



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:16 am GMT

PDB ID : 1OE8  
Title : 28KDA GLUTATHIONE S-TRANSFERASE FROM SCHISTOSOMA  
HAEMATOBIIUM (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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

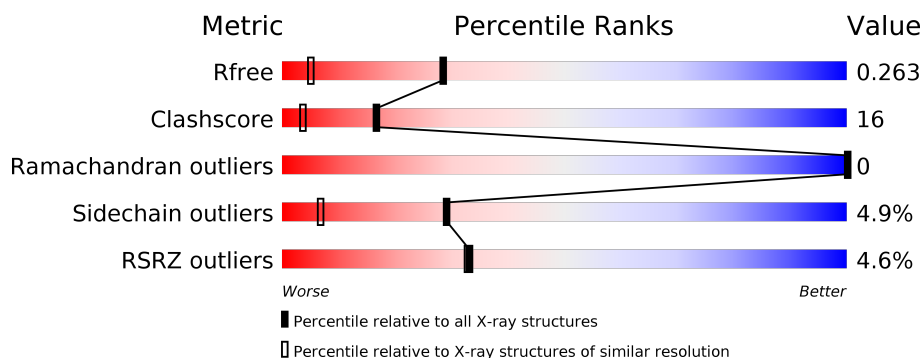
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (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 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  $\leq 5\%$ . 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	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>30%</div> <div>7%</div> <div>••</div> </div> </div>
1	B	211	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>28%</div> <div>8%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

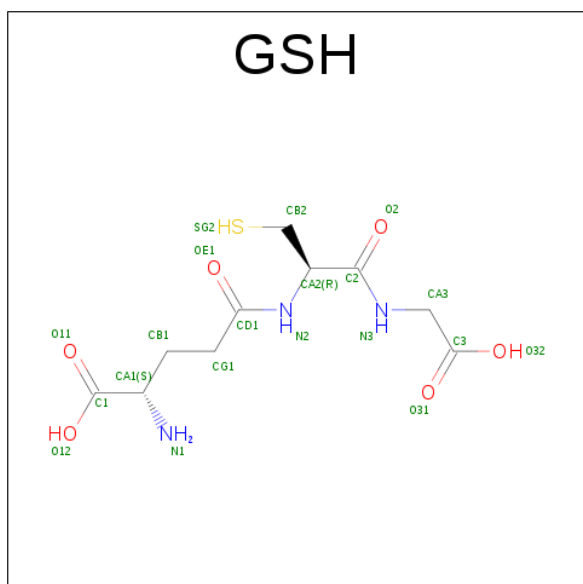
There are 3 unique types of molecules in this entry. The entry contains 3684 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: GSH) (formula:  $C_{10}H_{17}N_3O_6S$ ).



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		

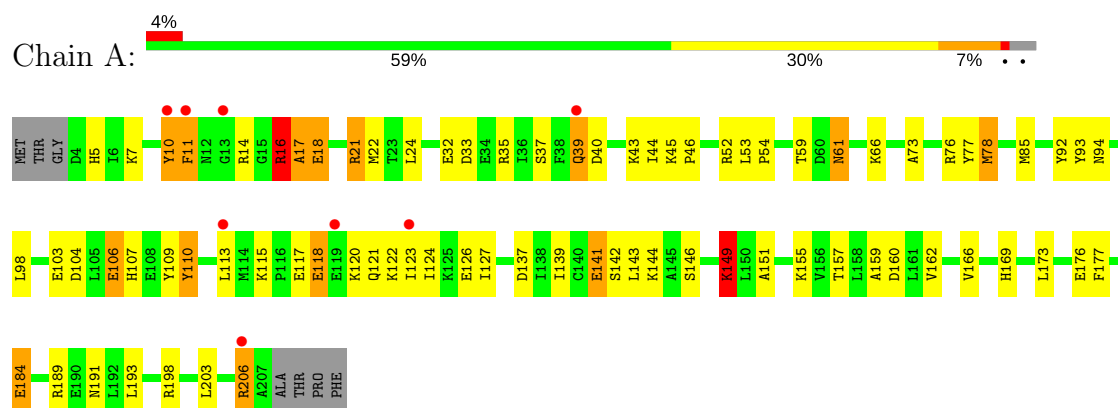
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	159	Total 159	O 159	0	0
3	B	157	Total 157	O 157	0	0

