



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:29 PM UTC

PDB ID : 7Y55 / pdb_00007y55
Title : Crystal structure of a glutathione S-transferase Tau1 from Pinus densata in complex with GSH
Authors : Qu, C.; Zeng, Q.Y.
Deposited on : 2022-06-16
Resolution : 2.19 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

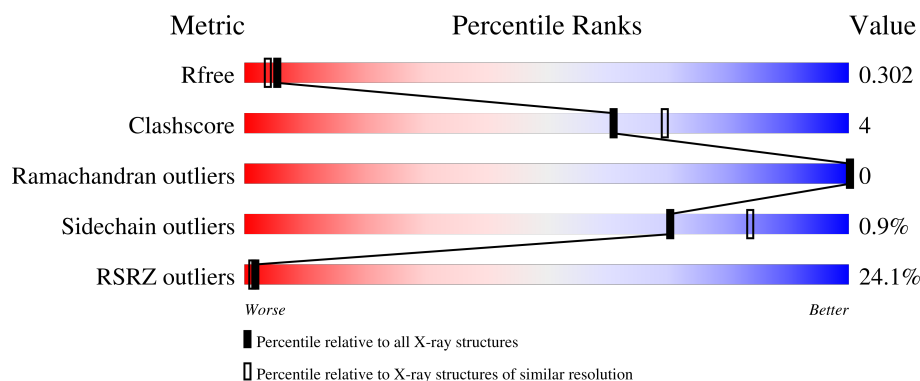
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	237	
1	B	237	
1	C	237	
1	D	237	

2 Entry composition [i](#)

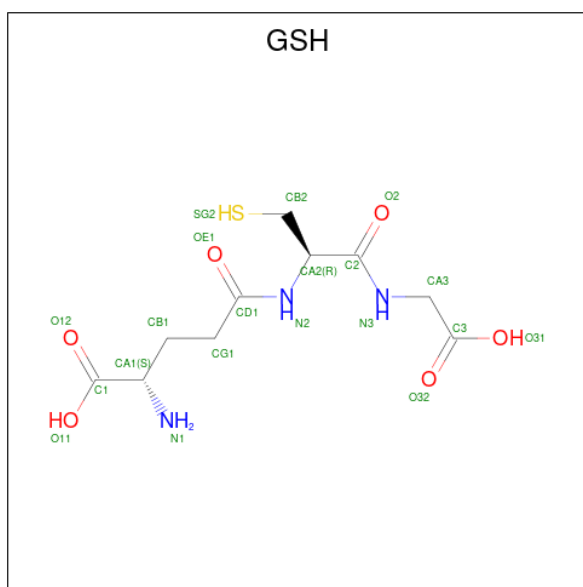
There are 3 unique types of molecules in this entry. The entry contains 14837 atoms, of which 7327 are hydrogens and 0 are deuteriums.

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 PdGSTU1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	224	Total	C	H	N	O	S	0	0	0
			3655	1191	1824	305	324	11			
1	B	224	Total	C	H	N	O	S	0	0	0
			3655	1191	1824	305	324	11			
1	C	223	Total	C	H	N	O	S	0	0	0
			3639	1186	1817	304	321	11			
1	D	221	Total	C	H	N	O	S	0	0	0
			3609	1177	1802	301	318	11			

- Molecule 2 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			35	10	15	3	6	1		
2	B	1	Total	C	H	N	O	S	0	0
			35	10	15	3	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	S	0	0
			35	10	15	3	6	1		
2	D	1	Total	C	H	N	O	S	0	0
			35	10	15	3	6	1		

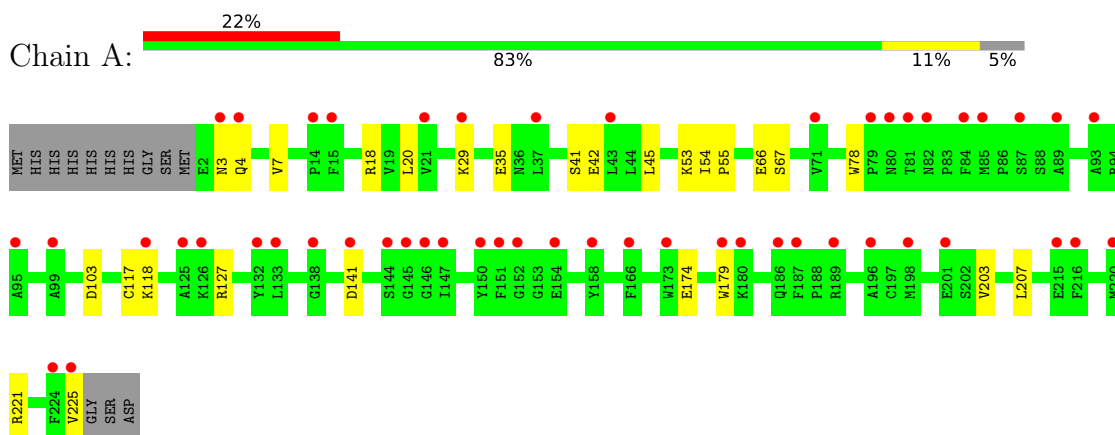
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	30	Total	O	0	0
			30	30		
3	C	47	Total	O	0	0
			47	47		
3	D	37	Total	O	0	0
			37	37		

