



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:08 PM UTC

PDB ID : 1OE8 / pdb_00001oe8
Title : 28kDa glutathione S-transferase from Schistosoma haematobium (glutathione saturated)
Authors : Johnson, K.A.; Angelucci, F.; Tsernoglou, D.
Deposited on : 2003-03-19
Resolution : 1.65 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

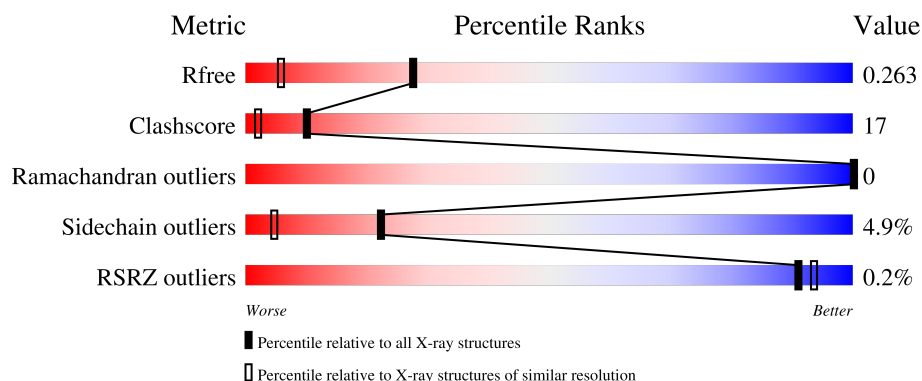
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	211	
1	B	211	

2 Entry composition [i](#)

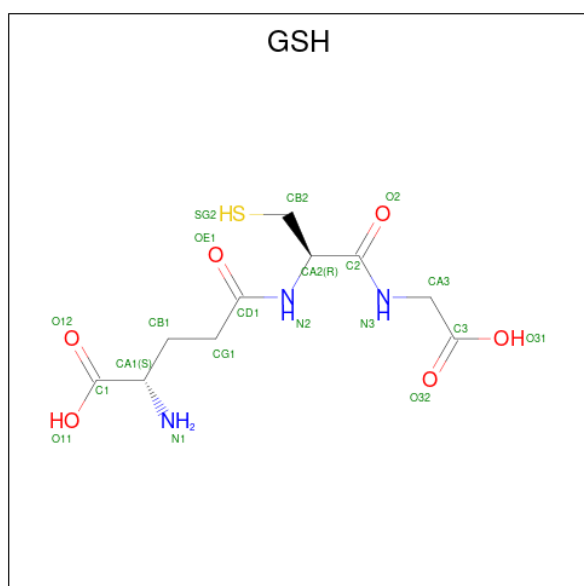
There are 3 unique types of molecules in this entry. The entry contains 3684 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	204	Total	C	N	O	S	0	7	0
			1662	1066	285	303	8			
1	B	205	Total	C	N	O	S	0	7	0
			1666	1068	286	304	8			

- 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	159	Total 159	O 159	0	0
3	B	157	Total 157	O 157	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 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.

• Molecule 1: GLUTATHIONE S-TRANSFERASE



• Molecule 1: GLUTATHIONE S-TRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.14Å 77.70Å 53.20Å 90.00° 93.40° 90.00°	Depositor
Resolution (Å)	25.00 – 1.65 25.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.0 (25.00-1.65) 98.5 (25.00-1.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.280 0.215 , 0.263	Depositor DCC
R_{free} test set	2621 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.477 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3684	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	1.61	15/1724 (0.9%)	2.54	117/2324 (5.0%)
1	B	1.59	14/1728 (0.8%)	2.43	108/2329 (4.6%)
All	All	1.60	29/3452 (0.8%)	2.48	225/4653 (4.8%)

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	2
1	B	0	1
All	All	0	3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	TYR	CA-CB	10.19	1.59	1.52
1	A	182	TYR	CA-CB	8.85	1.58	1.52
1	A	142	SER	C-O	-7.23	1.15	1.24
1	A	162	VAL	C-N	6.76	1.42	1.33
1	B	74	ILE	C-N	6.52	1.42	1.33
1	A	159	ALA	C-N	6.50	1.42	1.33
1	A	74	ILE	C-N	6.46	1.42	1.33
1	B	162	VAL	C-N	6.23	1.42	1.33
1	A	150	LEU	N-CA	5.98	1.53	1.45
1	A	191	ASN	C-N	5.81	1.41	1.33
1	A	20	ILE	C-O	-5.69	1.17	1.24
1	B	190	GLU	N-CA	5.68	1.53	1.46
1	B	70	GLU	C-N	5.47	1.40	1.33
1	A	20	ILE	CA-C	5.46	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	193	LEU	N-CA	5.40	1.53	1.46
1	B	103	GLU	N-CA	5.39	1.53	1.46
1	B	163	LEU	CA-CB	5.37	1.61	1.53
1	A	103	GLU	N-CA	5.34	1.53	1.46
1	A	79	ALA	C-O	5.32	1.30	1.24
1	B	54	PRO	N-CD	5.29	1.55	1.47
1	A	193	LEU	N-CA	5.29	1.53	1.46
1	A	79	ALA	C-N	-5.25	1.27	1.33
1	A	192	LEU	CA-CB	5.23	1.61	1.53
1	B	83	HIS	C-O	-5.20	1.17	1.23
1	B	71	SER	CA-C	-5.16	1.46	1.52
1	B	56	VAL	C-O	-5.13	1.18	1.24
1	A	21	ARG	CD-NE	-5.12	1.39	1.46
1	B	43	LYS	CA-CB	5.05	1.61	1.53
1	B	21	ARG	CD-NE	-5.03	1.39	1.46