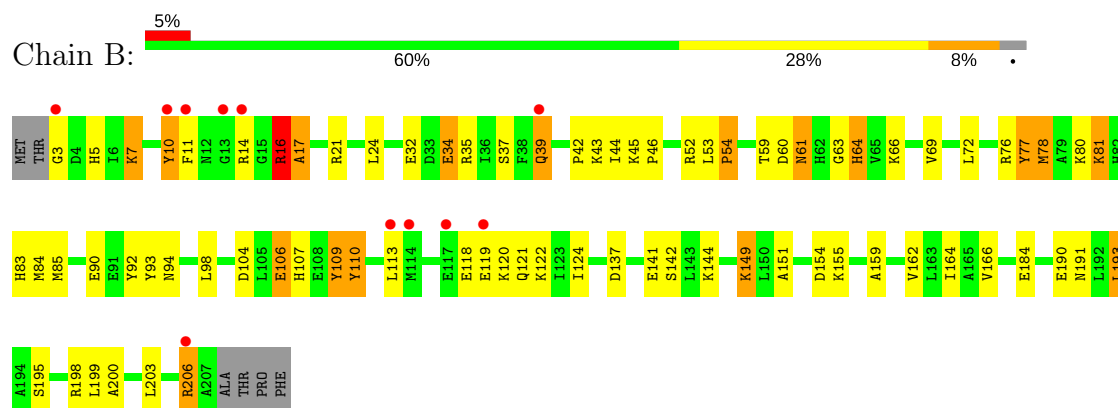
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	53.14Å 77.70Å 53.20Å 90.00° 93.40° 90.00°	Depositor
Resolution (Å)	25.00 – 1.65 27.42 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.0 (25.00-1.65) 98.5 (27.42-1.65)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	2614 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.477 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3684	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 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	1.22	4/1724 (0.2%)	2.42	75/2324 (3.2%)
1	B	1.20	4/1728 (0.2%)	2.24	69/2329 (3.0%)
All	All	1.21	8/3452 (0.2%)	2.34	144/4653 (3.1%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10[A]	TYR	CD1-CE1	-6.76	1.29	1.39
1	A	10[B]	TYR	CD1-CE1	-6.76	1.29	1.39
1	B	10[A]	TYR	CD1-CE1	-6.25	1.29	1.39
1	B	10[B]	TYR	CD1-CE1	-6.25	1.29	1.39
1	A	142	SER	CB-OG	5.79	1.49	1.42
1	A	93	TYR	CG-CD2	5.77	1.46	1.39
1	B	142	SER	CB-OG	5.47	1.49	1.42
1	B	54	PRO	N-CD	5.29	1.55	1.47