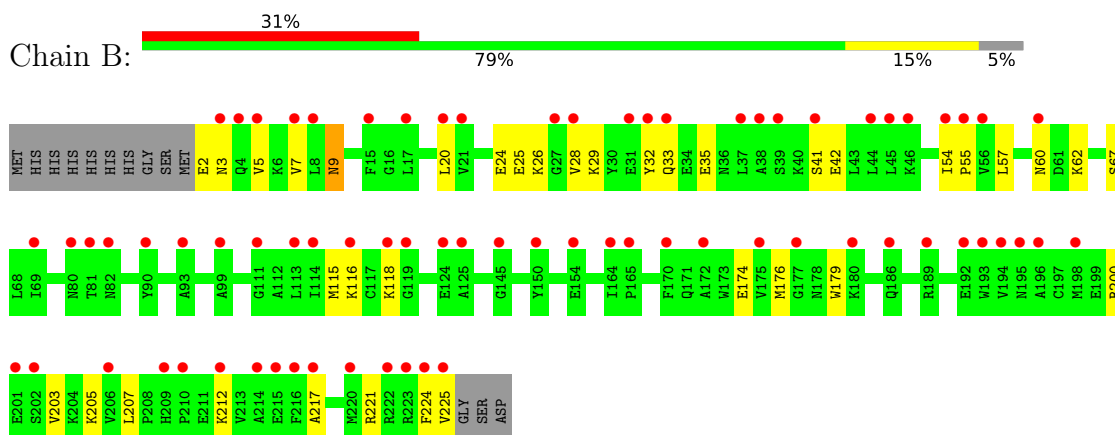
3 Residue-property plots [i](#)

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.

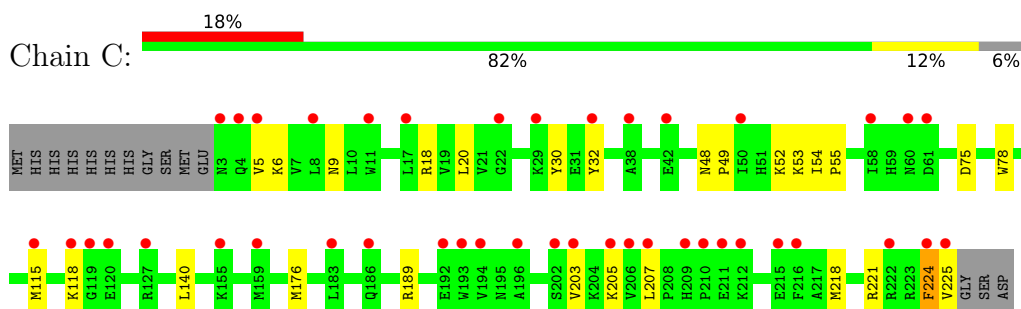
• Molecule 1: PdGSTU1



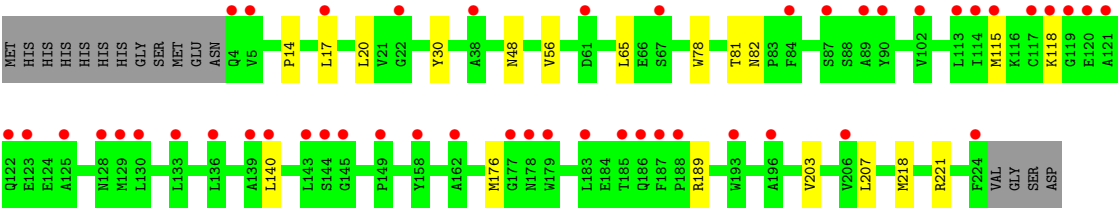
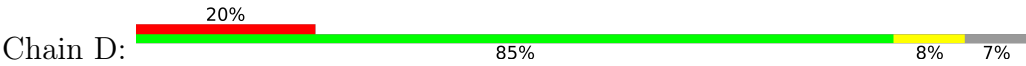
• Molecule 1: PdGSTU1



• Molecule 1: PdGSTU1



● Molecule 1: PdGSTU1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.40Å 55.51Å 119.75Å 90.00° 112.50° 90.00°	Depositor
Resolution (Å)	38.43 – 2.19 38.43 – 2.19	Depositor EDS
% Data completeness (in resolution range)	93.5 (38.43-2.19) 93.4 (38.43-2.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692+SVN	Depositor
R, R_{free}	0.276 , 0.302 0.278 , 0.302	Depositor DCC
R_{free} test set	2000 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14837	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0106e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.52	0/1881	0.86	3/2540 (0.1%)
1	B	0.51	0/1881	0.91	2/2540 (0.1%)
1	C	0.51	0/1872	0.94	6/2528 (0.2%)
1	D	0.51	0/1857	0.91	4/2507 (0.2%)
All	All	0.51	0/7491	0.91	15/10115 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78	TRP	CA-C-N	5.58	126.44	120.47
1	D	78	TRP	C-N-CA	5.58	126.44	120.47
1	C	224	PHE	N-CA-C	-5.58	101.92	109.95
1	D	48	ASN	CA-C-N	5.55	125.17	119.56
1	D	48	ASN	C-N-CA	5.55	125.17	119.56
1	C	5	VAL	N-CA-C	5.45	115.96	108.12
1	C	48	ASN	CA-C-N	5.34	124.96	119.56
1	C	48	ASN	C-N-CA	5.34	124.96	119.56
1	B	224	PHE	N-CA-C	-5.32	102.17	110.42
1	A	78	TRP	CA-C-N	5.30	124.99	119.64
1	A	78	TRP	C-N-CA	5.30	124.99	119.64
1	C	78	TRP	CA-C-N	5.27	126.11	120.47
1	C	78	TRP	C-N-CA	5.27	126.11	120.47
1	B	9	ASN	N-CA-C	5.07	116.55	108.79
1	A	4	GLN	N-CA-C	5.05	119.31	113.20

There are no chirality outliers.

There are no planarity outliers.

