



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:13 PM UTC

PDB ID : 6GSY / pdb_00006gsy
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

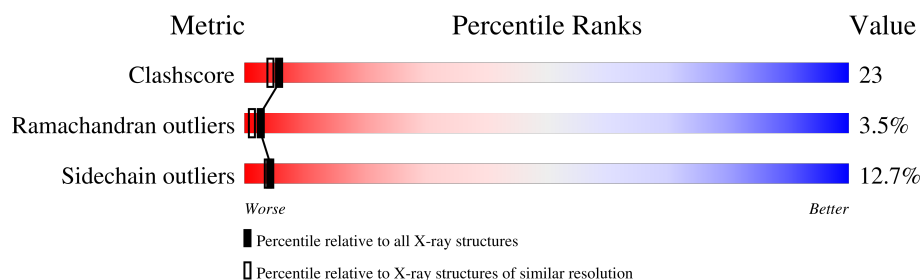
1 Overall quality at a glance

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	
1	B	217	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4074 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.

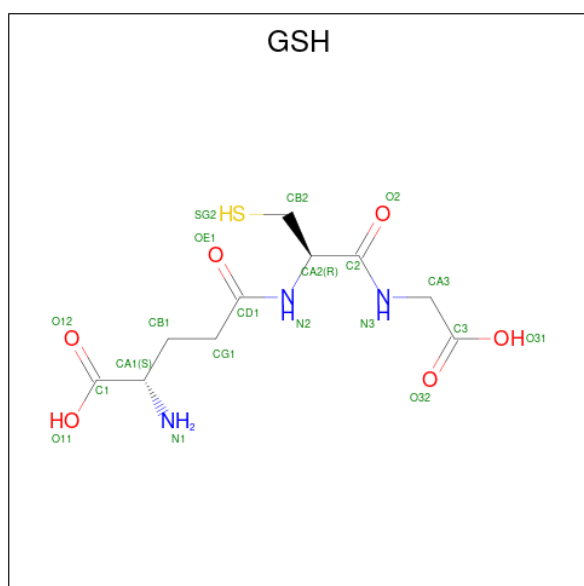
- Molecule 1 is a protein called MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1816	1177	303	325	11			
1	B	217	Total	C	N	O	S	0	0	0
			1816	1177	303	325	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	PHE	TYR	engineered mutation	UNP P04905
B	6	PHE	TYR	engineered mutation	UNP P04905

- 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		

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

- Molecule 3 is water.

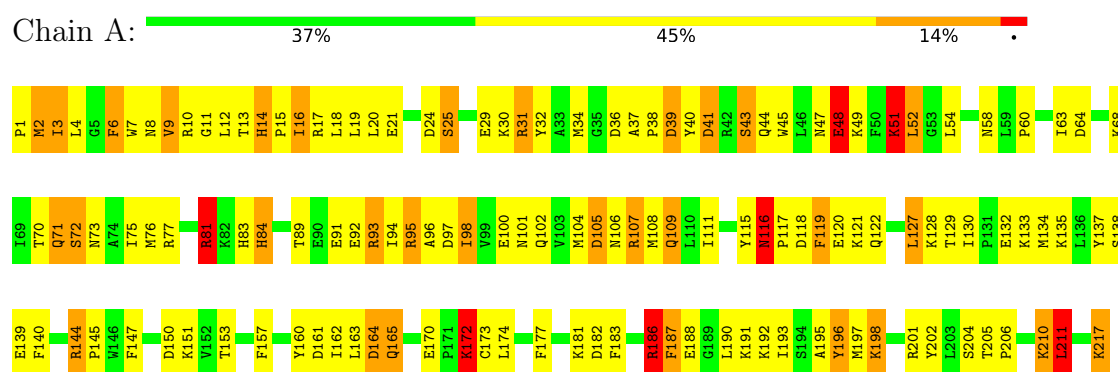
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	209	Total	O	0	0
			209	209		
3	B	193	Total	O	0	0
			193	193		

3 Residue-property plots

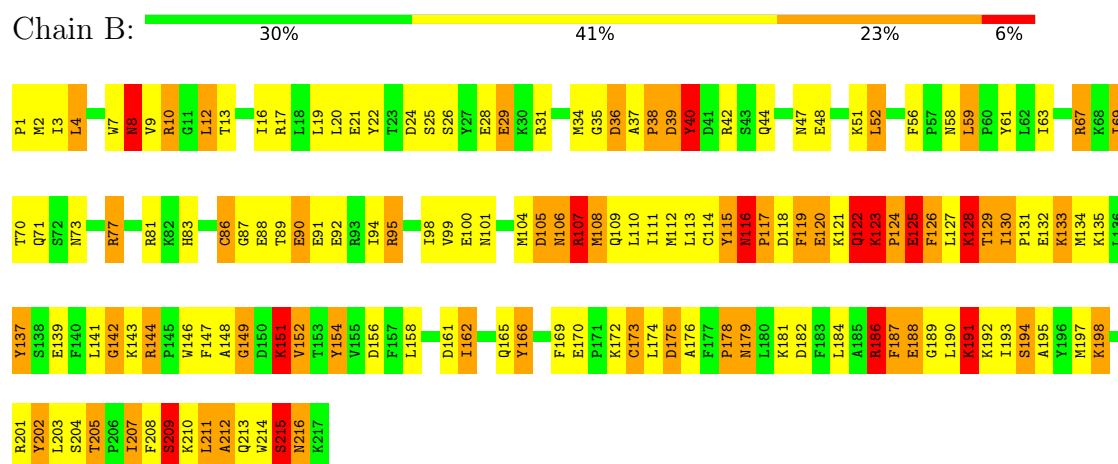
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	87.84Å 69.70Å 81.57Å 90.00° 105.38° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	88.3 (6.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4074	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	1.38	11/1865 (0.6%)	2.41	124/2513 (4.9%)
1	B	1.33	2/1865 (0.1%)	2.52	124/2513 (4.9%)
All	All	1.36	13/3730 (0.3%)	2.46	248/5026 (4.9%)