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	HIS	CA-CB-CG	-16.83	96.97	113.80
1	B	21	ARG	CD-NE-CZ	13.57	143.39	124.40
1	A	107	HIS	CA-CB-CG	-13.46	100.34	113.80
1	A	146	SER	O-C-N	11.63	136.58	122.86
1	A	94	ASN	CA-CB-CG	-10.97	101.63	112.60
1	A	159	ALA	CA-C-O	10.95	132.62	120.90
1	A	139	ILE	O-C-N	10.84	132.38	121.87
1	B	94	ASN	CA-CB-CG	-10.54	102.06	112.60
1	A	159	ALA	O-C-N	-10.11	111.57	122.09
1	A	189	ARG	O-C-N	9.76	132.63	122.09
1	A	47	THR	CA-C-N	-9.71	114.11	123.04
1	A	47	THR	C-N-CA	-9.71	114.11	123.04
1	A	143	LEU	O-C-N	9.49	132.18	122.12
1	A	146	SER	CA-C-O	-9.14	111.60	121.56
1	B	66	LYS	O-C-N	8.94	133.93	123.30
1	B	83	HIS	CA-CB-CG	-8.91	104.89	113.80
1	B	139	ILE	O-C-N	8.86	130.60	121.91
1	A	139	ILE	CA-C-O	-8.66	111.94	120.95
1	A	11[A]	PHE	CA-CB-CG	8.62	122.42	113.80
1	A	11[B]	PHE	CA-CB-CG	8.62	122.42	113.80
1	B	190	GLU	O-C-N	-8.52	113.08	122.12
1	A	7	LYS	O-C-N	8.49	133.40	123.30
1	A	106	GLU	CA-C-O	-8.47	111.57	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ARG	NE-CZ-NH2	-8.41	111.63	119.20
1	B	78[A]	MET	CA-C-O	8.41	129.33	120.42
1	B	78[B]	MET	CA-C-O	8.41	129.33	120.42
1	B	4	ASP	N-CA-C	8.40	122.61	110.10
1	A	21	ARG	CD-NE-CZ	8.35	136.09	124.40
1	A	189	ARG	CA-C-O	-8.21	112.24	120.70
1	B	189	ARG	O-C-N	8.20	130.52	122.07
1	A	20	ILE	O-C-N	8.19	130.42	121.90
1	B	71	SER	N-CA-C	8.11	120.84	111.11
1	A	83	HIS	CA-CB-CG	-8.10	105.70	113.80
1	B	48	ILE	O-C-N	-8.06	113.63	121.12
1	A	48	ILE	O-C-N	-8.00	114.33	121.61
1	B	195	SER	CA-C-O	7.80	128.98	119.31
1	B	189	ARG	CA-C-O	-7.62	112.82	120.82
1	B	21	ARG	NE-CZ-NH2	-7.57	112.38	119.20
1	A	149	LYS	O-C-N	7.55	132.80	122.46
1	A	52	ARG	CD-NE-CZ	-7.53	113.85	124.40
1	A	55	ALA	CA-C-N	-7.51	112.70	123.06
1	A	55	ALA	C-N-CA	-7.51	112.70	123.06
1	B	146	SER	CA-C-O	-7.36	113.75	121.55
1	A	191	ASN	O-C-N	-7.36	114.49	122.07
1	B	78[A]	MET	O-C-N	-7.33	113.79	122.15
1	B	78[B]	MET	O-C-N	-7.33	113.79	122.15
1	A	64	HIS	CA-C-O	-7.33	112.70	121.05
1	B	191	ASN	O-C-N	-7.29	114.56	122.07
1	A	149	LYS	CG-CD-CE	7.26	128.00	111.30
1	B	164	ILE	CA-C-O	-7.23	113.19	120.85
1	B	106	GLU	CG-CD-OE1	7.22	135.01	118.40
1	A	118	GLU	CA-C-O	-7.13	113.33	120.82
1	A	18	GLU	CG-CD-OE2	7.07	134.66	118.40
1	A	177	PHE	CA-CB-CG	-7.03	106.77	113.80
1	B	64	HIS	O-C-N	7.00	131.28	123.01
1	A	66	LYS	CA-C-N	-6.99	111.61	122.87
1	A	66	LYS	C-N-CA	-6.99	111.61	122.87
1	B	172	ASP	CA-C-O	-6.98	113.15	120.55
1	A	191	ASN	CA-C-O	6.90	128.06	120.82
1	A	66	LYS	O-C-N	6.89	131.50	123.30
1	A	84	MET	CA-C-O	-6.79	112.52	120.53
1	B	139	ILE	CA-C-O	-6.75	114.02	121.17
1	B	21	ARG	NE-CZ-NH1	6.72	128.22	121.50
1	A	90	GLU	CB-CG-CD	6.69	123.98	112.60
1	A	136	LEU	CA-C-O	-6.69	113.33	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ASP	N-CA-C	-6.68	104.07	111.82
1	A	78[A]	MET	CA-C-O	6.66	127.48	120.42
1	A	78[B]	MET	CA-C-O	6.66	127.48	120.42
1	A	91	GLU	CA-C-O	-6.66	113.50	120.55
1	B	129	ASN	OD1-CG-ND2	6.64	129.24	122.60
1	B	55	ALA	CA-C-N	-6.63	113.78	122.99
1	B	55	ALA	C-N-CA	-6.63	113.78	122.99
1	B	64	HIS	CA-C-O	-6.59	113.54	121.05
1	B	7	LYS	O-C-N	6.55	131.02	123.29