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	1831	1824	1823	15	0
1	B	1831	1824	1823	22	0
1	C	1822	1817	1817	16	0
1	D	1807	1802	1802	9	0
2	A	20	15	15	4	0
2	B	20	15	15	1	0
2	C	20	15	15	1	0
2	D	20	15	15	0	0
3	A	25	0	0	2	0
3	B	30	0	0	4	0
3	C	47	0	0	4	0
3	D	37	0	0	0	0
All	All	7510	7327	7325	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:SER:N	2:A:301:GSH:O11	2.16	0.77
1:A:117:CYS:SG	3:A:425:HOH:O	2.49	0.70
1:A:221:ARG:O	1:A:225:VAL:N	2.26	0.69
1:C:103:ASP:OD2	3:C:401:HOH:O	2.13	0.67
1:B:212:LYS:NZ	3:B:403:HOH:O	2.29	0.65
1:C:189:ARG:NH1	3:C:402:HOH:O	2.29	0.64
1:C:49:PRO:O	1:C:52:LYS:NZ	2.29	0.64
1:C:6:LYS:NZ	3:C:403:HOH:O	2.29	0.64
1:B:62:LYS:HG2	1:D:81:THR:HG21	1.83	0.61
1:C:115:MET:O	1:C:221:ARG:NH1	2.35	0.59
1:D:203:VAL:HG13	1:D:207:LEU:HD22	1.84	0.59
1:C:203:VAL:HG13	1:C:207:LEU:HD22	1.87	0.56
1:B:2:GLU:N	3:B:404:HOH:O	2.38	0.56
1:C:205:LYS:NZ	3:C:404:HOH:O	2.38	0.55
1:A:127:ARG:NH1	3:A:402:HOH:O	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASN:HD22	1:A:29:LYS:HE2	1.74	0.53
1:B:203:VAL:HG13	1:B:207:LEU:HD22	1.90	0.53
1:D:140:LEU:HD23	1:D:189:ARG:HB3	1.92	0.52
1:A:54:ILE:HD11	2:A:301:GSH:HB23	1.93	0.51
1:C:140:LEU:HD23	1:C:189:ARG:HB3	1.93	0.50
1:A:18:ARG:NH2	1:A:103:ASP:OD1	2.40	0.49
1:B:24:GLU:OE1	1:B:205:LYS:NZ	2.36	0.49
1:C:20:LEU:HD22	1:C:30:TYR:CE2	2.49	0.47
1:A:66:GLU:HA	2:A:301:GSH:HN11	1.80	0.47
1:D:115:MET:O	1:D:221:ARG:NH1	2.47	0.47
1:C:176:MET:HG2	1:C:218:MET:SD	2.55	0.47
1:A:54:ILE:HB	1:A:55:PRO:HA	1.96	0.46
1:B:3:ASN:ND2	1:B:29:LYS:HE2	2.31	0.46
1:B:174:GLU:HA	1:B:179:TRP:CD1	2.50	0.46
1:A:174:GLU:HA	1:A:179:TRP:CD1	2.52	0.45
1:D:176:MET:HG2	1:D:218:MET:SD	2.56	0.45
1:C:9:ASN:HB3	1:C:32:TYR:CE1	2.52	0.45
1:B:7:VAL:HG11	1:B:20:LEU:HD21	1.98	0.45
1:C:224:PHE:O	1:C:225:VAL:C	2.60	0.44
1:B:5:VAL:HG13	1:B:57:LEU:HD11	1.98	0.44
1:C:54:ILE:HB	1:C:55:PRO:HA	2.00	0.44
1:A:7:VAL:HG11	1:A:20:LEU:HD21	2.00	0.43
1:D:14:PRO:HA	1:D:17:LEU:HD12	1.99	0.43
1:B:42:GLU:OE2	3:B:402:HOH:O	2.21	0.43
1:B:54:ILE:HB	1:B:55:PRO:HA	2.01	0.43
1:B:25:GLU:OE1	1:B:200:ARG:NH2	2.50	0.43
1:C:75:ASP:OD2	1:C:85:MET:HG2	2.19	0.43
1:B:116:LYS:NZ	3:B:409:HOH:O	2.51	0.43
1:B:26:LYS:HB2	1:B:28:VAL:HG23	2.00	0.43
1:A:203:VAL:HG13	1:A:207:LEU:HD22	2.01	0.42
1:D:81:THR:HG22	1:D:82:ASN:OD1	2.19	0.42
1:D:56:VAL:HG22	1:D:65:LEU:CD2	2.50	0.42
1:B:67:SER:OG	2:B:301:GSH:O12	2.25	0.42
1:B:35:GLU:OE2	1:B:41:SER:OG	2.37	0.42
1:B:176:MET:CE	1:B:217:ALA:HB1	2.50	0.41
1:A:53:LYS:HD3	2:A:301:GSH:HB13	2.02	0.41
1:C:53:LYS:HA	2:C:301:GSH:HA31	2.03	0.41
1:D:20:LEU:HD22	1:D:30:TYR:CE2	2.56	0.41
1:B:9:ASN:HB3	1:B:32:TYR:CE1	2.55	0.41
1:A:35:GLU:OE2	1:A:41:SER:OG	2.29	0.41
1:B:3:ASN:HD22	1:B:29:LYS:HE2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:NH2	1:C:103:ASP:OD1	2.45	0.41
1:B:115:MET:O	1:B:221:ARG:NH1	2.48	0.40
1:B:33:GLN:NE2	1:B:35:GLU:OE2	2.44	0.40
1:A:42:GLU:HA	1:A:45:LEU:HD12	2.04	0.40
1:B:203:VAL:CG1	1:B:207:LEU:HD22	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/237 (94%)	214 (96%)	8 (4%)	0	100	100
1	B	222/237 (94%)	213 (96%)	9 (4%)	0	100	100
1	C	221/237 (93%)	215 (97%)	6 (3%)	0	100	100
1	D	219/237 (92%)	212 (97%)	7 (3%)	0	100	100
All	All	884/948 (93%)	854 (97%)	30 (3%)	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	193/204 (95%)	191 (99%)	2 (1%)	68	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	193/204 (95%)	190 (98%)	3 (2%)	55	71
1	C	192/204 (94%)	191 (100%)	1 (0%)	81	90
1	D	190/204 (93%)	189 (100%)	1 (0%)	81	90
All	All	768/816 (94%)	761 (99%)	7 (1%)	70	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LYS
1	A	141	ASP
1	B	60	ASN
1	B	118	LYS
1	B	225	VAL
1	C	118	LYS
1	D	118	LYS

