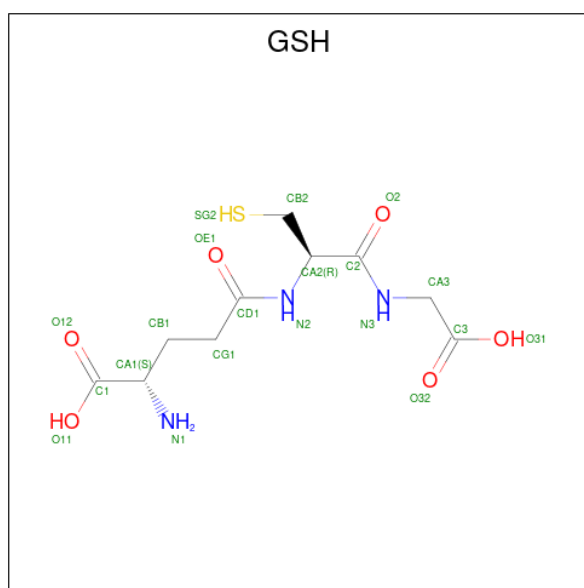
There are 3 unique types of molecules in this entry. The entry contains 4096 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1818	1177	303	327	11			
1	B	217	Total	C	N	O	S	0	0	0
			1818	1177	303	327	11			

- 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		
2	B	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	229	Total 229	O 229	0	0
3	B	191	Total 191	O 191	0	0

3 Residue-property plots

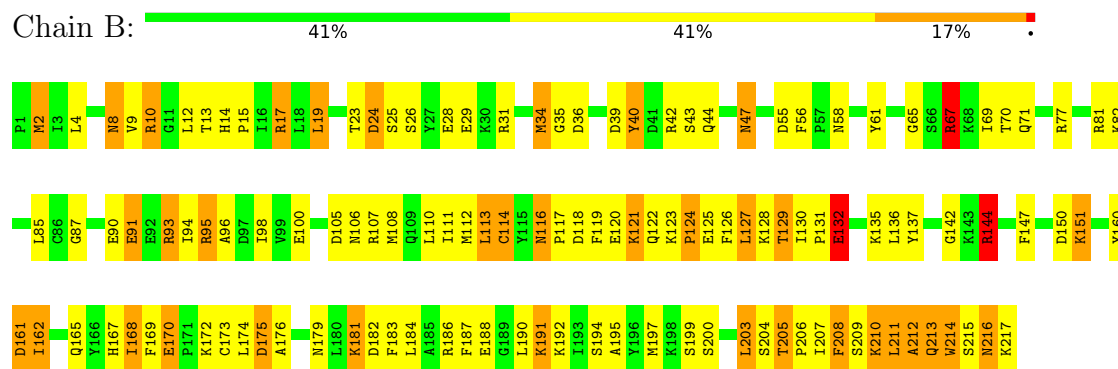
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3



• Molecule 1: MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.24Å 69.44Å 81.28Å 90.00° 106.01° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	75.0 (6.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4096	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	1.25	4/1867 (0.2%)	2.30	102/2515 (4.1%)
1	B	1.23	0/1867	2.31	107/2515 (4.3%)
All	All	1.24	4/3734 (0.1%)	2.30	209/5030 (4.2%)

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	5
1	B	0	3
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	PHE	N-CA	6.50	1.54	1.46
1	A	130	ILE	CA-CB	6.11	1.57	1.54
1	A	160	TYR	N-CA	5.25	1.52	1.46
1	A	6	TYR	CA-CB	5.07	1.62	1.53