1	B	81	LYS	O-C-N	-6.51	114.60	122.22
1	B	35	ARG	NE-CZ-NH1	-6.50	115.00	121.50
1	B	66	LYS	CA-C-O	-6.49	113.35	120.36
1	B	191	ASN	CA-C-O	6.47	127.61	120.82
1	B	177	PHE	CA-CB-CG	-6.46	107.34	113.80
1	B	66	LYS	CA-C-N	-6.43	112.52	122.87
1	B	66	LYS	C-N-CA	-6.43	112.52	122.87
1	A	179	THR	CA-C-O	6.38	128.14	120.81
1	A	160	ASP	CA-C-O	-6.37	113.80	120.55
1	B	8	VAL	CA-C-O	-6.35	113.67	120.59
1	A	59	THR	CA-C-O	-6.32	113.37	120.32
1	B	151	ALA	O-C-N	-6.30	115.44	122.12
1	B	52	ARG	CD-NE-CZ	-6.28	115.61	124.40
1	B	142	SER	O-C-N	6.28	128.53	122.07
1	B	202	TYR	CA-C-N	6.27	129.19	120.29
1	B	202	TYR	C-N-CA	6.27	129.19	120.29
1	A	129	ASN	CA-CB-CG	-6.27	106.33	112.60
1	A	64	HIS	O-C-N	6.26	130.40	123.01
1	B	146	SER	O-C-N	6.25	130.50	122.81
1	B	195	SER	O-C-N	-6.23	113.86	122.46
1	B	49	PRO	O-C-N	6.21	131.03	122.64
1	B	90	GLU	CB-CG-CD	6.20	123.14	112.60
1	A	76	ARG	N-CA-CB	-6.19	100.69	110.28
1	A	21	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	A	7	LYS	CA-C-O	-6.15	113.72	120.36
1	A	82	HIS	ND1-CE1-NE2	6.14	114.54	108.40
1	A	151	ALA	O-C-N	-6.14	115.61	122.12
1	A	149	LYS	CA-C-N	-6.12	110.98	122.73
1	A	149	LYS	C-N-CA	-6.12	110.98	122.73
1	B	11[A]	PHE	O-C-N	6.10	130.32	122.03
1	B	11[B]	PHE	O-C-N	6.10	130.32	122.03
1	B	104	ASP	N-CA-C	-6.09	104.75	111.82
1	A	121	GLN	CB-CA-C	-6.08	100.69	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ARG	CB-CG-CD	-6.04	97.41	111.30
1	B	48	ILE	CB-CA-C	-6.04	103.91	110.85
1	A	11[A]	PHE	O-C-N	6.02	130.22	122.03
1	A	11[B]	PHE	O-C-N	6.02	130.22	122.03
1	A	12	ASN	OD1-CG-ND2	6.00	128.60	122.60
1	A	106	GLU	N-CA-C	-6.00	104.74	111.28
1	A	88	THR	CA-C-O	-5.99	114.63	121.58
1	B	170	VAL	N-CA-C	-5.99	104.67	110.42
1	B	85	MET	CA-CB-CG	5.95	126.00	114.10
1	B	16[A]	ARG	N-CA-C	5.95	119.80	112.54
1	B	16[B]	ARG	N-CA-C	5.95	119.80	112.54
1	B	84	MET	CA-C-O	-5.93	113.36	120.65
1	A	177	PHE	N-CA-C	5.93	118.50	111.33
1	A	134	VAL	CA-C-O	5.89	127.08	120.95
1	A	143	LEU	CA-C-O	-5.89	114.31	120.55
1	A	8	VAL	CA-C-O	-5.88	114.18	120.59
1	A	80	LYS	O-C-N	5.88	128.13	122.07
1	B	188	HIS	O-C-N	-5.88	115.97	122.09
1	B	190	GLU	CA-C-O	5.88	126.78	120.55
1	A	190	GLU	O-C-N	-5.87	116.02	122.07
1	B	91	GLU	CA-C-O	-5.86	114.34	120.55
1	A	175	LYS	O-C-N	-5.85	114.78	122.39
1	B	76	ARG	O-C-N	5.83	129.44	122.27
1	A	48	ILE	CB-CA-C	-5.80	104.38	110.53
1	B	143	LEU	O-C-N	5.78	128.25	122.12
1	B	174	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	27	ALA	CA-C-O	-5.77	111.72	119.11
1	B	57	LYS	CA-C-N	-5.76	115.63	123.12
1	B	57	LYS	C-N-CA	-5.76	115.63	123.12
1	A	55	ALA	CA-C-O	-5.76	114.38	121.06
1	B	21	ARG	CB-CG-CD	-5.73	98.11	111.30
1	B	40	ASP	O-C-N	5.72	129.49	122.34
1	A	20	ILE	CA-C-O	-5.71	114.71	121.05
1	A	206	ARG	CD-NE-CZ	5.71	132.39	124.40
1	B	59	THR	OG1-CB-CG2	-5.69	97.92	109.30
1	B	170	VAL	CA-C-O	-5.69	115.14	121.17
1	A	149	LYS	CA-C-O	-5.67	112.64	119.27
1	B	43	LYS	N-CA-C	5.66	117.53	111.36
1	B	163	LEU	CA-C-N	-5.64	112.41	120.42
1	B	163	LEU	C-N-CA	-5.64	112.41	120.42
1	B	61	ASN	O-C-N	-5.62	115.11	122.59
1	B	105	LEU	O-C-N	-5.60	115.77	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	GLU	O-C-N	5.58	128.03	122.12