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	5
All	All	0	10

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	ASN	C-O	7.61	1.34	1.24
1	A	100	GLU	N-CA	7.03	1.54	1.46
1	A	96	ALA	N-CA	5.83	1.53	1.46
1	A	138	SER	N-CA	5.78	1.53	1.46
1	A	14	HIS	N-CA	5.71	1.52	1.46
1	B	187	PHE	N-CA	5.46	1.53	1.46
1	A	17	ARG	N-CA	5.43	1.53	1.46
1	A	160	TYR	N-CA	5.36	1.52	1.46
1	A	16	ILE	CA-CB	5.32	1.61	1.54
1	A	157	PHE	N-CA	5.21	1.52	1.46
1	A	107	ARG	N-CA	5.16	1.52	1.46
1	A	164	ASP	N-CA	5.11	1.52	1.46
1	A	129	THR	CA-CB	5.00	1.61	1.53

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ASN	CA-CB-CG	23.71	136.31	112.60
1	B	95	ARG	CD-NE-CZ	16.41	147.38	124.40
1	B	186	ARG	CD-NE-CZ	15.70	146.38	124.40
1	A	201	ARG	CD-NE-CZ	15.50	146.10	124.40
1	A	186	ARG	CD-NE-CZ	14.77	145.08	124.40
1	B	36	ASP	CA-CB-CG	13.72	126.32	112.60
1	B	105	ASP	CA-CB-CG	13.71	126.31	112.60
1	A	182	ASP	CA-CB-CG	13.28	125.88	112.60
1	B	186	ARG	NE-CZ-NH1	12.90	134.40	121.50
1	B	107	ARG	NE-CZ-NH2	-12.05	108.35	119.20
1	B	188	GLU	CA-CB-CG	11.84	137.78	114.10
1	B	191	LYS	CA-CB-CG	11.66	137.42	114.10
1	A	71	GLN	OE1-CD-NE2	-10.77	111.83	122.60
1	B	67	ARG	CD-NE-CZ	10.63	139.29	124.40
1	A	58	ASN	OD1-CG-ND2	-10.50	112.10	122.60
1	B	179	ASN	CA-CB-CG	9.88	122.48	112.60
1	B	88	GLU	CA-CB-CG	9.28	132.65	114.10
1	B	114	CYS	CB-CA-C	9.24	126.11	110.86
1	A	47	ASN	CA-C-O	-9.22	108.34	119.49
1	A	9	VAL	CA-C-O	9.13	130.59	121.64
1	B	4	LEU	CA-C-O	-9.10	110.62	120.36
1	B	101	ASN	O-C-N	-9.02	111.87	122.15
1	A	157	PHE	CA-CB-CG	8.75	122.55	113.80
1	B	107	ARG	NH1-CZ-NH2	8.74	130.67	119.30
1	B	116	ASN	CB-CA-C	8.67	127.25	110.17
1	B	152	VAL	N-CA-CB	8.64	120.93	110.31
1	A	106	ASN	CA-CB-CG	8.48	121.08	112.60
1	B	89	THR	CA-CB-OG1	-8.37	97.04	109.60
1	A	48	GLU	CA-CB-CG	8.33	130.76	114.10
1	B	201	ARG	CD-NE-CZ	8.31	136.04	124.40
1	B	81	ARG	NE-CZ-NH1	8.31	129.81	121.50
1	A	4	LEU	CA-C-N	-8.27	116.29	122.33
1	A	4	LEU	C-N-CA	-8.27	116.29	122.33
1	B	16	ILE	O-C-N	8.27	130.50	121.90
1	A	13	THR	CA-CB-OG1	-8.23	97.25	109.60
1	B	24	ASP	CA-CB-CG	8.19	120.79	112.60
1	A	116	ASN	OD1-CG-ND2	7.81	130.41	122.60
1	B	186	ARG	NH1-CZ-NH2	-7.75	109.22	119.30
1	B	106	ASN	N-CA-CB	7.75	121.63	110.16
1	A	96	ALA	CB-CA-C	7.72	123.01	110.88
1	A	186	ARG	NE-CZ-NH1	7.70	129.20	121.50
1	A	202	TYR	CB-CA-C	7.69	122.19	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	GLU	CB-CG-CD	7.68	125.65	112.60
1	A	89	THR	CA-CB-OG1	-7.67	98.09	109.60
1	A	101	ASN	CA-CB-CG	-7.66	104.94	112.60
1	B	101	ASN	CA-C-O	7.61	128.49	120.42
1	B	56	PHE	CA-CB-CG	7.60	121.40	113.80
1	A	186	ARG	NH1-CZ-NH2	-7.58	109.44	119.30
1	B	73	ASN	CA-CB-CG	7.58	120.18	112.60
1	B	101	ASN	CA-C-N	7.55	130.73	120.54
1	B	101	ASN	C-N-CA	7.55	130.73	120.54
1	B	8	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	A	170	GLU	O-C-N	7.48	127.25	121.27
1	B	63	ILE	CA-C-O	-7.45	112.55	120.53
1	A	14	HIS	CA-CB-CG	7.45	121.25	113.80
1	A	186	ARG	CA-CB-CG	7.44	128.99	114.10
1	B	115	TYR	CA-CB-CG	7.44	127.29	113.90
1	B	87	GLY	CA-C-O	-7.39	113.92	121.90
1	A	205	THR	O-C-N	7.37	126.43	121.71
1	B	186	ARG	NE-CZ-NH2	-7.36	112.58	119.20
1	A	177	PHE	N-CA-C	7.30	121.78	108.94
1	A	122	GLN	OE1-CD-NE2	7.23	129.83	122.60
1	A	116	ASN	CB-CA-C	7.21	119.15	109.42
1	A	102	GLN	OE1-CD-NE2	7.21	129.81	122.60
1	A	211	LEU	N-CA-CB	-7.19	99.13	110.28
1	A	47	ASN	CA-CB-CG	7.17	119.77	112.60
1	B	147	PHE	N-CA-C	7.14	119.92	111.71
1	B	121	LYS	N-CA-CB	7.08	122.46	110.49
1	B	101	ASN	CB-CG-ND2	7.07	127.00	116.40
1	A	97	ASP	CA-CB-CG	7.02	119.62	112.60
1	B	28	GLU	CA-C-O	-6.98	113.28	121.44
1	A	119	PHE	CA-CB-CG	6.95	120.75	113.80
1	A	72	SER	CA-CB-OG	6.92	124.93	111.10
1	B	149	GLY	N-CA-C	6.88	121.48	111.24
1	A	147	PHE	N-CA-C	6.82	119.55	111.71