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ARG	NE-CZ-NH1	12.48	133.98	121.50
1	A	144	ARG	NE-CZ-NH1	11.04	132.54	121.50
1	A	153	THR	CA-C-O	-10.56	109.24	121.49
1	B	81	ARG	NE-CZ-NH2	-9.94	110.26	119.20
1	B	95	ARG	CD-NE-CZ	9.55	137.77	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ASN	CA-C-O	-9.39	109.49	120.10
1	A	77	ARG	CD-NE-CZ	9.26	137.36	124.40
1	B	39	ASP	N-CA-C	9.25	122.35	111.71
1	A	119	PHE	CA-C-N	9.23	133.03	120.38
1	A	119	PHE	C-N-CA	9.23	133.03	120.38
1	A	73	ASN	CA-C-O	-8.85	111.04	120.42
1	A	186	ARG	NE-CZ-NH1	8.85	130.35	121.50
1	A	24	ASP	CA-CB-CG	-8.80	103.80	112.60
1	B	71	GLN	OE1-CD-NE2	-8.65	113.95	122.60
1	A	97	ASP	O-C-N	-8.49	113.26	122.09
1	B	137	TYR	CA-C-O	8.28	129.52	120.82
1	B	67	ARG	CD-NE-CZ	8.09	135.72	124.40
1	B	213	GLN	N-CA-C	-7.98	102.82	114.39
1	A	99	VAL	CA-C-O	7.98	129.25	120.95
1	A	101	ASN	OD1-CG-ND2	-7.92	114.69	122.60
1	B	58	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	A	107	ARG	NE-CZ-NH2	7.84	126.26	119.20
1	B	100	GLU	CG-CD-OE1	7.73	136.19	118.40
1	B	183	PHE	O-C-N	7.72	130.43	122.09
1	B	9	VAL	CA-CB-CG1	7.70	123.48	110.40
1	A	170	GLU	O-C-N	7.53	127.30	121.27
1	A	88	GLU	CB-CG-CD	7.40	125.18	112.60
1	B	77	ARG	NE-CZ-NH2	-7.34	112.60	119.20
1	B	144	ARG	NE-CZ-NH2	-7.30	112.63	119.20
1	B	210	LYS	N-CA-C	-7.29	104.51	113.19
1	A	72	SER	N-CA-C	7.27	120.13	111.33
1	B	58	ASN	CA-CB-CG	7.26	119.86	112.60
1	A	56	PHE	O-C-N	7.26	127.93	121.32
1	B	151	LYS	CB-CA-C	7.15	125.44	109.56
1	B	116	ASN	CB-CA-C	7.11	118.05	109.31
1	A	120	GLU	N-CA-C	7.09	119.91	111.33
1	B	43	SER	N-CA-C	7.08	119.85	111.71
1	B	67	ARG	NE-CZ-NH1	7.01	128.51	121.50
1	A	13	THR	CA-C-O	-7.00	111.16	119.35
1	A	101	ASN	CB-CG-ND2	6.95	126.82	116.40
1	B	87	GLY	N-CA-C	-6.93	103.20	112.14
1	B	93	ARG	NH1-CZ-NH2	6.92	128.30	119.30
1	B	71	GLN	CG-CD-NE2	6.86	126.69	116.40
1	A	175	ASP	CA-C-O	-6.85	113.63	120.82
1	B	69	ILE	N-CA-C	6.75	118.52	108.46
1	B	61	TYR	CA-C-O	-6.73	113.79	121.40
1	B	93	ARG	NE-CZ-NH1	-6.72	114.78	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	PHE	N-CA-C	6.71	119.43	111.71
1	B	183	PHE	CA-C-O	-6.71	113.79	120.70
1	B	17	ARG	CD-NE-CZ	-6.71	115.01	124.40
1	B	2	MET	N-CA-C	-6.69	100.62	110.52
1	B	168	ILE	N-CA-C	-6.68	103.97	110.72
1	B	98	ILE	CA-C-O	-6.66	114.16	121.29
1	A	153	THR	N-CA-C	-6.66	99.73	109.18
1	B	186	ARG	CA-C-N	6.60	129.41	120.44
1	B	186	ARG	C-N-CA	6.60	129.41	120.44
1	A	73	ASN	O-C-N	6.57	129.64	122.15
1	B	94	ILE	CA-C-O	-6.49	114.29	121.17
1	A	74	ALA	CA-C-N	6.48	128.72	120.56
1	A	74	ALA	C-N-CA	6.48	128.72	120.56
1	B	47	ASN	N-CA-CB	6.47	120.19	110.22
1	B	182	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	123	LYS	CB-CG-CD	6.45	126.13	111.30
1	B	28	GLU	CA-C-O	-6.44	113.90	121.44
1	A	195	ALA	CA-C-N	6.43	129.54	120.28
1	A	195	ALA	C-N-CA	6.43	129.54	120.28
1	B	181	LYS	CA-C-O	-6.40	113.72	120.63
1	A	211	LEU	CA-C-O	-6.35	113.69	120.42
1	A	90	GLU	CA-C-N	6.34	129.11	120.54
1	A	90	GLU	C-N-CA	6.34	129.11	120.54