1	A	203	LEU	O-C-N	5.58	128.51	122.15
1	A	154	ASP	N-CA-CB	-5.53	102.27	110.61
1	A	7	LYS	CA-C-N	-5.49	115.88	122.90
1	A	7	LYS	C-N-CA	-5.49	115.88	122.90
1	A	84	MET	O-C-N	5.44	129.48	122.19
1	A	95	VAL	O-C-N	5.43	127.23	121.91
1	A	162	VAL	CA-C-N	-5.43	113.01	120.28
1	A	162	VAL	C-N-CA	-5.43	113.01	120.28
1	A	95	VAL	CB-CA-C	-5.42	105.03	111.97
1	A	136	LEU	N-CA-C	-5.42	105.46	111.36
1	B	93	TYR	CA-C-O	5.41	126.69	120.90
1	B	33	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	201	LYS	CA-C-O	5.38	126.47	120.82
1	B	47	THR	CA-C-N	-5.37	114.86	123.46
1	B	47	THR	C-N-CA	-5.37	114.86	123.46
1	A	26	ALA	CA-C-O	5.37	126.17	120.10
1	B	202	TYR	O-C-N	-5.35	116.56	122.07
1	B	149	LYS	O-C-N	5.33	129.97	122.41
1	B	65	VAL	N-CA-CB	-5.32	101.37	111.21
1	B	162	VAL	CA-C-N	-5.32	113.15	120.28
1	B	162	VAL	C-N-CA	-5.32	113.15	120.28
1	A	95	VAL	N-CA-C	-5.32	105.32	110.42
1	A	66	LYS	CA-C-O	-5.31	114.62	120.36
1	B	149	LYS	CB-CG-CD	5.31	123.51	111.30
1	A	160	ASP	O-C-N	5.29	127.72	122.12
1	A	123	ILE	CA-CB-CG1	5.27	119.36	110.40
1	B	66	LYS	N-CA-C	-5.27	100.31	108.90
1	A	137	ASP	N-CA-CB	-5.25	102.38	110.16
1	A	172	ASP	CA-C-O	-5.25	114.17	120.10
1	A	160	ASP	CB-CA-C	-5.24	102.09	110.79
1	B	188	HIS	CG-CD2-NE2	5.24	112.44	107.20
1	A	183	PRO	O-C-N	-5.22	115.97	122.23
1	B	136	LEU	N-CA-C	-5.22	105.67	111.36
1	B	142	SER	CA-C-O	-5.20	115.36	120.82
1	B	48	ILE	N-CA-CB	-5.20	104.84	111.39
1	B	172	ASP	CB-CA-C	-5.18	102.19	110.79
1	A	95	VAL	CA-C-O	-5.17	115.68	121.17
1	A	33	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	103	GLU	CA-CB-CG	-5.16	103.78	114.10
1	A	11[A]	PHE	CA-C-N	-5.15	114.98	122.65
1	A	11[A]	PHE	C-N-CA	-5.15	114.98	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11[B]	PHE	CA-C-N	-5.15	114.98	122.65
1	A	11[B]	PHE	C-N-CA	-5.15	114.98	122.65
1	B	61	ASN	CA-C-N	5.14	130.45	122.49
1	B	61	ASN	C-N-CA	5.14	130.45	122.49
1	B	92	TYR	CA-C-O	-5.14	115.10	120.55
1	B	118	GLU	CA-C-O	-5.13	115.43	121.07
1	A	137	ASP	CA-CB-CG	-5.12	107.47	112.60
1	A	23	THR	CA-CB-OG1	-5.11	101.93	109.60
1	A	102	ALA	CA-C-O	-5.11	115.14	120.55
1	B	35	ARG	CB-CA-C	5.10	118.17	109.75
1	A	170	VAL	N-CA-C	-5.09	105.53	110.42
1	A	128	LEU	CA-C-O	5.08	125.63	119.38
1	A	157	THR	N-CA-CB	5.08	119.25	111.22
1	B	79	ALA	CA-C-O	-5.08	115.16	120.55
1	A	193	LEU	N-CA-C	-5.08	105.93	111.82
1	B	127	ILE	CA-C-O	5.08	125.96	120.47
1	A	93	TYR	CG-CD2-CE2	-5.08	113.59	121.20
1	B	15	GLY	O-C-N	5.08	128.44	123.31
1	A	86	GLY	N-CA-C	-5.07	106.61	112.29
1	A	152	VAL	O-C-N	5.07	127.95	123.03
1	B	169	HIS	ND1-CE1-NE2	5.07	113.47	108.40
1	A	30	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	104	ASP	CA-C-O	-5.07	114.14	119.97
1	B	9	ILE	CA-C-N	-5.05	113.72	122.10
1	B	9	ILE	C-N-CA	-5.05	113.72	122.10
1	B	112	THR	N-CA-C	5.04	119.28	113.18
1	B	35	ARG	CA-C-O	5.04	125.92	120.43
1	A	202	TYR	CA-C-N	5.04	127.44	120.29
1	A	202	TYR	C-N-CA	5.04	127.44	120.29
1	B	15	GLY	N-CA-C	-5.03	104.20	111.20
1	B	105	LEU	CA-C-O	5.03	125.75	120.42
1	B	21	ARG	CG-CD-NE	-5.03	100.94	112.00
1	A	201	LYS	CA-C-O	5.01	126.09	120.82
1	A	187	LYS	CA-C-O	5.01	125.86	120.55