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16[A]	ARG	CD-NE-CZ	35.16	172.83	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16[B]	ARG	CD-NE-CZ	35.16	172.83	123.60
1	B	16[A]	ARG	CD-NE-CZ	18.62	149.66	123.60
1	B	16[B]	ARG	CD-NE-CZ	18.62	149.66	123.60
1	A	21	ARG	NE-CZ-NH2	-17.34	111.63	120.30
1	B	16[A]	ARG	NE-CZ-NH1	17.19	128.90	120.30
1	B	16[B]	ARG	NE-CZ-NH1	17.19	128.90	120.30
1	B	21	ARG	NE-CZ-NH1	15.84	128.22	120.30
1	B	21	ARG	NE-CZ-NH2	-15.83	112.38	120.30
1	A	21	ARG	NE-CZ-NH1	14.73	127.67	120.30
1	B	21	ARG	CD-NE-CZ	14.14	143.39	123.60
1	B	10[A]	TYR	CG-CD1-CE1	13.71	132.26	121.30
1	B	10[B]	TYR	CG-CD1-CE1	13.71	132.26	121.30
1	B	10[A]	TYR	CB-CG-CD2	13.38	129.03	121.00
1	B	10[B]	TYR	CB-CG-CD2	13.38	129.03	121.00
1	A	93	TYR	CB-CG-CD2	-11.72	113.97	121.00
1	A	10[A]	TYR	CG-CD1-CE1	11.42	130.44	121.30
1	A	10[B]	TYR	CG-CD1-CE1	11.42	130.44	121.30
1	A	52	ARG	NE-CZ-NH2	-11.05	114.77	120.30
1	B	35	ARG	NE-CZ-NH1	-10.61	115.00	120.30
1	A	76	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	B	107	HIS	CA-CB-CG	-9.78	96.97	113.60
1	A	93	TYR	CG-CD2-CE2	-9.64	113.59	121.30
1	A	52	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	A	110	TYR	CB-CG-CD2	9.35	126.61	121.00
1	B	10[A]	TYR	CD1-CE1-CZ	-9.23	111.50	119.80
1	B	10[B]	TYR	CD1-CE1-CZ	-9.23	111.50	119.80
1	A	206	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	A	21	ARG	CD-NE-CZ	8.92	136.09	123.60
1	A	106	GLU	OE1-CD-OE2	-8.92	112.59	123.30
1	A	77	TYR	CB-CG-CD1	-8.89	115.67	121.00
1	B	52	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	10[A]	TYR	CB-CG-CD2	8.71	126.23	121.00
1	A	10[B]	TYR	CB-CG-CD2	8.71	126.23	121.00
1	A	146	SER	O-C-N	8.68	136.58	122.70
1	B	34	GLU	OE1-CD-OE2	-8.62	112.96	123.30
1	B	104	ASP	CB-CG-OD1	-8.53	110.62	118.30
1	A	110	TYR	CB-CG-CD1	-8.51	115.90	121.00
1	A	141	GLU	OE1-CD-OE2	-8.48	113.13	123.30
1	B	106	GLU	CG-CD-OE1	8.36	135.01	118.30
1	A	92	TYR	CB-CG-CD2	-8.26	116.04	121.00
1	A	18	GLU	CG-CD-OE2	8.18	134.66	118.30
1	A	93	TYR	CB-CG-CD1	8.12	125.87	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	TYR	CD1-CE1-CZ	-7.87	112.71	119.80
1	A	107	HIS	CA-CB-CG	-7.80	100.34	113.60
1	A	10[A]	TYR	CD1-CE1-CZ	-7.67	112.89	119.80
1	A	10[B]	TYR	CD1-CE1-CZ	-7.67	112.89	119.80
1	A	104	ASP	CB-CG-OD1	-7.64	111.43	118.30
1	A	198	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	16[A]	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	B	16[B]	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	B	77	TYR	CB-CG-CD1	-7.58	116.45	121.00
1	A	93	TYR	CZ-CE2-CD2	7.57	126.61	119.80
1	B	85	MET	CA-CB-CG	7.47	126.00	113.30
1	B	198	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	B	52	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	A	35	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	B	106	GLU	OE1-CD-OE2	-7.25	114.59	123.30
1	B	109	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	B	110	TYR	CB-CG-CD2	7.05	125.23	121.00
1	A	11[A]	PHE	CB-CG-CD2	7.03	125.72	120.80
1	A	11[B]	PHE	CB-CG-CD2	7.03	125.72	120.80
1	B	66	LYS	O-C-N	7.02	133.93	122.70
1	A	16[A]	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	16[B]	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	52	ARG	CD-NE-CZ	-6.96	113.85	123.60
1	A	159	ALA	O-C-N	-6.95	111.57	122.70
1	B	93	TYR	CG-CD2-CE2	-6.87	115.81	121.30
1	B	206	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	103	GLU	OE1-CD-OE2	-6.76	115.19	123.30