1	A	122	GLN	CA-C-N	6.34	130.36	120.97
1	A	122	GLN	C-N-CA	6.34	130.36	120.97
1	A	129	THR	CA-C-N	6.32	125.39	120.33
1	A	129	THR	C-N-CA	6.32	125.39	120.33
1	A	33	ALA	N-CA-CB	-6.32	100.71	110.56
1	B	132	GLU	CB-CG-CD	6.29	123.29	112.60
1	B	12	LEU	O-C-N	6.28	129.72	122.25
1	B	121	LYS	CB-CA-C	-6.27	100.38	110.79
1	B	184	LEU	CA-C-O	-6.21	113.09	120.10
1	B	96	ALA	CA-C-N	6.19	128.49	120.44
1	B	96	ALA	C-N-CA	6.19	128.49	120.44
1	B	174	LEU	N-CA-CB	-6.19	101.27	110.61
1	A	41	ASP	CA-C-O	-6.18	113.87	120.92
1	B	194	SER	CA-C-N	6.18	128.47	120.44
1	B	194	SER	C-N-CA	6.18	128.47	120.44
1	B	213	GLN	N-CA-CB	6.18	119.14	110.98
1	A	183	PHE	N-CA-C	-6.15	104.65	111.36
1	A	58	ASN	CA-CB-CG	6.14	118.74	112.60
1	A	10	ARG	CA-C-O	-6.12	114.39	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ASP	CA-CB-CG	-6.11	106.49	112.60
1	A	77	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	A	26	SER	CA-C-O	-6.09	113.84	120.36
1	B	110	LEU	CB-CA-C	6.09	120.52	110.90
1	A	206	PRO	CA-C-N	6.06	130.62	121.65
1	A	206	PRO	C-N-CA	6.06	130.62	121.65
1	B	136	LEU	CA-C-O	-6.00	114.19	120.55
1	A	144	ARG	NE-CZ-NH2	-6.00	113.80	119.20
1	A	122	GLN	OE1-CD-NE2	5.99	128.59	122.60
1	A	30	LYS	N-CA-C	-5.98	98.53	108.34
1	A	191	LYS	CA-C-O	-5.97	114.74	121.00
1	A	140	PHE	CA-C-O	-5.94	114.19	120.55
1	A	204	SER	CA-CB-OG	-5.94	99.22	111.10
1	A	66	SER	CA-C-N	5.91	129.75	121.24
1	A	66	SER	C-N-CA	5.91	129.75	121.24
1	B	167	HIS	CA-CB-CG	-5.90	107.90	113.80
1	B	4	LEU	CA-C-O	-5.88	114.02	120.43
1	A	150	ASP	CA-CB-CG	-5.88	106.72	112.60
1	B	56	PHE	CA-CB-CG	5.86	119.66	113.80
1	B	10	ARG	O-C-N	5.84	128.40	122.09
1	B	81	ARG	CA-C-O	5.84	126.68	119.97
1	B	150	ASP	CA-C-N	-5.83	112.66	122.29
1	B	150	ASP	C-N-CA	-5.83	112.66	122.29
1	A	123	LYS	CG-CD-CE	5.79	124.62	111.30
1	A	96	ALA	CA-C-N	5.79	128.35	120.54
1	A	96	ALA	C-N-CA	5.79	128.35	120.54
1	A	55	ASP	CA-CB-CG	-5.78	106.82	112.60
1	B	181	LYS	N-CA-CB	5.77	118.71	110.06
1	A	26	SER	O-C-N	5.76	129.78	123.22
1	B	120	GLU	CA-C-N	5.75	127.99	120.28
1	B	120	GLU	C-N-CA	5.75	127.99	120.28
1	A	73	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	B	194	SER	CB-CA-C	5.71	120.27	110.79
1	A	214	TRP	CA-C-N	5.70	131.06	122.68
1	A	214	TRP	C-N-CA	5.70	131.06	122.68
1	B	95	ARG	CG-CD-NE	5.70	124.53	112.00
1	B	12	LEU	CA-C-O	-5.69	112.88	119.59
1	A	132	GLU	CA-C-O	-5.68	114.40	120.42
1	A	3	ILE	CA-C-O	-5.64	114.53	120.39
1	B	67	ARG	O-C-N	-5.63	115.87	122.96
1	B	114	CYS	CA-C-O	-5.62	114.92	120.82
1	A	197	MET	N-CA-CB	-5.62	101.57	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	NH1-CZ-NH2	-5.61	112.00	119.30
1	B	65	GLY	O-C-N	5.60	129.99	122.70
1	B	82	LYS	O-C-N	5.60	128.54	122.15
1	A	165	GLN	N-CA-C	5.58	118.08	111.33
1	A	164	ASP	CA-C-O	-5.57	115.15	121.00
1	A	31	ARG	CA-C-O	-5.57	114.82	120.84
1	B	214	TRP	CA-C-O	5.56	127.11	120.28
1	A	183	PHE	O-C-N	5.55	128.47	122.15
1	B	40	TYR	CA-CB-CG	5.54	123.88	113.90
1	A	28	GLU	N-CA-C	-5.53	100.87	109.72
1	B	205	THR	CA-CB-OG1	-5.53	101.30	109.60