1	A	51	LYS	CA-CB-CG	6.82	127.73	114.10
1	B	58	ASN	O-C-N	6.75	130.04	123.29
1	B	137	TYR	CA-C-O	6.75	127.91	120.82
1	B	202	TYR	CB-CA-C	6.74	120.41	109.90
1	A	76	MET	CA-C-O	-6.71	113.72	120.90
1	B	20	LEU	CA-C-O	-6.70	113.73	120.90
1	B	25	SER	CA-C-O	6.68	128.84	121.56
1	A	11	GLY	CA-C-N	6.65	132.66	122.29
1	A	11	GLY	C-N-CA	6.65	132.66	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	THR	CA-C-O	-6.64	114.23	120.34
1	B	81	ARG	NH1-CZ-NH2	-6.63	110.68	119.30
1	A	106	ASN	CA-C-O	-6.62	113.53	120.55
1	B	77	ARG	NE-CZ-NH2	-6.61	113.25	119.20
1	B	86	CYS	CA-C-O	-6.55	113.64	121.56
1	A	58	ASN	O-C-N	6.54	129.41	123.26
1	B	114	CYS	CA-C-O	-6.49	113.98	120.80
1	A	2	MET	N-CA-C	-6.47	101.99	110.53
1	A	95	ARG	CD-NE-CZ	6.46	133.44	124.40
1	A	91	GLU	CG-CD-OE2	-6.41	103.66	118.40
1	A	47	ASN	N-CA-CB	6.37	121.15	110.32
1	A	40	TYR	N-CA-CB	-6.37	101.59	111.65
1	B	44	GLN	CA-C-O	6.32	127.46	120.63
1	B	142	GLY	CA-C-N	6.31	132.27	122.49
1	B	142	GLY	C-N-CA	6.31	132.27	122.49
1	A	77	ARG	NE-CZ-NH1	6.30	127.80	121.50
1	A	119	PHE	CA-C-N	6.29	130.26	120.82
1	A	119	PHE	C-N-CA	6.29	130.26	120.82
1	A	77	ARG	N-CA-C	6.28	119.11	111.82
1	A	24	ASP	CA-C-O	6.27	128.74	121.28
1	A	165	GLN	OE1-CD-NE2	6.26	128.86	122.60
1	A	14	HIS	CA-C-O	6.26	124.09	118.33
1	A	89	THR	CA-C-O	-6.25	114.33	121.58
1	A	183	PHE	O-C-N	6.20	128.45	122.07
1	B	70	THR	N-CA-CB	6.19	122.32	111.55
1	A	64	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	147	PHE	CA-CB-CG	6.17	119.97	113.80
1	B	51	LYS	CA-C-O	-6.17	112.12	119.15
1	A	205	THR	CA-C-O	-6.15	114.84	120.50
1	A	71	GLN	CG-CD-NE2	6.14	125.61	116.40
1	A	181	LYS	CA-C-O	6.12	127.04	120.55
1	A	198	LYS	N-CA-CB	6.09	119.81	110.61
1	B	40	TYR	CA-CB-CG	6.08	124.85	113.90
1	B	77	ARG	CA-C-O	6.08	126.97	120.10
1	A	77	ARG	CD-NE-CZ	6.07	132.89	124.40
1	B	182	ASP	O-C-N	6.07	129.73	122.27
1	A	39	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	31	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	B	162	ILE	CA-C-O	-6.04	114.77	121.17
1	B	190	LEU	CB-CA-C	6.00	119.69	109.72
1	A	24	ASP	CA-CB-CG	-5.99	106.61	112.60
1	B	187	PHE	N-CA-C	-5.99	104.72	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASP	N-CA-C	-5.96	104.85	111.71
1	B	69	ILE	CA-CB-CG1	5.96	120.53	110.40
1	B	187	PHE	CA-C-N	5.95	130.21	120.63
1	B	187	PHE	C-N-CA	5.95	130.21	120.63
1	B	101	ASN	CA-CB-CG	5.94	118.54	112.60
1	A	172	LYS	N-CA-C	5.91	120.35	113.20
1	A	6	PHE	O-C-N	5.91	129.46	123.26
1	A	127	LEU	CA-C-O	-5.90	112.07	120.51
1	B	99	VAL	N-CA-CB	5.87	117.03	110.51
1	A	18	LEU	CA-C-O	-5.86	114.33	120.55
1	B	9	VAL	CA-C-N	5.86	128.41	120.44
1	B	9	VAL	C-N-CA	5.86	128.41	120.44
1	B	77	ARG	CD-NE-CZ	5.85	132.60	124.40
1	A	165	GLN	N-CA-CB	5.85	118.49	110.01
1	A	153	THR	CA-C-O	-5.84	114.92	121.40
1	B	133	LYS	CA-C-N	5.82	128.40	120.54
1	B	133	LYS	C-N-CA	5.82	128.40	120.54
1	A	73	ASN	CA-CB-CG	5.80	118.40	112.60
1	B	105	ASP	N-CA-CB	5.80	118.42	110.01
1	A	137	TYR	O-C-N	5.80	128.27	122.12
1	A	96	ALA	CA-C-N	5.77	128.33	120.54
1	A	96	ALA	C-N-CA	5.77	128.33	120.54
1	B	162	ILE	O-C-N	5.76	127.56	121.91
1	A	63	ILE	CB-CG1-CD1	5.76	125.90	113.80
1	A	24	ASP	CA-C-N	5.75	129.64	121.42
1	A	24	ASP	C-N-CA	5.75	129.64	121.42
1	B	31	ARG	CA-C-N	5.71	128.82	120.71
1	B	31	ARG	C-N-CA	5.71	128.82	120.71
1	A	164	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	128	LYS	N-CA-C	-5.71	106.16	113.01
1	A	107	ARG	CA-C-N	5.69	127.84	120.44
1	A	107	ARG	C-N-CA	5.69	127.84	120.44
1	A	187	PHE	CA-C-N	5.69	127.91	120.28
1	A	187	PHE	C-N-CA	5.69	127.91	120.28
1	B	83	HIS	CA-CB-CG	-5.67	108.13	113.80
1	B	10	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	B	156	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	115	TYR	N-CA-CB	5.65	119.08	109.87