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

Mol	Chain	Res	Type
1	A	60	ASN
1	A	109	ASN
1	C	82	ASN
1	D	80	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	C	301	-	18,19,19	1.68	2 (11%)	21,24,24	1.69	4 (19%)
2	GSH	B	301	-	18,19,19	1.64	2 (11%)	21,24,24	1.66	5 (23%)
2	GSH	A	301	-	18,19,19	1.71	3 (16%)	21,24,24	1.74	3 (14%)
2	GSH	D	301	-	18,19,19	1.63	2 (11%)	21,24,24	1.57	5 (23%)

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	C	301	-	-	7/24/24/24	-
2	GSH	B	301	-	-	6/24/24/24	-
2	GSH	A	301	-	-	5/24/24/24	-
2	GSH	D	301	-	-	7/24/24/24	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	GSH	CD1-N2	4.20	1.42	1.34
2	C	301	GSH	CD1-N2	4.00	1.42	1.34
2	C	301	GSH	C2-N3	3.92	1.42	1.33
2	B	301	GSH	CD1-N2	3.91	1.42	1.34
2	D	301	GSH	CD1-N2	3.89	1.42	1.34
2	D	301	GSH	C2-N3	3.82	1.42	1.33
2	B	301	GSH	C2-N3	3.62	1.42	1.33
2	A	301	GSH	C2-N3	3.57	1.42	1.33
2	A	301	GSH	CB2-SG2	-2.25	1.76	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	GSH	CA2-CB2-SG2	-4.71	108.85	114.16
2	A	301	GSH	CA2-CB2-SG2	-4.17	109.45	114.16
2	A	301	GSH	CG1-CB1-CA1	-3.73	105.31	113.86
2	D	301	GSH	CB2-CA2-N2	-3.61	106.14	111.28
2	B	301	GSH	CA2-CB2-SG2	-3.34	110.39	114.16
2	D	301	GSH	CG1-CB1-CA1	-3.27	106.36	113.86
2	B	301	GSH	C2-CA2-N2	-3.24	102.34	111.11
2	B	301	GSH	CG1-CB1-CA1	-3.16	106.61	113.86
2	B	301	GSH	CA2-C2-N3	3.01	123.00	116.54
2	A	301	GSH	CG1-CD1-N2	2.74	120.70	115.86
2	C	301	GSH	CG1-CD1-N2	2.54	120.33	115.86
2	D	301	GSH	CA2-C2-N3	2.23	121.32	116.54
2	D	301	GSH	CA2-CB2-SG2	-2.22	111.65	114.16
2	C	301	GSH	OE1-CD1-N2	-2.10	119.39	122.95
2	C	301	GSH	O11-C1-O12	-2.08	119.36	124.08
2	D	301	GSH	O31-C3-CA3	2.07	120.70	112.81
2	B	301	GSH	O2-C2-N3	-2.04	118.65	122.98

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	GSH	O12-C1-CA1-N1
2	B	301	GSH	N2-CA2-CB2-SG2
2	B	301	GSH	C2-CA2-CB2-SG2
2	C	301	GSH	N2-CA2-CB2-SG2
2	C	301	GSH	C2-CA2-CB2-SG2
2	D	301	GSH	O12-C1-CA1-N1
2	D	301	GSH	N2-CA2-CB2-SG2
2	D	301	GSH	C2-CA2-CB2-SG2
2	A	301	GSH	O11-C1-CA1-N1
2	A	301	GSH	CA1-CB1-CG1-CD1
2	B	301	GSH	O11-C1-CA1-N1
2	D	301	GSH	O11-C1-CA1-N1
2	C	301	GSH	O31-C3-CA3-N3
2	C	301	GSH	O32-C3-CA3-N3
2	B	301	GSH	CA1-CB1-CG1-CD1
2	C	301	GSH	O2-C2-CA2-N2
2	C	301	GSH	N1-CA1-CB1-CG1
2	C	301	GSH	N3-C2-CA2-N2
2	A	301	GSH	O11-C1-CA1-CB1

Continued on next page...

Continued from previous page...

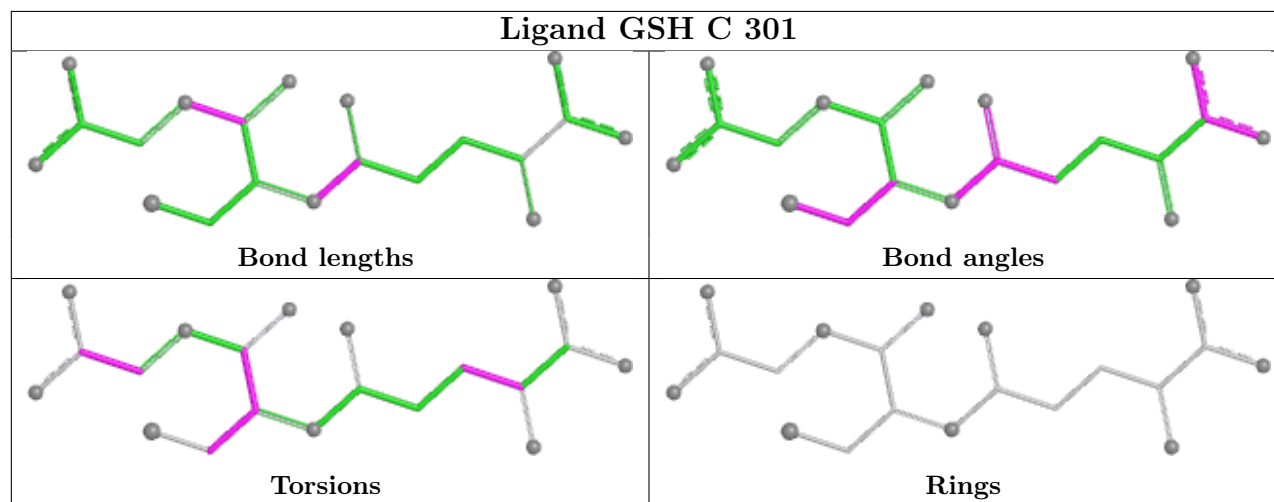
Mol	Chain	Res	Type	Atoms
2	A	301	GSH	O12-C1-CA1-CB1
2	D	301	GSH	O12-C1-CA1-CB1
2	D	301	GSH	O11-C1-CA1-CB1
2	B	301	GSH	N1-CA1-CB1-CG1
2	D	301	GSH	N1-CA1-CB1-CG1
2	A	301	GSH	O12-C1-CA1-N1