1	A	1	PRO	N-CA-CB	-5.53	96.92	103.00
1	B	44	GLN	CB-CA-C	5.53	120.85	110.63
1	A	71	GLN	CG-CD-NE2	5.50	124.65	116.40
1	A	102	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	A	87	GLY	N-CA-C	-5.49	105.62	111.93
1	B	13	THR	CA-CB-OG1	-5.46	101.41	109.60
1	B	70	THR	CA-C-O	-5.46	114.99	121.60
1	A	91	GLU	CG-CD-OE2	-5.41	105.96	118.40
1	B	91	GLU	CB-CG-CD	5.40	121.78	112.60
1	A	118	ASP	CA-CB-CG	-5.38	107.22	112.60
1	B	214	TRP	CB-CA-C	5.37	119.05	109.65
1	A	42	ARG	NE-CZ-NH2	-5.37	114.37	119.20
1	B	160	TYR	CA-C-O	5.37	126.45	120.82
1	B	190	LEU	N-CA-C	-5.37	103.05	110.35
1	B	77	ARG	CD-NE-CZ	5.36	131.90	124.40
1	B	105	ASP	O-C-N	5.36	127.60	122.03
1	B	195	ALA	CA-C-O	-5.34	115.21	120.82
1	A	10	ARG	CD-NE-CZ	-5.34	116.92	124.40
1	B	168	ILE	O-C-N	5.33	127.32	121.83
1	B	2	MET	O-C-N	5.33	128.91	122.94
1	B	204	SER	CA-CB-OG	-5.32	100.47	111.10
1	B	55	ASP	O-C-N	5.29	128.19	122.15
1	B	9	VAL	N-CA-CB	5.29	122.15	112.36
1	B	176	ALA	N-CA-C	5.29	119.36	113.01
1	B	36	ASP	CA-C-O	5.28	128.01	121.94
1	A	69	ILE	N-CA-CB	-5.27	102.79	111.44
1	A	135	LYS	O-C-N	-5.27	116.53	122.12
1	A	133	LYS	CB-CG-CD	5.26	123.39	111.30
1	B	194	SER	CA-CB-OG	5.25	121.60	111.10
1	A	177	PHE	N-CA-C	5.25	118.52	108.97
1	A	191	LYS	O-C-N	5.24	127.48	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	46	LEU	CB-CA-C	5.22	120.59	110.46
1	A	97	ASP	CA-C-O	5.22	126.48	120.90
1	B	90	GLU	CG-CD-OE1	5.21	130.38	118.40
1	A	181	LYS	N-CA-C	-5.20	105.61	111.28
1	A	56	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	28	GLU	CA-CB-CG	5.19	124.49	114.10
1	A	186	ARG	CA-C-N	5.19	127.50	120.65
1	A	186	ARG	C-N-CA	5.19	127.50	120.65
1	B	31	ARG	CA-C-O	-5.18	115.25	120.84
1	A	86	CYS	CA-C-O	-5.16	115.20	121.28
1	B	175	ASP	CA-CB-CG	-5.15	107.45	112.60
1	B	132	GLU	CB-CA-C	5.13	120.86	110.38
1	A	193	ILE	CA-C-O	5.12	126.18	120.71
1	B	25	SER	N-CA-C	-5.12	103.78	110.53
1	A	191	LYS	N-CA-CB	5.11	117.37	109.91
1	A	186	ARG	NH1-CZ-NH2	-5.11	112.66	119.30
1	A	174	LEU	N-CA-CB	-5.09	102.92	110.61
1	B	208	PHE	CA-CB-CG	-5.09	108.71	113.80
1	B	29	GLU	CB-CA-C	-5.08	99.32	109.33
1	A	43	SER	N-CA-C	5.08	118.25	111.75
1	A	33	ALA	CA-C-O	-5.08	115.47	121.66
1	A	41	ASP	CA-CB-CG	-5.06	107.54	112.60
1	A	116	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	34	MET	CA-C-O	-5.05	115.21	121.11
1	A	4	LEU	CA-C-O	-5.04	114.93	120.43
1	B	199	SER	CA-C-O	-5.03	115.50	121.89
1	B	44	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	187	PHE	N-CA-CB	5.03	117.36	110.07
1	A	36	ASP	CA-C-O	-5.02	115.79	121.72
1	B	47	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	8	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	B	106	ASN	CA-C-N	5.01	127.25	120.44
1	B	106	ASN	C-N-CA	5.01	127.25	120.44
1	A	86	CYS	CA-C-N	-5.00	115.35	120.10
1	A	86	CYS	C-N-CA	-5.00	115.35	120.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	165	GLN	Mainchain
1	A	178	PRO	Mainchain
1	A	186	ARG	Sidechain
1	A	42	ARG	Sidechain
1	B	144	ARG	Sidechain
1	B	161	ASP	Mainchain
1	B	17	ARG	Sidechain