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	THR	Mainchain
1	A	73	ALA	Mainchain
1	B	84	MET	Mainchain

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	1662	0	1700	55	0
1	B	1666	0	1703	63	0
2	A	20	0	15	1	0
2	B	20	0	15	1	0
3	A	159	0	0	16	1
3	B	157	0	0	13	1
All	All	3684	0	3433	118	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 17.

All (118) 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:64:HIS:ND1	3:B:2067:HOH:O	1.72	1.17
1:A:14:ARG:HD3	1:A:206:ARG:NH1	1.67	1.10
1:B:5:HIS:ND1	3:B:2004:HOH:O	1.83	1.08
1:B:98[B]:LEU:HD22	3:B:2117:HOH:O	1.53	1.06
1:B:11[A]:PHE:CD1	3:B:2038:HOH:O	2.07	1.05
1:B:11[A]:PHE:CE1	3:B:2038:HOH:O	2.14	0.98
1:A:155:LYS:HD3	3:A:2124:HOH:O	1.63	0.97
1:A:5:HIS:ND1	3:A:2001:HOH:O	1.98	0.89
1:A:144:LYS:NZ	3:A:2113:HOH:O	2.04	0.88
1:A:98[B]:LEU:HD13	1:A:151:ALA:HB1	1.59	0.84
1:A:141:GLU:OE1	3:A:2113:HOH:O	1.94	0.83
1:A:14:ARG:HD3	1:A:206:ARG:CZ	2.08	0.83
1:A:106:GLU:OE2	1:A:166[B]:VAL:HG22	1.77	0.83
1:B:106:GLU:OE1	1:B:166[B]:VAL:HG22	1.79	0.82
1:B:3:GLY:HA3	1:B:61:ASN:HB3	1.64	0.80
1:A:98[B]:LEU:HD12	3:A:2115:HOH:O	1.82	0.80
1:B:90:GLU:OE2	3:B:2088:HOH:O	1.99	0.79
1:B:5:HIS:CE1	3:B:2004:HOH:O	2.30	0.76
1:B:7:LYS:HD3	1:B:34:GLU:OE2	1.86	0.75
1:B:90:GLU:OE2	3:B:2089:HOH:O	2.04	0.75
1:B:14:ARG:HD3	1:B:206:ARG:CZ	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:CD	3:A:2124:HOH:O	2.24	0.73
1:A:98[A]:LEU:HD22	1:A:151:ALA:HB1	1.68	0.72
1:B:98[A]:LEU:CD1	1:B:151:ALA:HB1	2.23	0.69
1:B:16[B]:ARG:NH1	2:B:301:GSH:SG2	2.65	0.69
1:A:149:LYS:N	1:A:149:LYS:HD2	2.07	0.69
1:B:63:GLY:O	3:B:2066:HOH:O	2.10	0.68
1:B:162:VAL:HG13	3:B:2099:HOH:O	1.94	0.66
1:B:98[B]:LEU:HD23	1:B:151:ALA:HB1	1.79	0.64
1:A:155:LYS:CE	3:A:2124:HOH:O	2.44	0.64
1:B:74:ILE:CG2	1:B:78[A]:MET:HE3	2.28	0.64
1:A:43:LYS:HE3	1:A:44:ILE:HD11	1.79	0.63
1:A:117:GLU:O	1:A:121:GLN:HG2	1.98	0.63
1:B:43:LYS:HE3	1:B:44:ILE:HD11	1.83	0.61
1:B:120:LYS:O	1:B:124:ILE:HG13	2.04	0.58
1:A:118:GLU:O	1:A:122:LYS:HE2	2.03	0.58
1:B:18:GLU:HG3	1:B:22:MET:HE3	1.87	0.57
1:A:53:LEU:HB3	1:A:54:PRO:HA	1.87	0.57
1:B:10[A]:TYR:CD2	1:B:17:ALA:CB	2.88	0.57
1:B:98[A]:LEU:HD13	1:B:151:ALA:HB1	1.86	0.57
1:B:24:LEU:HD21	1:B:78[A]:MET:SD	2.45	0.56
1:B:10[A]:TYR:HD2	1:B:17:ALA:HB3	1.70	0.56
1:A:24:LEU:HD21	1:A:78[A]:MET:SD	2.46	0.55
1:A:37:SER:OG	1:A:39[B]:GLN:HG2	2.07	0.55
1:A:122:LYS:N	1:A:122:LYS:HD3	2.22	0.54
1:B:149:LYS:N	1:B:149:LYS:HD2	2.23	0.54
1:B:10[A]:TYR:HD2	1:B:17:ALA:CB	2.21	0.54
1:A:16[B]:ARG:NH1	2:A:301:GSH:SG2	2.80	0.54
1:A:120:LYS:O	1:A:124:ILE:HG13	2.07	0.54
1:A:16[A]:ARG:CZ	3:A:2006:HOH:O	2.55	0.53
1:B:37:SER:OG	1:B:39[B]:GLN:HG2	2.08	0.53
1:A:122:LYS:CD	3:A:2103:HOH:O	2.55	0.53
1:A:5:HIS:HE1	1:A:32:GLU:OE1	1.92	0.53
1:B:193:LEU:HD21	1:B:203:LEU:HD12	1.91	0.52
1:A:43:LYS:HG3	1:A:44:ILE:N	2.23	0.52
1:A:59:THR:HG21	3:A:2011:HOH:O	2.09	0.52
1:B:14:ARG:HD3	1:B:206:ARG:NH2	2.24	0.52
1:B:10[A]:TYR:CD2	1:B:17:ALA:HB2	2.44	0.51
1:A:5:HIS:CE1	3:A:2001:HOH:O	2.51	0.51
1:A:10[A]:TYR:CD2	1:A:17:ALA:CB	2.93	0.51
1:A:109:TYR:CZ	1:A:113:LEU:HD21	2.46	0.51
1:B:14:ARG:HD3	1:B:206:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:THR:HG22	3:A:2057:HOH:O	2.11	0.50
1:A:10[A]:TYR:CD2	1:A:17:ALA:HB2	2.47	0.50
1:B:43:LYS:HE3	1:B:44:ILE:CD1	2.41	0.49
1:A:10[A]:TYR:HD2	1:A:17:ALA:HB3	1.77	0.49
1:A:16[A]:ARG:NH1	3:A:2006:HOH:O	2.46	0.49
1:A:106:GLU:HG3	1:A:110:TYR:CZ	2.48	0.49
1:A:14:ARG:HD3	1:A:206:ARG:HH12	1.69	0.49
1:A:22:MET:HE2	1:A:203:LEU:HD21	1.94	0.49
1:A:144:LYS:HG3	1:A:184:GLU:HG2	1.94	0.49
1:B:98[A]:LEU:HD12	1:B:151:ALA:HB1	1.95	0.48
1:B:109:TYR:CZ	1:B:113:LEU:HD21	2.48	0.48
1:B:120:LYS:HZ2	1:B:124:ILE:HD11	1.79	0.47
1:A:45:LYS:HB3	1:A:46:PRO:HD3	1.97	0.47
1:A:10[A]:TYR:HD2	1:A:17:ALA:CB	2.28	0.47
1:A:68:MET:HE1	1:A:77:TYR:CD1	2.50	0.47
1:B:120:LYS:NZ	1:B:124:ILE:HD11	2.31	0.46
1:B:106:GLU:HG3	1:B:110:TYR:CZ	2.50	0.46
1:B:43:LYS:NZ	3:B:2045:HOH:O	2.25	0.46
1:B:74:ILE:HG23	1:B:78[A]:MET:HE3	1.96	0.46
1:A:61:ASN:C	1:A:61:ASN:ND2	2.74	0.46
1:B:45:LYS:N	1:B:46:PRO:HD2	2.31	0.46
1:B:80:LYS:HD2	3:B:2078:HOH:O	2.16	0.45
1:B:162:VAL:O	1:B:166[B]:VAL:HG23	2.17	0.45
1:A:127:ILE:HD11	1:A:173:LEU:CD1	2.47	0.45
1:B:122:LYS:N	1:B:122:LYS:HD3	2.31	0.44
1:B:53:LEU:HB3	1:B:54:PRO:HA	2.00	0.44
1:B:98[B]:LEU:CD2	1:B:151:ALA:HB1	2.47	0.44
1:A:122:LYS:HD3	3:A:2103:HOH:O	2.18	0.44
1:A:21:ARG:NH1	3:A:2010:HOH:O	2.23	0.44
1:A:106:GLU:OE1	1:A:169:HIS:ND1	2.51	0.44
1:A:18:GLU:OE1	1:A:21:ARG:NH1	2.40	0.43
1:A:118:GLU:O	1:A:122:LYS:HG2	2.17	0.43
1:B:184:GLU:H	1:B:184:GLU:CD	2.26	0.43
1:A:98[A]:LEU:CD2	1:A:151:ALA:HB1	2.42	0.43
1:A:14:ARG:CD	1:A:206:ARG:NH1	2.60	0.42
1:A:43:LYS:HE3	1:A:44:ILE:CD1	2.48	0.42
1:B:98[A]:LEU:HD13	1:B:159:ALA:HB1	2.02	0.42
1:B:72:LEU:HA	1:B:72:LEU:HD23	1.85	0.42
1:B:10[A]:TYR:HE2	1:B:17:ALA:H	1.65	0.42
1:B:193:LEU:CD2	1:B:200:ALA:HA	2.49	0.42
1:B:98[B]:LEU:CD2	3:B:2117:HOH:O	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:CD2	1:B:203:LEU:HD12	2.50	0.41
1:B:5:HIS:HE1	1:B:32:GLU:OE2	2.04	0.41
1:B:77:TYR:O	1:B:81:LYS:HG3	2.21	0.41
1:A:184:GLU:H	1:A:184:GLU:CD	2.29	0.41
1:A:122:LYS:HD2	3:A:2103:HOH:O	2.19	0.41
1:B:68:MET:HE1	1:B:77:TYR:CD1	2.56	0.40
1:A:61:ASN:C	1:A:61:ASN:HD22	2.28	0.40
1:B:119:GLU:HA	1:B:119:GLU:OE1	2.21	0.40
1:B:164:ILE:CD1	1:B:199:LEU:HD21	2.52	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)
3:A:2058:HOH:O	3:B:2144:HOH:O[2_556]	2.11	0.09