1	A	24	ASP	CB-CA-C	5.64	119.74	111.73
1	A	107	ARG	O-C-N	-5.63	116.15	122.12
1	A	107	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	A	134	MET	O-C-N	5.60	128.54	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	PHE	CA-C-N	5.58	126.82	119.84
1	A	177	PHE	C-N-CA	5.58	126.82	119.84
1	B	116	ASN	CA-C-N	5.58	126.82	119.84
1	B	116	ASN	C-N-CA	5.58	126.82	119.84
1	A	81	ARG	CA-C-O	5.58	126.47	120.55
1	A	58	ASN	CA-C-O	-5.58	115.02	121.26
1	B	194	SER	CA-C-N	5.57	128.01	120.38
1	B	194	SER	C-N-CA	5.57	128.01	120.38
1	A	84	HIS	CB-CA-C	-5.57	103.98	112.11
1	A	52	LEU	O-C-N	5.55	128.96	122.24
1	A	217	LYS	CA-CB-CG	5.54	125.19	114.10
1	B	182	ASP	CA-C-O	-5.54	113.60	119.97
1	B	166	TYR	CB-CA-C	5.54	119.98	110.79
1	B	16	ILE	CA-C-O	-5.45	115.00	121.05
1	A	43	SER	CB-CA-C	-5.45	99.58	110.42
1	A	163	LEU	O-C-N	5.44	128.97	122.27
1	B	13	THR	CA-CB-OG1	-5.43	101.45	109.60
1	A	83	HIS	CA-CB-CG	-5.42	108.38	113.80
1	B	120	GLU	CA-CB-CG	5.42	124.94	114.10
1	A	70	THR	N-CA-C	-5.41	101.54	109.81
1	A	97	ASP	CA-C-O	5.40	126.67	120.90
1	B	73	ASN	CB-CA-C	5.39	119.42	110.90
1	A	100	GLU	CG-CD-OE2	-5.38	106.04	118.40
1	A	2	MET	CA-C-O	-5.37	115.64	121.87
1	A	195	ALA	CA-C-N	5.37	127.42	120.44
1	A	195	ALA	C-N-CA	5.37	127.42	120.44
1	B	125	GLU	N-CA-C	5.36	122.21	110.80
1	A	105	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	152	VAL	O-C-N	5.34	128.50	122.67
1	A	92	GLU	N-CA-C	5.33	117.09	111.28
1	B	190	LEU	CA-C-N	5.33	127.74	120.54
1	B	190	LEU	C-N-CA	5.33	127.74	120.54
1	B	193	ILE	N-CA-CB	5.33	117.39	110.57
1	A	81	ARG	CA-C-N	5.29	127.81	120.29
1	A	81	ARG	C-N-CA	5.29	127.81	120.29
1	A	196	TYR	CA-C-N	5.29	129.06	120.60
1	A	196	TYR	C-N-CA	5.29	129.06	120.60
1	B	59	LEU	O-C-N	5.29	127.60	121.10
1	A	105	ASP	CA-C-O	5.28	126.88	121.07
1	B	101	ASN	N-CA-C	5.28	117.12	111.36
1	B	141	LEU	O-C-N	5.28	127.50	122.07
1	A	95	ARG	NE-CZ-NH1	5.24	126.74	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	ARG	CD-NE-CZ	-5.22	117.10	124.40
1	A	34	MET	CA-C-O	-5.21	115.11	121.78
1	B	143	LYS	CB-CA-C	-5.21	101.37	110.17
1	A	188	GLU	CA-C-N	5.19	131.59	121.41
1	A	188	GLU	C-N-CA	5.19	131.59	121.41
1	B	191	LYS	O-C-N	5.19	127.49	122.09
1	B	151	LYS	N-CA-C	5.19	118.52	110.17
1	A	210	LYS	CA-C-N	5.19	128.19	120.31
1	A	210	LYS	C-N-CA	5.19	128.19	120.31
1	A	30	LYS	N-CA-C	-5.17	99.98	108.41
1	B	17	ARG	CA-C-O	5.17	126.03	120.55
1	A	91	GLU	CG-CD-OE1	5.17	130.28	118.40
1	B	152	VAL	N-CA-C	-5.15	102.86	109.30
1	B	126	PHE	CB-CA-C	5.15	118.69	110.09
1	B	3	ILE	CA-C-N	5.14	129.60	122.77
1	B	3	ILE	C-N-CA	5.14	129.60	122.77
1	B	187	PHE	CB-CA-C	5.14	118.82	110.24
1	A	34	MET	N-CA-C	-5.13	102.60	110.14
1	B	116	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	B	22	TYR	N-CA-C	5.12	116.86	111.28
1	B	123	LYS	CB-CA-C	5.10	120.21	110.17
1	B	146	TRP	CA-C-N	5.08	127.60	120.28
1	B	146	TRP	C-N-CA	5.08	127.60	120.28
1	B	130	ILE	CB-CA-C	5.07	120.59	111.36
1	A	172	LYS	CA-C-N	5.06	131.20	121.18
1	A	172	LYS	C-N-CA	5.06	131.20	121.18
1	A	109	GLN	CB-CG-CD	5.05	121.19	112.60
1	A	4	LEU	CA-C-O	-5.05	114.93	120.43
1	A	96	ALA	O-C-N	-5.05	116.87	122.07
1	B	90	GLU	CA-C-O	5.04	126.12	120.82
1	B	81	ARG	CD-NE-CZ	5.03	131.44	124.40
1	B	61	TYR	CA-CB-CG	5.03	122.95	113.90
1	A	70	THR	CA-C-O	-5.02	115.75	121.68
1	B	10	ARG	O-C-N	5.02	127.51	122.09
1	B	29	GLU	O-C-N	5.02	129.42	123.24
1	B	21	GLU	N-CA-C	5.01	116.43	111.07
1	B	158	LEU	CA-C-O	-5.01	114.68	120.24
1	B	81	ARG	CA-CB-CG	5.01	124.11	114.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	81	ARG	Sidechain
1	A	93	ARG	Sidechain
1	A	98	ILE	Mainchain
1	B	107	ARG	Sidechain
1	B	144	ARG	Sidechain
1	B	154	TYR	Mainchain
1	B	186	ARG	Sidechain