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	1818	0	1805	50	0
1	B	1818	0	1805	63	1
2	A	20	0	15	0	0
2	B	20	0	15	0	0
3	A	229	0	0	5	0
3	B	191	0	0	6	0
All	All	4096	0	3640	113	1

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 15.

All (113) 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:123:LYS:HG2	1:B:127:LEU:HD21	1.39	1.03
1:A:95:ARG:HH22	1:A:144:ARG:HH21	1.06	0.92
1:B:125:GLU:HA	1:B:128:LYS:HE3	1.55	0.88
1:A:140:PHE:O	1:A:144:ARG:NH2	2.06	0.88
1:A:95:ARG:HH22	1:A:144:ARG:NH2	1.73	0.87
1:B:212:ALA:HB3	1:B:216:ASN:HB3	1.58	0.84
1:B:34:MET:HE2	1:B:40:TYR:HB3	1.60	0.84
1:A:95:ARG:NH2	1:A:144:ARG:HH21	1.76	0.83
1:A:8:ASN:HD22	1:A:8:ASN:H	1.32	0.76
1:B:108:MET:O	1:B:112:MET:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LYS:NZ	1:A:139:GLU:OE2	2.21	0.73
1:A:8:ASN:HD22	1:A:8:ASN:N	1.86	0.72
1:A:95:ARG:NH2	1:A:144:ARG:HE	1.87	0.72
1:B:95:ARG:NH2	1:B:144:ARG:HE	1.89	0.71
1:B:170:GLU:HB3	1:B:173:CYS:HB3	1.73	0.71
1:A:95:ARG:NH2	1:A:144:ARG:NH2	2.34	0.71
1:B:216:ASN:HD22	1:B:217:LYS:N	1.91	0.69
1:A:37:ALA:HB1	1:A:38:PRO:HA	1.74	0.68
1:A:144:ARG:HD2	1:A:149:GLY:HA2	1.77	0.67
1:B:216:ASN:HD22	1:B:216:ASN:C	2.02	0.66
1:B:91:GLU:O	1:B:95:ARG:HG3	1.96	0.65
1:B:8:ASN:HD22	1:B:8:ASN:H	1.45	0.65
1:A:123:LYS:N	1:A:124:PRO:HD2	2.17	0.60
1:A:106:ASN:ND2	1:A:137:TYR:OH	2.30	0.60
1:A:104:MET:O	1:A:108:MET:HG2	2.01	0.60
1:A:116:ASN:OD1	1:A:118:ASP:HB2	2.02	0.59
1:B:93:ARG:HD3	3:B:345:HOH:O	2.01	0.59
1:A:115:TYR:HE1	1:A:211:LEU:HB2	1.67	0.59
1:B:35:GLY:O	1:B:40:TYR:HA	2.04	0.57
1:B:118:ASP:CG	1:B:121:LYS:HD2	2.30	0.57
1:B:19:LEU:HD22	1:B:23:THR:HG23	1.88	0.56
1:B:127:LEU:HD22	1:B:169:PHE:HE1	1.70	0.56
1:A:13:THR:HG23	1:A:16:ILE:HD12	1.86	0.56
1:A:167:HIS:NE2	1:A:171:PRO:O	2.39	0.56
1:B:8:ASN:HD22	1:B:8:ASN:N	2.02	0.56
1:A:95:ARG:NH2	1:A:144:ARG:NE	2.54	0.56
1:B:24:ASP:HB2	1:B:192:LYS:NZ	2.22	0.55
1:B:127:LEU:HD13	1:B:170:GLU:OE2	2.07	0.55
1:B:172:LYS:HD2	1:B:175:ASP:OD2	2.07	0.54
1:B:113:LEU:O	1:B:116:ASN:HB3	2.08	0.54
1:A:70:THR:O	1:A:71:GLN:HB2	2.06	0.53
1:B:2:MET:HE1	3:B:250:HOH:O	2.08	0.52
1:B:125:GLU:OE2	1:B:128:LYS:NZ	2.27	0.52
1:B:118:ASP:O	1:B:121:LYS:HB2	2.10	0.51
1:A:8:ASN:H	1:A:8:ASN:ND2	2.01	0.50
1:A:68:LYS:C	1:A:69:ILE:HG13	2.35	0.50
1:B:132:GLU:HG3	3:B:306:HOH:O	2.10	0.50
1:A:15:PRO:HG2	3:A:233:HOH:O	2.13	0.48
1:A:45:TRP:CZ2	1:A:49:LYS:HG3	2.48	0.48
1:B:19:LEU:HD21	1:B:85:LEU:HD13	1.96	0.48
1:B:132:GLU:OE2	1:B:135:LYS:HE3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:HD22	1:B:126:PHE:CG	2.49	0.48
1:A:119:PHE:HB2	1:A:213:GLN:HG3	1.96	0.48