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	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
1	B	210/211 (100%)	206 (98%)	4 (2%)	0	100	100
All	All	419/422 (99%)	410 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	182/181 (101%)	171 (94%)	11 (6%)	17	3
1	B	182/181 (101%)	171 (94%)	11 (6%)	17	3
All	All	364/362 (101%)	342 (94%)	22 (6%)	22	3

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

Mol	Chain	Res	Type
1	A	11[A]	PHE
1	A	11[B]	PHE
1	A	16[A]	ARG
1	A	16[B]	ARG
1	A	39[A]	GLN
1	A	39[B]	GLN
1	A	61	ASN
1	A	115	LYS
1	A	118	GLU
1	A	123	ILE
1	A	149	LYS
1	B	16[A]	ARG
1	B	16[B]	ARG
1	B	39[A]	GLN
1	B	39[B]	GLN
1	B	42	PRO
1	B	61	ASN
1	B	115	LYS
1	B	118	GLU
1	B	121	GLN
1	B	149	LYS
1	B	155	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	61	ASN
1	A	64	HIS
1	B	5	HIS
1	B	61	ASN

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Mol	Chain	Res	Type
1	B	64	HIS
1	B	82	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 ⓘ

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	A	301	-	18,19,19	1.56	4 (22%)	21,24,24	2.00	5 (23%)
2	GSH	B	301	-	18,19,19	1.49	4 (22%)	21,24,24	1.27	3 (14%)

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	301	-	-	0/24/24/24	-
2	GSH	B	301	-	-	2/24/24/24	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	GSH	CA2-C2	2.90	1.60	1.52
2	B	301	GSH	CA2-C2	2.83	1.60	1.52
2	A	301	GSH	CB2-CA2	2.83	1.56	1.53
2	B	301	GSH	CB2-CA2	2.66	1.55	1.53
2	A	301	GSH	O11-C1	-2.64	1.22	1.30
2	A	301	GSH	OE1-CD1	2.62	1.28	1.23
2	B	301	GSH	CB2-SG2	2.31	1.86	1.81
2	B	301	GSH	OE1-CD1	2.19	1.27	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	GSH	CA2-CB2-SG2	-4.70	108.86	114.16
2	A	301	GSH	CB2-CA2-C2	-3.96	100.89	109.50
2	A	301	GSH	CA2-N2-CD1	-3.26	113.51	121.68
2	A	301	GSH	C2-CA2-N2	-2.70	103.80	111.11
2	B	301	GSH	CB1-CG1-CD1	-2.66	107.14	113.06
2	B	301	GSH	C2-CA2-N2	-2.55	104.21	111.11
2	B	301	GSH	O11-C1-O12	2.41	129.54	124.08
2	A	301	GSH	OE1-CD1-N2	-2.39	118.90	122.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	GSH	N2-CA2-CB2-SG2
2	B	301	GSH	C2-CA2-CB2-SG2