1	B	77	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	1816	0	1805	54	3
1	B	1816	0	1805	118	4
2	A	20	0	15	2	0
2	B	20	0	14	2	0
3	A	209	0	0	3	0
3	B	193	0	0	11	0
All	All	4074	0	3639	170	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (170) 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:10:ARG:HD3	1:B:207:ILE:HD13	1.29	1.09
1:B:170:GLU:HB3	1:B:173:CYS:HB3	1.31	1.06
1:A:48:GLU:HG3	1:A:52:LEU:HD21	1.45	0.96
1:A:135:LYS:NZ	1:A:139:GLU:OE2	2.03	0.92
1:B:95:ARG:NH2	1:B:144:ARG:HE	1.70	0.88
1:A:140:PHE:O	1:A:144:ARG:NH1	2.10	0.83
1:B:120:GLU:HA	1:B:123:LYS:HG3	1.61	0.80
1:B:144:ARG:HD3	1:B:149:GLY:HA2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:HD13	1:B:166:TYR:HE1	1.49	0.75
1:B:144:ARG:CD	1:B:149:GLY:HA2	2.18	0.73
1:B:135:LYS:HD2	1:B:139:GLU:OE2	1.90	0.72
1:B:40:TYR:HE2	1:B:211:LEU:H	1.38	0.72
1:A:105:ASP:O	1:A:109:GLN:HG3	1.90	0.71
1:B:124:PRO:O	1:B:127:LEU:HB2	1.93	0.69
1:B:40:TYR:CE2	1:B:211:LEU:HB2	2.27	0.69
1:B:10:ARG:HB3	1:B:207:ILE:HA	1.75	0.69
1:B:123:LYS:HB3	1:B:124:PRO:CD	2.24	0.67
1:B:123:LYS:HB3	1:B:124:PRO:HD2	1.77	0.67
1:A:16:ILE:HD13	1:A:75:ILE:HG21	1.78	0.66
1:B:113:LEU:HD22	1:B:126:PHE:CD2	2.31	0.65
1:B:191:LYS:HE2	1:B:191:LYS:O	1.96	0.65
1:A:95:ARG:NH2	1:A:144:ARG:NH1	2.45	0.65
1:A:41:ASP:OD1	1:A:43:SER:OG	2.11	0.65
1:A:193:ILE:O	1:A:197:MET:HG3	1.97	0.65
1:A:95:ARG:NH2	1:A:144:ARG:HH11	1.96	0.64
1:B:123:LYS:O	1:B:127:LEU:HD23	1.97	0.63
1:A:32:TYR:HD2	1:A:44:GLN:HG2	1.64	0.62
1:A:95:ARG:HH22	1:A:144:ARG:HH11	1.47	0.62
1:B:86:CYS:HB2	3:B:300:HOH:O	1.98	0.62
1:B:12:LEU:HD12	1:B:12:LEU:H	1.65	0.62
1:B:105:ASP:O	1:B:109:GLN:HG3	1.99	0.62
1:B:95:ARG:HH21	1:B:144:ARG:HE	1.46	0.61
1:B:124:PRO:O	1:B:127:LEU:N	2.27	0.61
1:B:172:LYS:O	1:B:174:LEU:N	2.33	0.61
1:B:40:TYR:CE2	1:B:210:LYS:HB2	2.36	0.61
1:A:95:ARG:HH22	1:A:144:ARG:NH1	1.99	0.61
1:B:110:LEU:HD13	1:B:166:TYR:CE1	2.33	0.60
1:A:21:GLU:HG3	1:A:196:TYR:CG	2.36	0.60
1:B:130:ILE:HG22	1:B:134:MET:HE3	1.83	0.59
1:B:113:LEU:HD22	1:B:126:PHE:HD2	1.65	0.59
1:B:197:MET:HG2	1:B:202:TYR:CE1	2.37	0.59
1:B:40:TYR:HE2	1:B:210:LYS:HB2	1.67	0.59
1:B:170:GLU:CB	1:B:173:CYS:HB3	2.22	0.58
1:B:42:ARG:HD3	3:B:338:HOH:O	2.02	0.58
1:B:120:GLU:O	1:B:123:LYS:HB2	2.03	0.58
1:A:115:TYR:HE1	1:A:211:LEU:HB3	1.67	0.57
1:B:130:ILE:HD12	1:B:170:GLU:HG3	1.86	0.57
1:B:2:MET:HE1	3:B:370:HOH:O	2.05	0.57
1:B:161:ASP:O	1:B:165:GLN:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASP:O	1:B:40:TYR:C	2.48	0.57
1:B:111:ILE:HG12	1:B:208:PHE:CZ	2.40	0.56
1:A:9:VAL:HG12	1:A:206:PRO:HG2	1.87	0.56
1:B:123:LYS:CB	1:B:124:PRO:HD2	2.35	0.56
1:B:151:LYS:HG2	1:B:152:VAL:O	2.05	0.56
1:B:191:LYS:HE2	1:B:191:LYS:C	2.31	0.56
1:A:172:LYS:N	1:A:172:LYS:HD3	2.21	0.55
1:B:8:ASN:HD22	1:B:8:ASN:H	1.53	0.55
1:A:145:PRO:HA	1:A:186:ARG:NH1	2.21	0.55
1:B:34:MET:HE2	1:B:40:TYR:HD2	1.69	0.55
1:B:125:GLU:HA	1:B:128:LYS:HE2	1.88	0.55
1:B:142:GLY:O	1:B:179:ASN:ND2	2.40	0.55
1:A:21:GLU:HG3	1:A:196:TYR:CD1	2.42	0.55
1:B:127:LEU:C	1:B:129:THR:H	2.13	0.55
1:B:8:ASN:HD22	1:B:8:ASN:N	2.05	0.54
1:B:130:ILE:CG2	1:B:134:MET:HE3	2.37	0.54
1:A:36:ASP:OD1	1:A:210:LYS:HD3	2.07	0.54
1:A:81:ARG:HE	1:B:90:GLU:CD	2.15	0.54
1:A:10:ARG:NH2	1:A:164:ASP:OD2	2.39	0.53
1:A:173:CYS:SG	1:A:174:LEU:CD1	2.97	0.53
1:B:8:ASN:ND2	3:B:305:HOH:O	2.42	0.53
1:B:214:TRP:O	1:B:216:ASN:N	2.42	0.53
1:B:107:ARG:O	1:B:111:ILE:HG13	2.09	0.53
1:A:132:GLU:HB2	3:A:365:HOH:O	2.09	0.52
1:B:92:GLU:HG2	1:B:148:ALA:O	2.09	0.52
1:B:130:ILE:O	1:B:133:LYS:N	2.41	0.52
1:B:40:TYR:HE2	1:B:211:LEU:N	2.07	0.52
1:A:10:ARG:HG3	1:A:14:HIS:HB2	1.91	0.52
1:B:12:LEU:HD21	2:B:218:GSH:HB12	1.91	0.52
1:A:6:PHE:O	1:A:31:ARG:HA	2.10	0.52
1:B:100:GLU:OE1	1:B:154:TYR:OH	2.20	0.52
1:A:29:GLU:CD	1:A:31:ARG:HH21	2.18	0.51