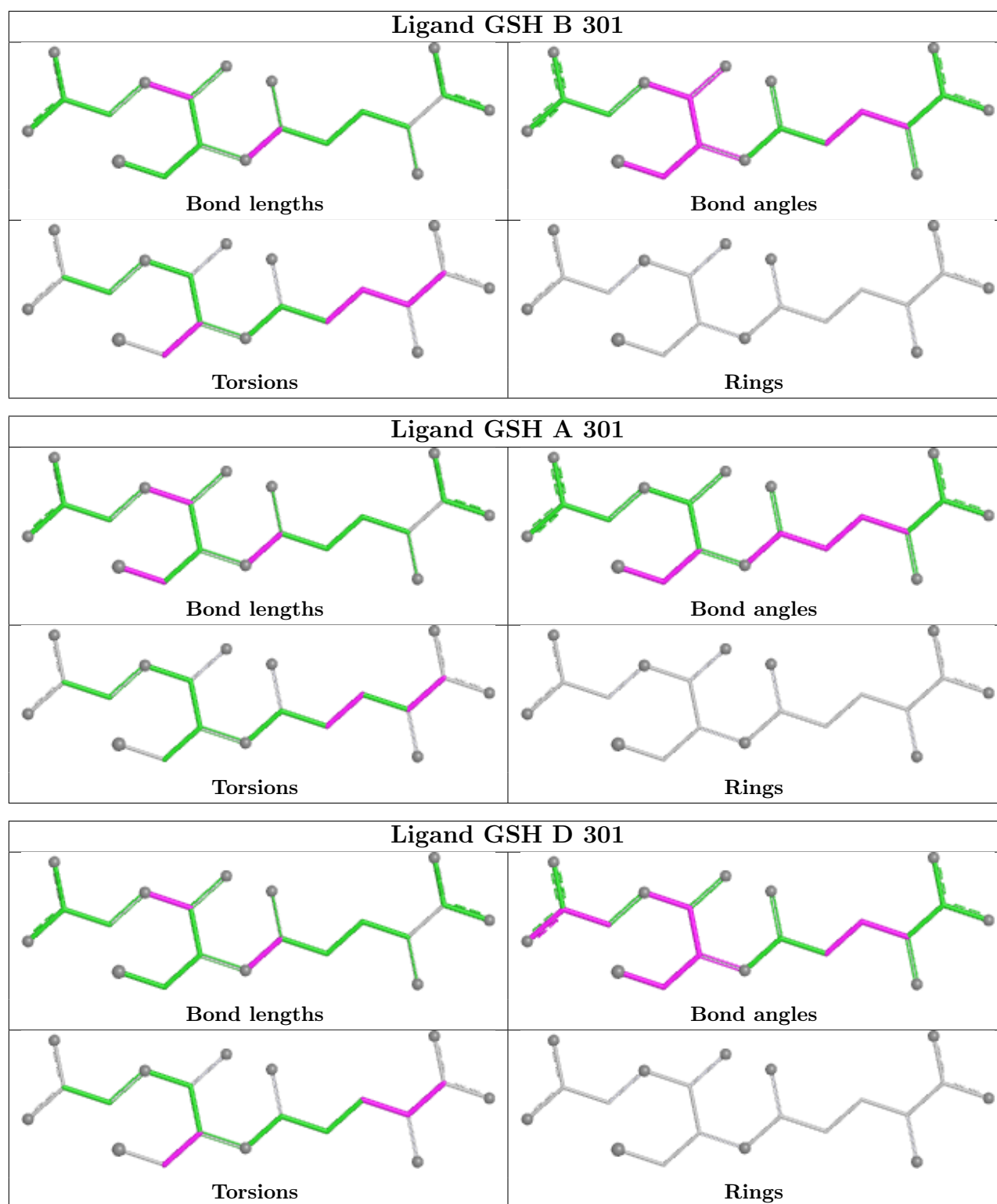
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	GSH	1	0
2	B	301	GSH	1	0
2	A	301	GSH	4	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	224/237 (94%)	1.33	51 (22%)	2 1	34, 51, 75, 95	0
1	B	224/237 (94%)	1.66	73 (32%)	1 0	38, 57, 83, 104	0
1	C	223/237 (94%)	1.24	43 (19%)	3 2	34, 46, 73, 97	0
1	D	221/237 (93%)	1.30	48 (21%)	2 1	34, 48, 72, 132	0
All	All	892/948 (94%)	1.38	215 (24%)	2 1	34, 50, 77, 132	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	ASN	7.7
1	C	4	GLN	6.4
1	B	224	PHE	6.2
1	B	220	MET	6.1
1	B	60	ASN	5.6
1	C	225	VAL	5.2
1	C	38	ALA	4.8
1	A	82	ASN	4.8
1	D	224	PHE	4.5
1	B	3	ASN	4.5
1	D	4	GLN	4.3
1	B	225	VAL	4.3
1	B	114	ILE	4.2
1	B	201	GLU	4.2
1	B	7	VAL	4.2
1	D	119	GLY	4.2
1	D	118	LYS	4.2
1	B	37	LEU	4.0
1	D	136	LEU	3.9
1	C	159	MET	3.9
1	D	22	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	187	PHE	3.8
1	B	81	THR	3.8
1	B	198	MET	3.8
1	B	5	VAL	3.7
1	C	120	GLU	3.7
1	D	186	GLN	3.7
1	A	198	MET	3.7
1	B	56	VAL	3.7
1	A	225	VAL	3.6
1	B	33	GLN	3.6
1	C	5	VAL	3.6
1	D	125	ALA	3.6
1	A	81	THR	3.6
1	A	95	ALA	3.5
1	B	206	VAL	3.5
1	B	216	PHE	3.5
1	A	180	LYS	3.4
1	B	111	GLY	3.4
1	B	118	LYS	3.4
1	B	202	SER	3.3
1	A	89	ALA	3.3
1	B	15	PHE	3.3
1	D	90	TYR	3.3
1	A	147	ILE	3.3
1	B	180	LYS	3.2
1	D	61	ASP	3.2
1	B	215	GLU	3.2
1	A	220	MET	3.1
1	A	4	GLN	3.1
1	D	38	ALA	3.1
1	A	3	ASN	3.1
1	B	90	TYR	3.0
1	B	116	LYS	3.0
1	B	217	ALA	3.0
1	D	89	ALA	3.0
1	A	146	GLY	3.0
1	A	224	PHE	3.0
1	B	172	ALA	3.0
1	D	121	ALA	3.0
1	D	120	GLU	3.0
1	B	189	ARG	2.9
1	B	124	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	22	GLY	2.9
1	C	212	LYS	2.9
1	A	71	VAL	2.9
1	A	166	PHE	2.9
1	C	224	PHE	2.9
1	B	82	ASN	2.9
1	A	80	ASN	2.9
1	A	173	TRP	2.9
1	B	209	HIS	2.9
1	B	192	GLU	2.8
1	B	186	GLN	2.8
1	B	196	ALA	2.8
1	C	207	LEU	2.8
1	A	79	PRO	2.8
1	B	210	PRO	2.8
1	C	203	VAL	2.8
1	B	20	LEU	2.7
1	B	223	ARG	2.7
1	C	50	ILE	2.7
1	C	11	TRP	2.7
1	B	8	LEU	2.7
1	D	187	PHE	2.7
1	B	150	TYR	2.7
1	A	144	SER	2.7
1	B	222	ARG	2.7
1	D	84	PHE	2.6
1	A	43	LEU	2.6
1	D	130	LEU	2.6
1	B	27	GLY	2.6
1	C	119	GLY	2.6
1	A	196	ALA	2.6
1	A	133	LEU	2.6
1	C	210	PRO	2.6
1	A	138	GLY	2.6
1	C	186	GLN	2.6
1	D	177	GLY	2.6
1	C	192	GLU	2.6
1	C	215	GLU	2.6
1	C	209	HIS	2.6
1	C	60	ASN	2.6
1	D	178	ASN	2.6
1	D	185	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	141	ASP	2.6
1	B	17	LEU	2.6
1	B	113	LEU	2.6
1	B	212	LYS	2.6
1	D	113	LEU	2.6
1	A	201	GLU	2.6
1	C	196	ALA	2.6
1	D	145	GLY	2.5
1	D	193	TRP	2.5
1	A	145	GLY	2.5
1	D	188	PRO	2.5
1	B	125	ALA	2.5
1	B	69	ILE	2.5
1	B	175	VAL	2.4
1	B	38	ALA	2.4
1	D	196	ALA	2.4
1	C	205	LYS	2.4
1	D	17	LEU	2.4
1	A	150	TYR	2.4
1	B	170	PHE	2.4
1	B	54	ILE	2.4
1	C	29	LYS	2.4
1	C	155	LYS	2.4
1	B	4	GLN	2.4
1	B	164	ILE	2.4
1	A	189	ARG	2.4
1	C	118	LYS	2.4
1	D	144	SER	2.4
1	A	179	TRP	2.4
1	B	193	TRP	2.4
1	C	211	GLU	2.3
1	D	183	LEU	2.3
1	D	87	SER	2.3
1	D	139	ALA	2.3
1	B	177	GLY	2.3
1	C	61	ASP	2.3
1	B	39	SER	2.3
1	A	152	GLY	2.3
1	D	179	TRP	2.3
1	D	115	MET	2.3
1	B	28	VAL	2.3
1	D	5	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	149	PRO	2.3
1	C	222	ARG	2.3
1	A	99	ALA	2.3
1	B	99	ALA	2.3
1	B	32	TYR	2.3
1	A	186	GLN	2.2
1	C	88	SER	2.2
1	D	117	CYS	2.2
1	C	183	LEU	2.2
1	A	154	GLU	2.2
1	A	151	PHE	2.2
1	A	29	LYS	2.2
1	B	194	VAL	2.2
1	C	194	VAL	2.2
1	A	125	ALA	2.2
1	B	45	LEU	2.2
1	C	17	LEU	2.2
1	C	32	TYR	2.2
1	C	127	ARG	2.2
1	A	85	MET	2.2
1	B	55	PRO	2.2
1	A	21	VAL	2.2
1	B	154	GLU	2.2
1	D	140	LEU	2.2
1	D	143	LEU	2.2
1	B	31	GLU	2.1
1	C	42	GLU	2.1
1	C	58	ILE	2.1
1	A	37	LEU	2.1
1	C	115	MET	2.1
1	D	158	TYR	2.1
1	D	114	ILE	2.1
1	B	145	GLY	2.1
1	A	126	LYS	2.1
1	B	41	SER	2.1
1	C	8	LEU	2.1
1	D	67	SER	2.1
1	B	80	ASN	2.1
1	D	129	MET	2.1
1	D	123	GLU	2.1
1	A	158	TYR	2.1
1	A	216	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	193	TRP	2.1
1	C	206	VAL	2.1
1	D	162	ALA	2.1
1	A	87	SER	2.1
1	C	202	SER	2.1
1	A	215	GLU	2.1
1	D	122	GLN	2.1
1	B	119	GLY	2.1
1	A	118	LYS	2.1
1	B	46	LYS	2.1
1	C	216	PHE	2.1
1	B	93	ALA	2.1
1	B	214	ALA	2.1
1	B	44	LEU	2.0
1	D	133	LEU	2.0
1	A	14	PRO	2.0
1	B	165	PRO	2.0
1	A	132	TYR	2.0
1	A	15	PHE	2.0
1	A	84	PHE	2.0
1	B	21	VAL	2.0
1	D	102	VAL	2.0
1	D	206	VAL	2.0
1	A	93	ALA	2.0
1	B	195	ASN	2.0
1	D	128	ASN	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](#)