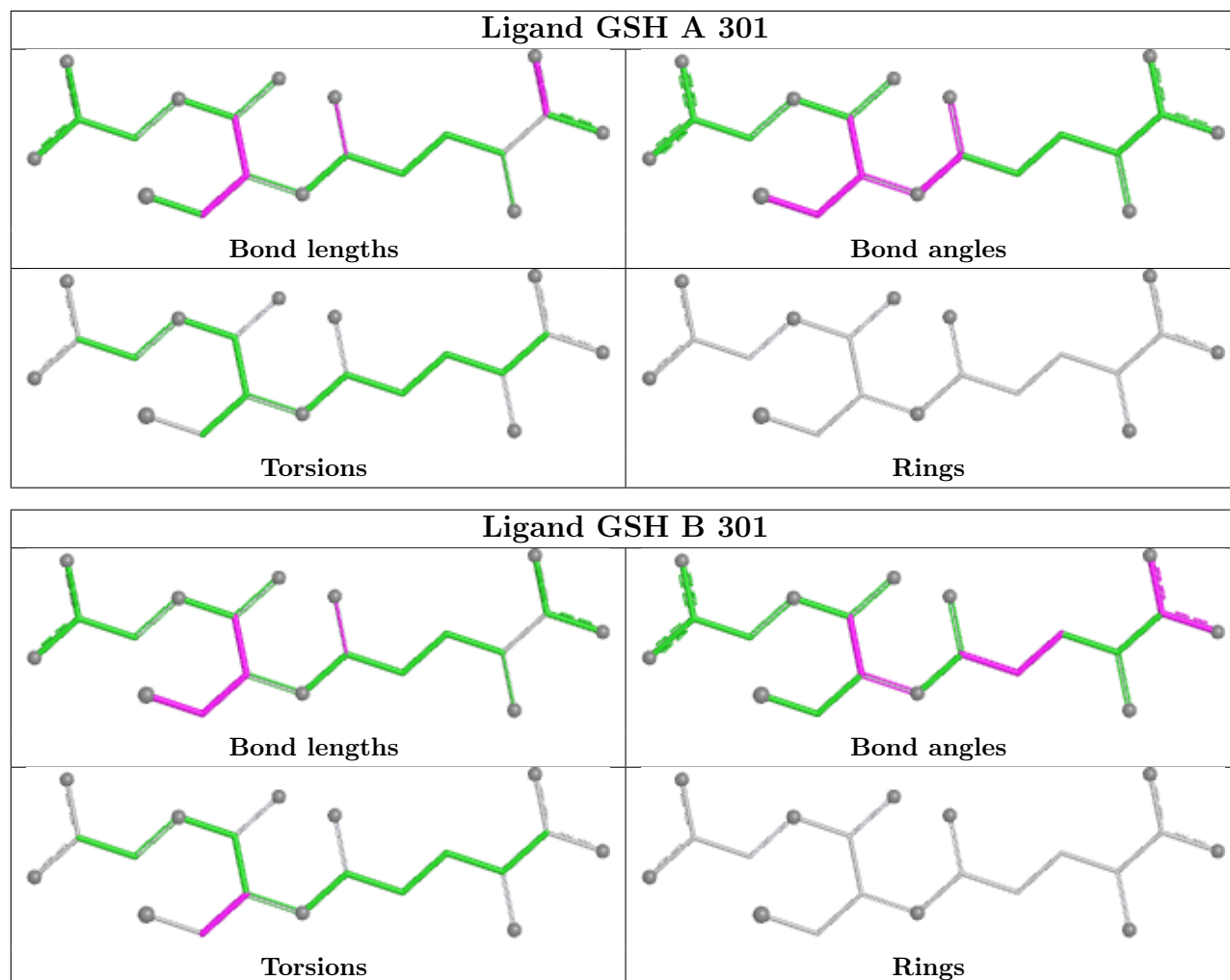
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GSH	1	0
2	B	301	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	204/211 (96%)	-0.87	0	100 100	14, 32, 52, 71	8 (3%)
1	B	205/211 (97%)	-0.85	1 (0%)	87 91	14, 31, 52, 68	9 (4%)
All	All	409/422 (96%)	-0.86	1 (0%)	91 93	14, 31, 52, 71	17 (4%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	GLY	2.7

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.