1:B:168:ILE:HG22	1:B:214:TRP:HZ2	1.79	0.47
1:A:39:ASP:OD1	1:A:39:ASP:N	2.47	0.46
1:A:58:ASN:ND2	3:A:320:HOH:O	2.40	0.46
1:A:205:THR:HA	1:A:206:PRO:C	2.40	0.46
1:B:123:LYS:HB3	1:B:124:PRO:CD	2.46	0.46
1:A:116:ASN:HA	1:A:117:PRO:HD2	1.79	0.45
1:B:216:ASN:C	1:B:216:ASN:ND2	2.73	0.45
1:B:130:ILE:N	1:B:131:PRO:CD	2.79	0.45
1:B:209:SER:OG	1:B:211:LEU:HB2	2.17	0.45
1:A:161:ASP:O	1:A:165:GLN:HG3	2.16	0.45
1:B:24:ASP:HB2	1:B:192:LYS:HZ1	1.80	0.45
1:B:10:ARG:HB3	1:B:207:ILE:HA	1.99	0.45
1:B:107:ARG:O	1:B:111:ILE:HG13	2.17	0.45
1:B:114:CYS:O	1:B:213:GLN:HG2	2.17	0.45
1:A:173:CYS:SG	1:A:174:LEU:HD13	2.56	0.45
1:B:19:LEU:HD22	1:B:23:THR:CG2	2.47	0.45
1:A:95:ARG:NH2	1:A:144:ARG:CZ	2.80	0.44
1:B:119:PHE:CB	1:B:213:GLN:HG3	2.47	0.44
1:A:67:ARG:NE	3:A:374:HOH:O	2.45	0.44
1:B:162:ILE:HD12	1:B:162:ILE:HA	1.82	0.44
1:A:116:ASN:C	1:A:118:ASP:N	2.74	0.43
1:A:152:VAL:HG23	3:A:268:HOH:O	2.18	0.43
1:A:153:THR:OG1	1:A:155:VAL:HG22	2.17	0.43
1:A:123:LYS:N	1:A:124:PRO:CD	2.80	0.43
1:B:112:MET:HE3	1:B:112:MET:HB3	1.87	0.43
1:B:205:THR:HA	1:B:206:PRO:C	2.43	0.43
1:B:203:LEU:HD23	1:B:203:LEU:C	2.44	0.43
1:A:191:LYS:HZ1	1:A:192:LYS:CE	2.31	0.43
1:B:95:ARG:NH2	1:B:144:ARG:NE	2.64	0.42
1:B:116:ASN:HA	1:B:117:PRO:HD3	1.81	0.42
1:A:100:GLU:OE1	1:A:154:TYR:OH	2.32	0.42
1:B:24:ASP:CG	1:B:192:LYS:NZ	2.78	0.42
1:B:208:PHE:HB3	1:B:212:ALA:HB2	2.01	0.42
1:B:125:GLU:O	1:B:129:THR:HG23	2.20	0.42
1:A:111:ILE:HG12	1:A:208:PHE:CE1	2.54	0.42
1:A:145:PRO:O	1:A:186:ARG:NH1	2.53	0.42
1:B:122:GLN:O	1:B:123:LYS:C	2.61	0.42
1:A:64:ASP:OD2	1:A:78:TYR:OH	2.33	0.42
1:B:191:LYS:O	1:B:191:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:HE3	1:A:76:MET:HB3	1.96	0.41
1:B:124:PRO:HA	3:B:357:HOH:O	2.19	0.41
1:B:95:ARG:NH1	3:B:312:HOH:O	2.53	0.41
1:A:113:LEU:HD22	1:A:126:PHE:CG	2.55	0.41
1:B:19:LEU:CD2	1:B:23:THR:HG23	2.50	0.41
1:B:128:LYS:O	1:B:131:PRO:HD2	2.21	0.41
1:B:161:ASP:O	1:B:165:GLN:HG3	2.20	0.41
1:A:118:ASP:O	1:A:119:PHE:C	2.64	0.41
1:B:47:ASN:ND2	3:B:294:HOH:O	2.53	0.41
1:B:188:GLU:HG2	1:B:197:MET:SD	2.61	0.41
1:A:205:THR:HB	1:A:206:PRO:HA	2.03	0.41
1:B:142:GLY:O	1:B:179:ASN:ND2	2.51	0.41
1:B:208:PHE:CB	1:B:212:ALA:HB2	2.51	0.41
1:A:47:ASN:HB3	3:A:331:HOH:O	2.20	0.40
1:B:214:TRP:O	1:B:215:SER:C	2.64	0.40
1:A:35:GLY:O	1:A:210:LYS:HD2	2.22	0.40
1:B:175:ASP:OD1	1:B:181:LYS:NZ	2.48	0.40
1:B:14:HIS:N	1:B:15:PRO:CD	2.84	0.40
1:A:10:ARG:HG3	1:A:14:HIS:HB2	2.02	0.40
1:A:150:ASP:C	1:A:151:LYS:HG3	2.45	0.40
1:B:24:ASP:CB	1:B:192:LYS:NZ	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ARG:NH1	1:B:67:ARG:NH1[2_555]	2.04	0.16