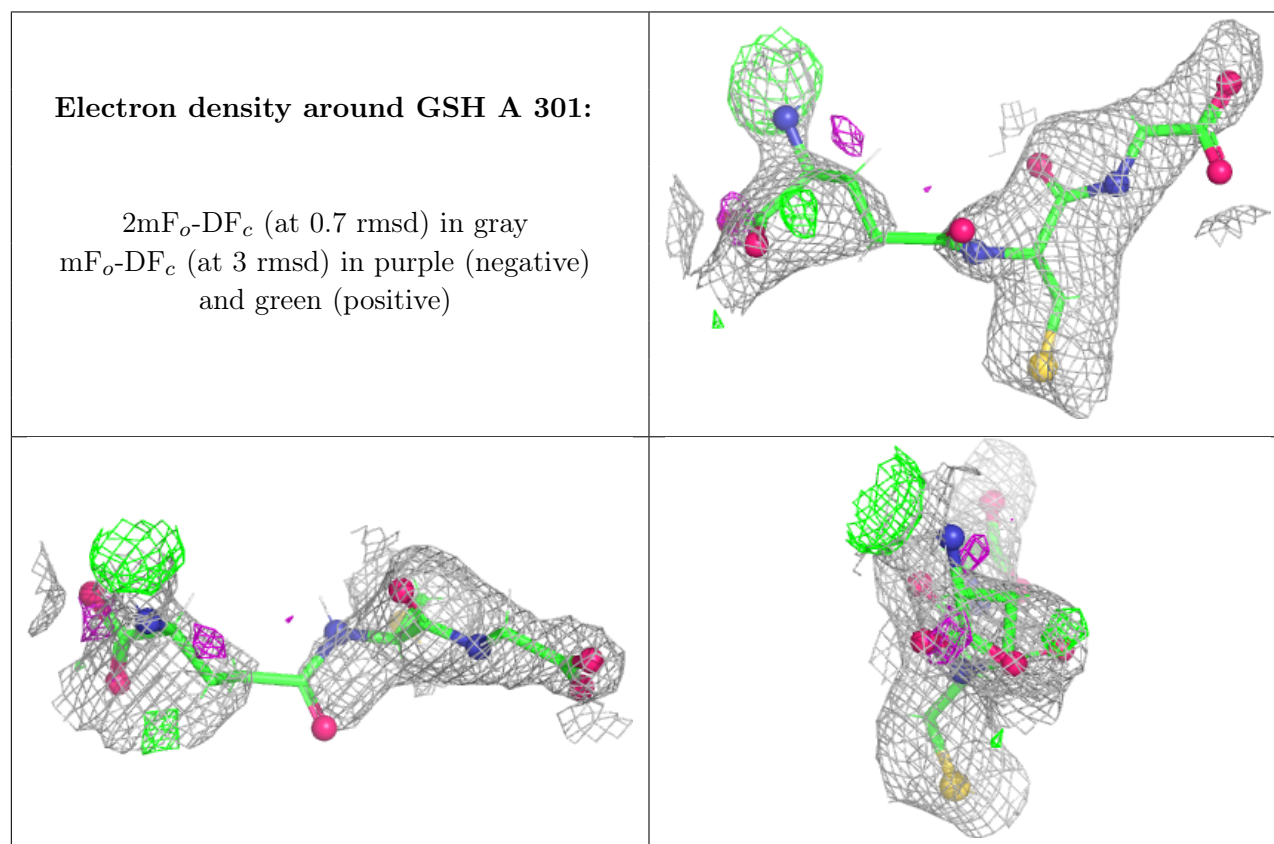
There are no oligosaccharides in this entry.