1	A	7	LYS	O-C-N	6.69	133.40	122.70
1	A	160	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	11[A]	PHE	CB-CG-CD1	-6.45	116.28	120.80
1	A	11[B]	PHE	CB-CG-CD1	-6.45	116.28	120.80
1	B	35	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	149	LYS	O-C-N	6.31	132.80	122.70
1	A	206	ARG	CD-NE-CZ	6.28	132.39	123.60
1	B	109	TYR	CG-CD1-CE1	-6.21	116.33	121.30
1	A	189	ARG	O-C-N	6.21	132.63	122.70
1	A	93	TYR	CD1-CE1-CZ	-6.20	114.22	119.80
1	A	78[A]	MET	CG-SD-CE	6.19	110.11	100.20
1	A	78[B]	MET	CG-SD-CE	6.19	110.11	100.20
1	B	110	TYR	CB-CG-CD1	-6.17	117.30	121.00
1	A	85	MET	CA-CB-CG	6.11	123.69	113.30
1	A	139	ILE	O-C-N	6.05	132.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	GLU	O-C-N	-6.01	113.08	122.70
1	A	159	ALA	CA-C-O	5.96	132.62	120.10
1	A	16[A]	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	16[B]	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	143	LEU	O-C-N	5.92	132.18	122.70
1	A	184	GLU	OE1-CD-OE2	-5.91	116.20	123.30
1	A	162	VAL	CG1-CB-CG2	-5.85	101.53	110.90
1	A	76	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	40	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	93	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	B	52	ARG	CD-NE-CZ	-5.71	115.61	123.60
1	B	137	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	B	184	GLU	OE1-CD-OE2	-5.67	116.49	123.30
1	A	184	GLU	CG-CD-OE1	5.67	129.64	118.30
1	B	77	TYR	CG-CD1-CE1	-5.65	116.78	121.30
1	A	18	GLU	OE1-CD-OE2	-5.63	116.54	123.30
1	B	77	TYR	CD1-CG-CD2	5.61	124.07	117.90
1	B	78[A]	MET	O-C-N	-5.57	113.79	122.70
1	B	78[B]	MET	O-C-N	-5.57	113.79	122.70
1	B	195	SER	O-C-N	-5.52	113.86	122.70
1	B	17	ALA	N-CA-CB	5.52	117.83	110.10
1	B	85	MET	CG-SD-CE	-5.51	91.38	100.20
1	A	76	ARG	N-CA-CB	-5.50	100.69	110.60
1	A	66	LYS	O-C-N	5.50	131.50	122.70
1	A	176	GLU	OE1-CD-OE2	5.47	129.87	123.30
1	A	21	ARG	CB-CG-CD	-5.46	97.41	111.60
1	A	137	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	76	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	B	193	LEU	CA-CB-CG	5.41	127.73	115.30
1	B	154	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	149	LYS	CG-CD-CE	5.37	128.00	111.90
1	B	69	VAL	CG1-CB-CG2	-5.36	102.32	110.90
1	B	64	HIS	O-C-N	5.36	131.28	122.70
1	A	94	ASN	CA-CB-CG	-5.35	101.63	113.40
1	B	10[A]	TYR	CD1-CG-CD2	-5.34	112.02	117.90
1	B	10[B]	TYR	CD1-CG-CD2	-5.34	112.02	117.90
1	B	92	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	B	59	THR	OG1-CB-CG2	-5.25	97.92	110.00
1	B	141	GLU	OE1-CD-OE2	-5.22	117.04	123.30
1	A	206	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	7	LYS	O-C-N	5.20	131.02	122.70
1	A	160	ASP	OD1-CG-OD2	5.19	133.17	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	ARG	CB-CG-CD	-5.19	98.11	111.60
1	B	21	ARG	CG-CD-NE	-5.17	100.94	111.80
1	A	17	ALA	CB-CA-C	-5.16	102.36	110.10
1	B	94	ASN	CA-CB-CG	-5.16	102.06	113.40
1	B	17	ALA	CB-CA-C	-5.15	102.37	110.10
1	A	106	GLU	CG-CD-OE2	5.15	128.59	118.30
1	B	144	LYS	CD-CE-NZ	5.14	123.53	111.70
1	A	191	ASN	O-C-N	-5.13	114.49	122.70
1	A	177	PHE	CB-CG-CD1	-5.12	117.21	120.80
1	B	83	HIS	CA-CB-CG	-5.12	104.89	113.60
1	A	33	ASP	CB-CG-OD2	5.12	122.90	118.30
1	B	60	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	191	ASN	O-C-N	-5.09	114.56	122.70
1	B	81	LYS	O-C-N	-5.06	114.60	122.70
1	A	193	LEU	CA-CB-CG	5.02	126.85	115.30
1	B	78[A]	MET	CA-CB-CG	-5.01	104.77	113.30
1	B	78[B]	MET	CA-CB-CG	-5.01	104.77	113.30