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	215/217 (99%)	210 (98%)	4 (2%)	1 (0%)	24	27
1	B	215/217 (99%)	205 (95%)	8 (4%)	2 (1%)	14	14
All	All	430/434 (99%)	415 (96%)	12 (3%)	3 (1%)	18	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	212	ALA
1	A	40	TYR
1	B	124	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	197/197 (100%)	184 (93%)	13 (7%)	15	18
1	B	197/197 (100%)	178 (90%)	19 (10%)	8	8
All	All	394/394 (100%)	362 (92%)	32 (8%)	11	12

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	8	ASN
1	A	14	HIS
1	A	19	LEU
1	A	30	LYS
1	A	46	LEU
1	A	123	LYS
1	A	143	LYS
1	A	152	VAL
1	A	162	ILE
1	A	191	LYS
1	A	204	SER
1	A	211	LEU

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Mol	Chain	Res	Type
1	B	8	ASN
1	B	19	LEU
1	B	26	SER
1	B	34	MET
1	B	42	ARG
1	B	67	ARG
1	B	113	LEU
1	B	127	LEU
1	B	129	THR
1	B	132	GLU
1	B	151	LYS
1	B	162	ILE
1	B	170	GLU
1	B	191	LYS
1	B	200	SER
1	B	203	LEU
1	B	210	LYS
1	B	211	LEU
1	B	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	47	ASN
1	A	58	ASN
1	A	106	ASN
1	A	179	ASN
1	B	8	ASN
1	B	47	ASN
1	B	106	ASN
1	B	122	GLN
1	B	216	ASN

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 ⓘ

2 ligands are 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	B	218	-	18,19,19	2.30	6 (33%)	21,24,24	3.06	10 (47%)
2	GSH	A	218	-	18,19,19	2.04	8 (44%)	21,24,24	2.50	7 (33%)

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	B	218	-	-	2/24/24/24	-
2	GSH	A	218	-	-	4/24/24/24	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	218	GSH	O12-C1	4.65	1.35	1.22
2	B	218	GSH	CB2-CA2	4.37	1.57	1.53
2	A	218	GSH	O12-C1	4.31	1.34	1.22
2	B	218	GSH	O32-C3	3.40	1.33	1.22
2	B	218	GSH	CA2-N2	2.91	1.51	1.45
2	A	218	GSH	O32-C3	2.84	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	218	GSH	CG1-CD1	-2.53	1.46	1.51
2	A	218	GSH	O11-C1	-2.49	1.22	1.30
2	A	218	GSH	CB2-CA2	2.44	1.55	1.53
2	B	218	GSH	O11-C1	-2.40	1.23	1.30
2	A	218	GSH	CB1-CG1	-2.37	1.45	1.52
2	A	218	GSH	CB1-CA1	2.14	1.57	1.53
2	B	218	GSH	CG1-CD1	-2.14	1.47	1.51
2	A	218	GSH	OE1-CD1	2.04	1.27	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	218	GSH	CA2-CB2-SG2	-7.23	106.01	114.16
2	A	218	GSH	CA2-CB2-SG2	-5.89	107.51	114.16
2	A	218	GSH	CB1-CG1-CD1	5.48	125.28	113.06
2	B	218	GSH	OE1-CD1-N2	4.76	131.01	122.95
2	B	218	GSH	CG1-CB1-CA1	-4.49	103.55	113.86
2	B	218	GSH	O31-C3-O32	-4.49	111.79	123.33
2	B	218	GSH	CB2-CA2-N2	-4.25	105.22	111.28
2	A	218	GSH	CA3-N3-C2	-4.08	111.09	121.38
2	B	218	GSH	OE1-CD1-CG1	-3.71	115.31	122.02
2	A	218	GSH	O31-C3-CA3	3.16	124.84	112.81
2	B	218	GSH	O31-C3-CA3	3.16	124.81	112.81
2	B	218	GSH	O2-C2-CA2	-3.13	113.93	120.48
2	B	218	GSH	C2-CA2-N2	-2.99	103.02	111.11
2	A	218	GSH	O31-C3-O32	-2.83	116.06	123.33
2	A	218	GSH	O2-C2-CA2	-2.46	115.33	120.48
2	A	218	GSH	OE1-CD1-N2	2.12	126.54	122.95
2	B	218	GSH	CA2-N2-CD1	-2.00	116.66	121.68

There are no chirality outliers.