1:A:71:GLN:OE1	2:A:218:GSH:N1	2.43	0.51
1:B:111:ILE:HG12	1:B:208:PHE:CE2	2.46	0.51
1:A:12:LEU:HD13	1:A:72:SER:OG	2.12	0.50
1:A:20:LEU:O	1:A:25:SER:HB2	2.11	0.50
1:B:106:ASN:ND2	1:B:137:TYR:OH	2.45	0.50
1:B:120:GLU:HA	1:B:123:LYS:CG	2.37	0.50
1:B:47:ASN:ND2	3:B:270:HOH:O	2.44	0.50
1:A:1:PRO:O	1:A:3:ILE:HD12	2.12	0.50
1:B:127:LEU:C	1:B:129:THR:N	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HB2	1:A:54:LEU:HG	1.93	0.50
1:B:130:ILE:O	1:B:131:PRO:C	2.55	0.49
1:A:2:MET:C	1:A:3:ILE:HD12	2.36	0.49
1:B:123:LYS:O	1:B:124:PRO:C	2.54	0.49
1:A:37:ALA:HB1	1:A:38:PRO:HA	1.95	0.49
1:B:210:LYS:O	1:B:216:ASN:HB2	2.13	0.49
1:B:125:GLU:N	1:B:128:LYS:HE2	2.27	0.48
1:B:59:LEU:H	2:B:218:GSH:HA31	1.78	0.48
1:A:51:LYS:HD3	3:A:229:HOH:O	2.12	0.48
1:B:116:ASN:CG	1:B:117:PRO:HD3	2.39	0.48
1:B:172:LYS:C	1:B:174:LEU:N	2.70	0.48
1:B:207:ILE:HB	1:B:215:SER:HB3	1.96	0.48
1:A:104:MET:O	1:A:108:MET:HG2	2.14	0.48
1:A:107:ARG:O	1:A:111:ILE:HG13	2.14	0.48
1:B:94:ILE:O	1:B:98:ILE:HG13	2.14	0.47
1:B:120:GLU:C	1:B:122:GLN:H	2.22	0.47
1:A:45:TRP:CZ2	1:A:49:LYS:HG3	2.49	0.47
1:A:94:ILE:O	1:A:98:ILE:HG13	2.15	0.47
1:B:91:GLU:O	1:B:95:ARG:HG3	2.14	0.47
1:B:40:TYR:CE2	1:B:211:LEU:N	2.82	0.47
1:B:116:ASN:OD1	1:B:117:PRO:HD2	2.16	0.46
1:A:36:ASP:OD1	1:A:210:LYS:NZ	2.44	0.46
1:B:86:CYS:HB2	3:B:322:HOH:O	2.16	0.46
1:A:161:ASP:O	1:A:165:GLN:HG3	2.16	0.46
1:B:111:ILE:O	1:B:112:MET:C	2.59	0.46
1:A:10:ARG:CG	1:A:14:HIS:HB2	2.46	0.45
1:B:12:LEU:HB3	1:B:107:ARG:HD2	1.98	0.45
1:B:40:TYR:OH	1:B:211:LEU:HA	2.17	0.45
1:B:208:PHE:O	1:B:209:SER:O	2.34	0.45
1:B:209:SER:O	1:B:216:ASN:HB2	2.16	0.45
1:A:111:ILE:HG23	1:A:115:TYR:CD2	2.52	0.45
1:B:194:SER:HA	3:B:401:HOH:O	2.17	0.45
1:B:172:LYS:C	1:B:174:LEU:H	2.23	0.45
1:B:172:LYS:O	1:B:175:ASP:N	2.27	0.45
1:B:214:TRP:O	1:B:215:SER:C	2.59	0.45
1:B:7:TRP:HB3	3:B:305:HOH:O	2.18	0.44
1:B:34:MET:C	1:B:35:GLY:O	2.59	0.44
1:A:109:GLN:OE1	1:A:133:LYS:HE2	2.17	0.44
1:A:145:PRO:O	1:A:186:ARG:NH1	2.39	0.44
1:B:181:LYS:HB3	3:B:393:HOH:O	2.17	0.44
1:B:130:ILE:H	1:B:130:ILE:HG13	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ALA:O	1:B:178:PRO:HD3	2.17	0.44
1:A:173:CYS:SG	1:A:174:LEU:HD13	2.58	0.44
1:A:14:HIS:N	1:A:15:PRO:CD	2.81	0.43
1:B:8:ASN:H	1:B:8:ASN:ND2	2.15	0.43
1:B:123:LYS:NZ	1:B:169:PHE:HZ	2.16	0.43
1:B:134:MET:HE1	1:B:166:TYR:HD2	1.83	0.43
1:A:116:ASN:HA	1:A:117:PRO:HD2	1.76	0.43
1:B:178:PRO:HD2	3:B:266:HOH:O	2.18	0.43
1:B:120:GLU:HA	1:B:123:LYS:HB2	2.00	0.43
1:B:187:PHE:C	1:B:189:GLY:H	2.26	0.43
1:A:162:ILE:HD12	1:A:162:ILE:HA	1.76	0.43
1:B:204:SER:OG	1:B:205:THR:HG23	2.19	0.43
1:B:34:MET:HE2	1:B:40:TYR:CD2	2.53	0.42
1:B:104:MET:O	1:B:108:MET:HG2	2.19	0.42
1:A:187:PHE:O	1:A:190:LEU:HD12	2.20	0.42
1:B:212:ALA:HB3	1:B:216:ASN:HB3	2.02	0.42
1:B:162:ILE:HD12	1:B:162:ILE:HA	1.88	0.42
1:A:7:TRP:C	1:A:9:VAL:H	2.27	0.42
1:A:12:LEU:HD11	1:A:60:PRO:CD	2.49	0.42
1:B:37:ALA:HA	1:B:38:PRO:C	2.43	0.42
1:B:123:LYS:NZ	1:B:169:PHE:CZ	2.86	0.42
1:B:209:SER:O	1:B:210:LYS:C	2.63	0.42
1:A:71:GLN:NE2	1:B:105:ASP:OD2	2.34	0.42
1:B:184:LEU:O	1:B:188:GLU:HG2	2.19	0.42
1:B:187:PHE:C	1:B:189:GLY:N	2.78	0.41
1:B:208:PHE:O	1:B:216:ASN:HA	2.19	0.41
1:B:129:THR:O	1:B:130:ILE:C	2.62	0.41
1:B:1:PRO:HG3	3:B:350:HOH:O	2.21	0.41
1:A:127:LEU:HA	1:A:130:ILE:HD12	2.03	0.41
1:B:4:LEU:HB3	1:B:29:GLU:HG2	2.02	0.41
1:B:48:GLU:O	1:B:52:LEU:HG	2.20	0.41
1:B:125:GLU:HA	1:B:128:LYS:HG3	2.02	0.41
1:B:195:ALA:HA	1:B:198:LYS:HE3	2.03	0.41
1:B:119:PHE:CG	1:B:213:GLN:HG3	2.56	0.41
1:B:115:TYR:O	1:B:116:ASN:HB2	2.21	0.41
2:A:218:GSH:HN12	1:B:105:ASP:CG	2.28	0.40
1:B:123:LYS:C	1:B:127:LEU:HD23	2.47	0.40
1:A:198:LYS:HB2	3:A:395:HOH:O	2.22	0.40
1:B:210:LYS:HA	1:B:216:ASN:O	2.21	0.40