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	52	0
1	B	1666	0	1703	56	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	12	1
All	All	3684	0	3433	108	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 16.

All (108) 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	0.95
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
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:HD2	1:A:149:LYS:N	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:A:122:LYS:N	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:120:LYS:O	1:A:124:ILE:HG13	2.07	0.54
1:A:16[B]:ARG:NH1	2:A:301:GSH:SG2	2.80	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:109:TYR:CZ	1:A:113:LEU:HD21	2.46	0.51
1:A:10[A]:TYR:CD2	1:A:17:ALA:CB	2.93	0.51
1:B:14:ARG:HD3	1:B:206:ARG:NH1	2.26	0.50
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: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:A:22:MET:HE2	1:A:203:LEU:HD21	1.95	0.48
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:118:GLU:O	1:A:122:LYS:HG2	2.17	0.43
1:A:18:GLU:OE1	1:A:21:ARG:NH1	2.40	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
1:B:193:LEU:CD2	1:B:203:LEU:HD12	2.50	0.41
1:A:61:ASN:C	1:A:61:ASN:ND2	2.74	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:122:LYS:HD2	3:A:2103:HOH:O	2.19	0.41
1:B:119:GLU:OE1	1:B:119:GLU:HA	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 ⓘ

### 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	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 ⓘ

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%)	170 (93%)	12 (7%)	19	3
1	B	182/181 (101%)	172 (94%)	10 (6%)	25	5
All	All	364/362 (101%)	342 (94%)	22 (6%)	29	4

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	126	GLU
1	A	149	LYS
1	B	16[A]	ARG
1	B	16[B]	ARG
1	B	39[A]	GLN
1	B	39[B]	GLN

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Mol	Chain	Res	Type
1	B	42	PRO
1	B	61	ASN
1	B	118	GLU
1	B	121	GLN
1	B	149	LYS
1	B	155	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	61	ASN
1	A	101	GLN
1	A	129	ASN
1	B	5	HIS
1	B	61	ASN
1	B	101	GLN
1	B	129	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 carbohydrates 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	-	11,19,19	1.52	3 (27%)	14,24,24	2.46	6 (42%)
2	GSH	B	301	-	11,19,19	1.60	4 (36%)	14,24,24	1.36	2 (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	-	-	0/18/24/24	0/0/0/0
2	GSH	B	301	-	-	0/18/24/24	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	GSH	OE1-CD1	2.08	1.27	1.23
2	B	301	GSH	CB2-SG2	2.24	1.86	1.81
2	A	301	GSH	OE1-CD1	2.49	1.28	1.23
2	B	301	GSH	CB2-CA2	2.60	1.55	1.53
2	B	301	GSH	CA2-C2	2.68	1.60	1.52
2	A	301	GSH	CA2-C2	2.74	1.60	1.52
2	A	301	GSH	CB2-CA2	2.76	1.56	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	GSH	CA2-CB2-SG2	-4.53	108.86	114.15
2	A	301	GSH	CA3-N3-C2	-4.22	116.69	122.39
2	A	301	GSH	CB2-CA2-C2	-3.95	100.89	109.60
2	A	301	GSH	CA2-N2-CD1	-3.07	113.51	121.62
2	A	301	GSH	C2-CA2-N2	-2.69	103.80	111.20
2	B	301	GSH	CB1-CG1-CD1	-2.67	107.14	113.18
2	B	301	GSH	C2-CA2-N2	-2.54	104.21	111.20
2	A	301	GSH	OE1-CD1-N2	-2.36	118.90	122.97

There are no chirality outliers.

There are no torsion outliers.

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	204/211 (96%)	0.18	8 (3%)	40 42	21, 32, 52, 71	1 (0%)
1	B	205/211 (97%)	0.23	11 (5%)	26 25	20, 32, 52, 68	2 (0%)
All	All	409/422 (96%)	0.20	19 (4%)	33 33	20, 32, 52, 71	3 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	GLY	9.3
1	B	113	LEU	4.0
1	B	206	ARG	3.8
1	A	10[A]	TYR	3.7
1	A	13	GLY	3.7
1	B	10[A]	TYR	3.3
1	B	14	ARG	3.3
1	B	119	GLU	3.0
1	A	206	ARG	2.8
1	A	123	ILE	2.7
1	B	3	GLY	2.7
1	B	11[A]	PHE	2.5
1	A	113	LEU	2.5
1	B	114	MET	2.4
1	B	117	GLU	2.4
1	A	11[A]	PHE	2.3
1	B	39[A]	GLN	2.1
1	A	39[A]	GLN	2.0
1	A	119	GLU	2.0

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GSH	A	301	20/20	0.88	0.15	0.25	25,36,42,50	0
2	GSH	B	301	20/20	0.88	0.14	0.06	24,35,41,51	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.