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.

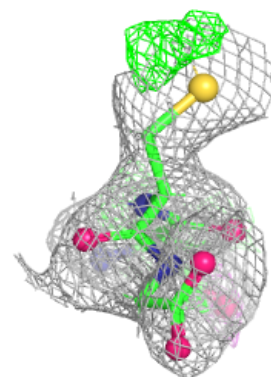
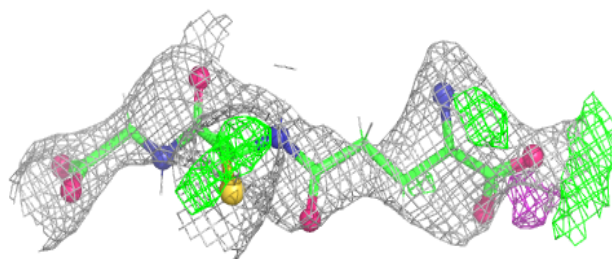
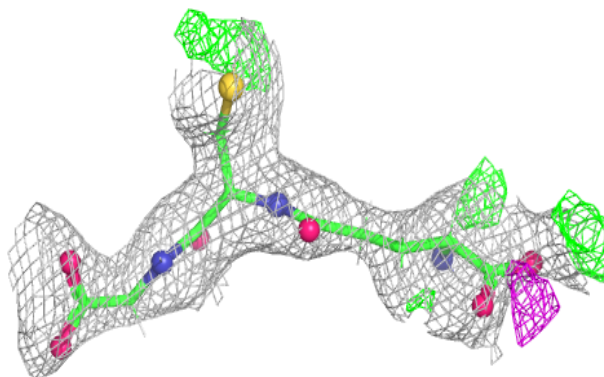
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GSH	A	301	20/20	0.65	0.20	42,69,93,94	0
2	GSH	D	301	20/20	0.66	0.20	55,65,74,92	0
2	GSH	C	301	20/20	0.71	0.24	43,63,114,120	0
2	GSH	B	301	20/20	0.71	0.25	80,100,131,132	0

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.