All (4) 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:A:191:LYS:CD	1:B:118:ASP:OD1[3_455]	1.30	0.90
1:B:67:ARG:NH2	1:B:67:ARG:NH2[2_555]	1.83	0.37
1:A:191:LYS:CE	1:B:118:ASP:OD1[3_455]	2.01	0.19
1:A:191:LYS:NZ	1:B:118:ASP:CG[3_455]	2.18	0.02

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	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	24	27
1	B	215/217 (99%)	183 (85%)	18 (8%)	14 (6%)	1	0
All	All	430/434 (99%)	386 (90%)	29 (7%)	15 (4%)	3	1

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	ASP
1	B	122	GLN
1	B	123	LYS
1	B	173	CYS
1	B	209	SER
1	B	212	ALA
1	B	215	SER
1	B	38	PRO
1	B	40	TYR
1	B	117	PRO
1	B	124	PRO
1	B	125	GLU
1	A	119	PHE
1	B	71	GLN
1	B	116	ASN

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%)	174 (88%)	23 (12%)	5	5
1	B	197/197 (100%)	170 (86%)	27 (14%)	3	3
All	All	394/394 (100%)	344 (87%)	50 (13%)	4	4

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	8	ASN
1	A	19	LEU
1	A	25	SER
1	A	39	ASP
1	A	41	ASP
1	A	48	GLU
1	A	51	LYS
1	A	68	LYS
1	A	84	HIS
1	A	93	ARG
1	A	116	ASN
1	A	118	ASP
1	A	120	GLU
1	A	121	LYS
1	A	128	LYS
1	A	150	ASP
1	A	151	LYS
1	A	172	LYS
1	A	192	LYS
1	A	204	SER
1	A	211	LEU
1	A	217	LYS
1	B	8	ASN
1	B	12	LEU
1	B	19	LEU
1	B	26	SER

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Mol	Chain	Res	Type
1	B	36	ASP
1	B	40	TYR
1	B	52	LEU
1	B	69	ILE
1	B	108	MET
1	B	119	PHE
1	B	122	GLN
1	B	123	LYS
1	B	128	LYS
1	B	129	THR
1	B	132	GLU
1	B	151	LYS
1	B	175	ASP
1	B	178	PRO
1	B	186	ARG
1	B	191	LYS
1	B	192	LYS
1	B	198	LYS
1	B	203	LEU
1	B	207	ILE
1	B	209	SER
1	B	211	LEU
1	B	215	SER

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	47	ASN
1	A	106	ASN
1	B	8	ASN
1	B	47	ASN
1	B	106	ASN
1	B	109	GLN
1	B	167	HIS

5.3.3 RNA ⓘ

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](#)

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	218	-	18,19,19	1.96	6 (33%)	21,24,24	2.74	10 (47%)
2	GSH	B	218	-	18,19,19	2.13	6 (33%)	21,24,24	2.91	11 (52%)