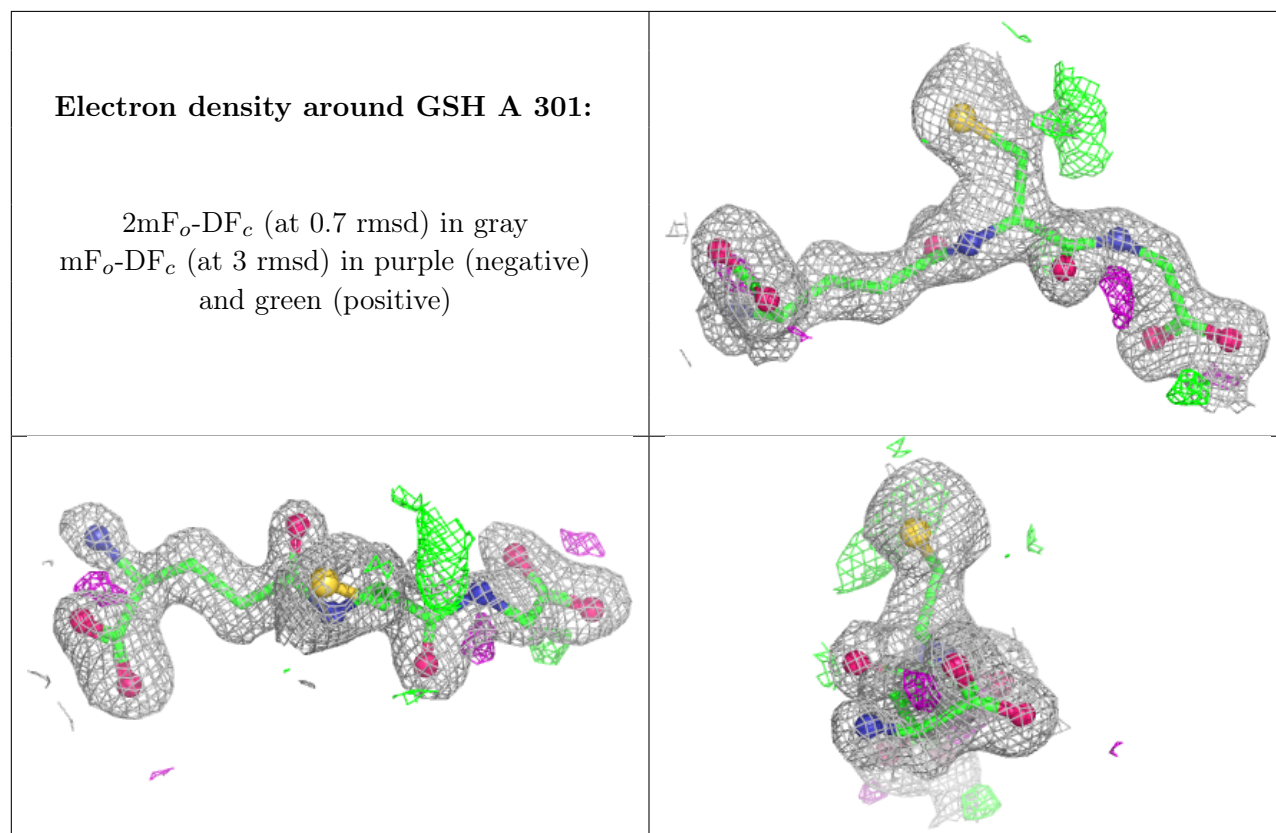
6.4 Ligands [i](#)

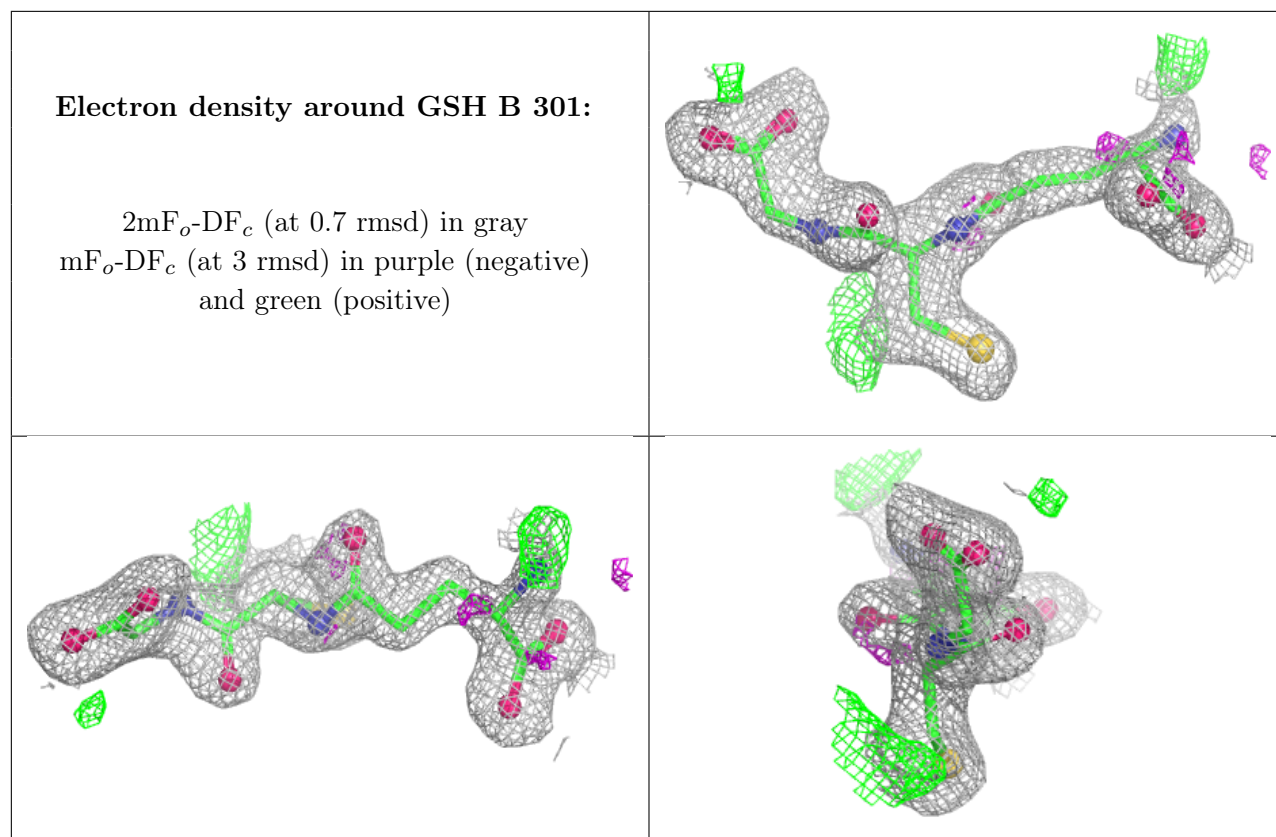
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	GSH	A	301	20/20	0.97	0.06	25,36,42,50	0
2	GSH	B	301	20/20	0.98	0.05	24,35,41,51	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.