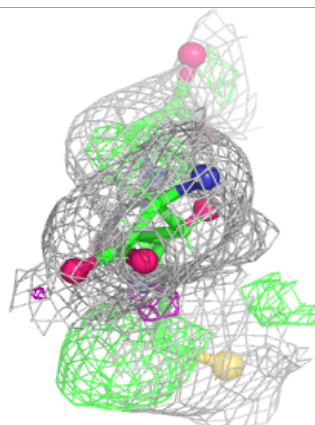
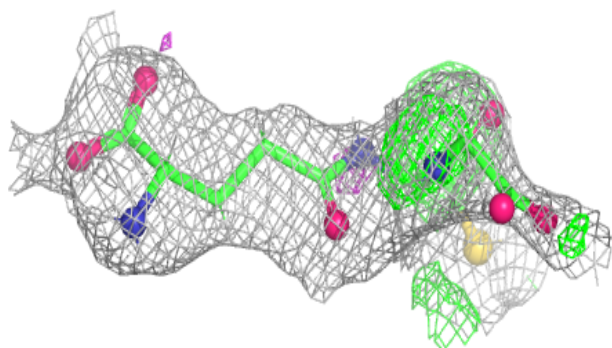
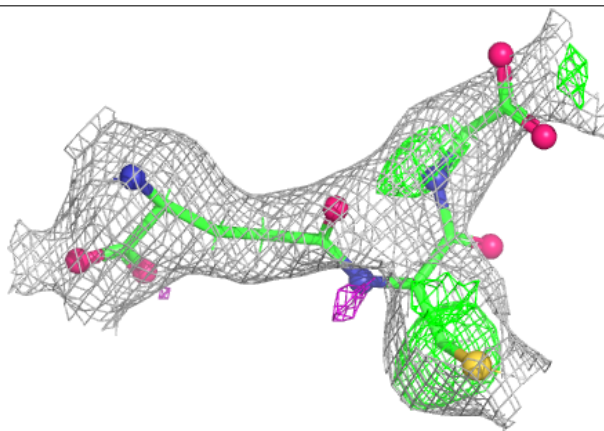


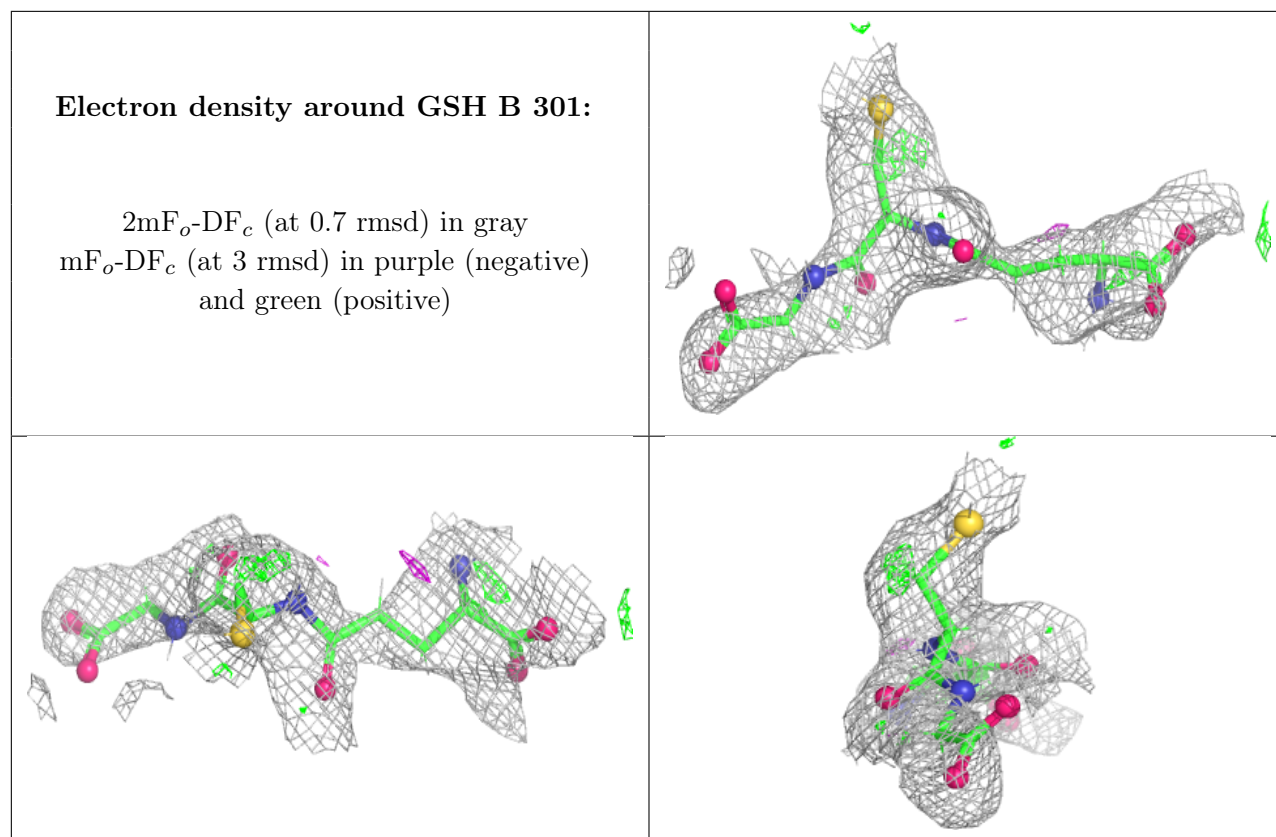
Electron density around GSH D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GSH C 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.