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	218	-	-	2/24/24/24	-
2	GSH	B	218	-	-	1/24/24/24	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	218	GSH	O12-C1	4.56	1.35	1.22
2	B	218	GSH	O12-C1	4.43	1.35	1.22
2	A	218	GSH	O32-C3	4.01	1.35	1.22
2	B	218	GSH	C2-N3	-3.41	1.25	1.33
2	B	218	GSH	O32-C3	3.37	1.33	1.22
2	B	218	GSH	O11-C1	-2.62	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	218	GSH	CA2-C2	2.41	1.59	1.52
2	B	218	GSH	CG1-CD1	-2.39	1.46	1.51
2	A	218	GSH	O11-C1	-2.39	1.23	1.30
2	A	218	GSH	CG1-CD1	-2.29	1.46	1.51
2	A	218	GSH	C2-N3	-2.23	1.28	1.33
2	A	218	GSH	CA3-N3	2.06	1.50	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	218	GSH	CA2-CB2-SG2	-6.96	106.32	114.16
2	B	218	GSH	O2-C2-N3	6.73	137.22	122.98
2	B	218	GSH	O2-C2-CA2	-6.46	106.96	120.48
2	A	218	GSH	OE1-CD1-CG1	-4.06	114.66	122.02
2	A	218	GSH	CB1-CG1-CD1	3.89	121.73	113.06
2	A	218	GSH	O31-C3-CA3	3.86	127.50	112.81
2	A	218	GSH	CB2-CA2-N2	3.73	116.60	111.28
2	B	218	GSH	CA3-N3-C2	3.67	130.65	121.38
2	B	218	GSH	CB2-CA2-N2	3.62	116.45	111.28
2	A	218	GSH	O31-C3-O32	-3.54	114.24	123.33
2	B	218	GSH	O31-C3-O32	-3.14	115.25	123.33
2	B	218	GSH	CG1-CB1-CA1	-3.05	106.86	113.86
2	A	218	GSH	CG1-CD1-N2	2.89	120.95	115.86
2	B	218	GSH	O31-C3-CA3	2.76	123.32	112.81
2	B	218	GSH	CA2-CB2-SG2	-2.76	111.05	114.16
2	A	218	GSH	CB1-CA1-N1	2.68	117.10	110.12
2	B	218	GSH	CB1-CG1-CD1	2.63	118.92	113.06
2	B	218	GSH	C2-CA2-N2	-2.60	104.07	111.11
2	A	218	GSH	CG1-CB1-CA1	-2.39	108.38	113.86
2	B	218	GSH	OE1-CD1-CG1	-2.25	117.95	122.02
2	A	218	GSH	CB2-CA2-C2	2.10	114.07	109.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

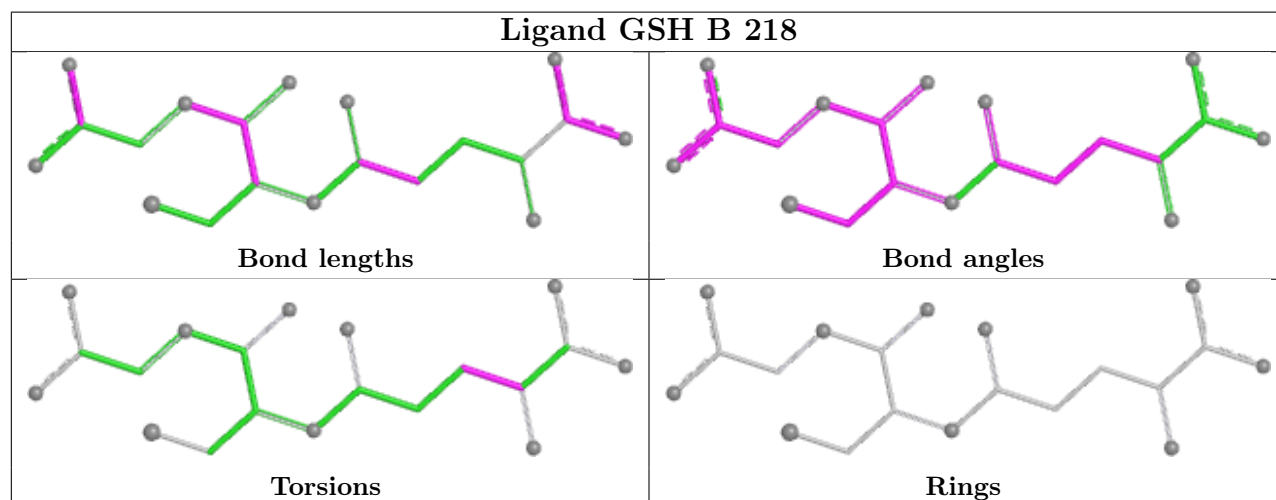
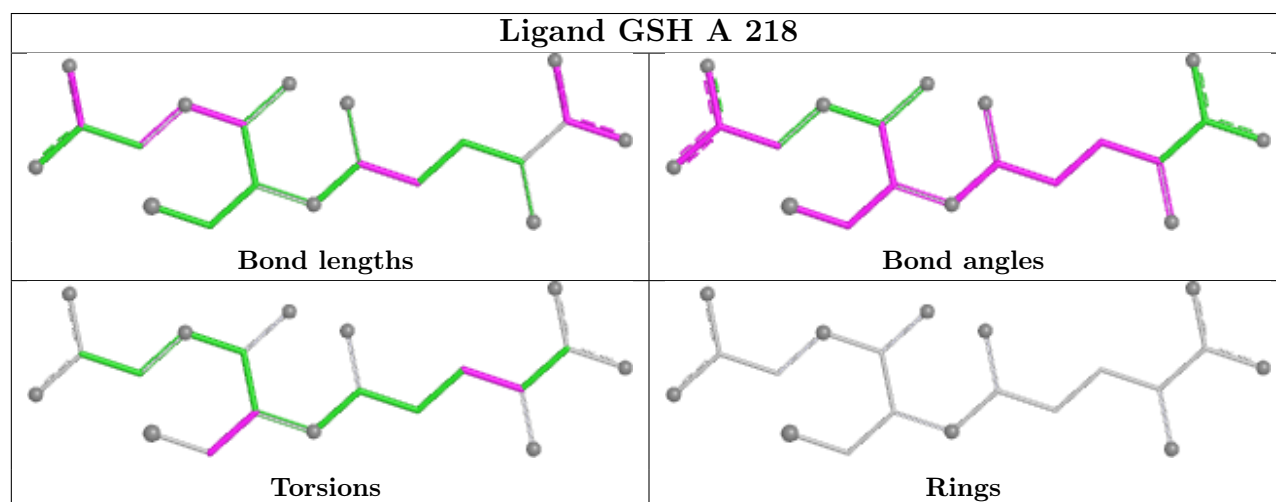
Mol	Chain	Res	Type	Atoms
2	A	218	GSH	N2-CA2-CB2-SG2
2	A	218	GSH	N1-CA1-CB1-CG1
2	B	218	GSH	C1-CA1-CB1-CG1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	218	GSH	2	0
2	B	218	GSH	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.