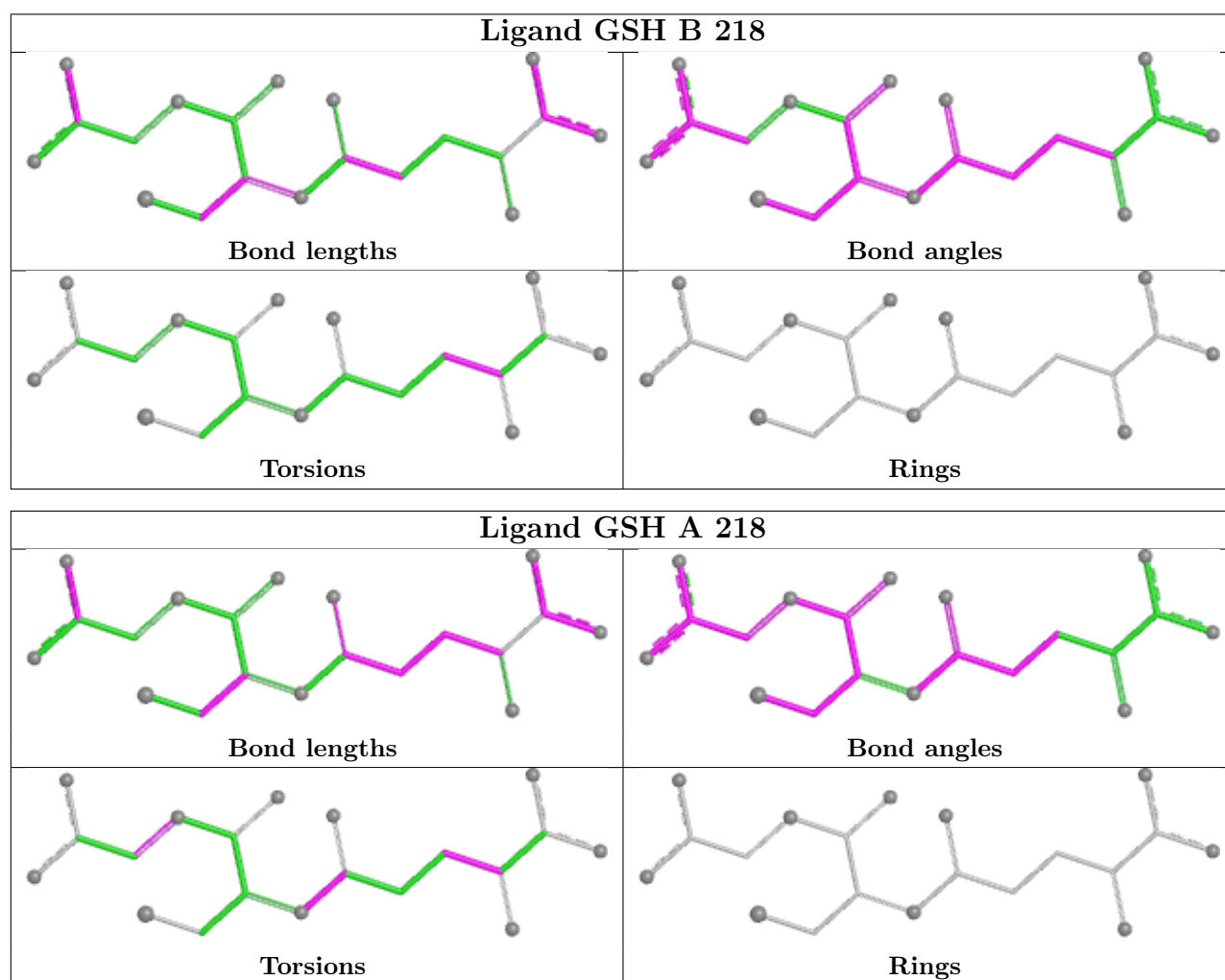
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	218	GSH	N1-CA1-CB1-CG1
2	B	218	GSH	C1-CA1-CB1-CG1
2	A	218	GSH	OE1-CD1-N2-CA2
2	A	218	GSH	CG1-CD1-N2-CA2
2	A	218	GSH	C1-CA1-CB1-CG1
2	A	218	GSH	C3-CA3-N3-C2

There are no ring outliers.

No monomer is involved in short contacts.

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.