



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2022 – 10:09 AM JST

PDB ID : 7Y55
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

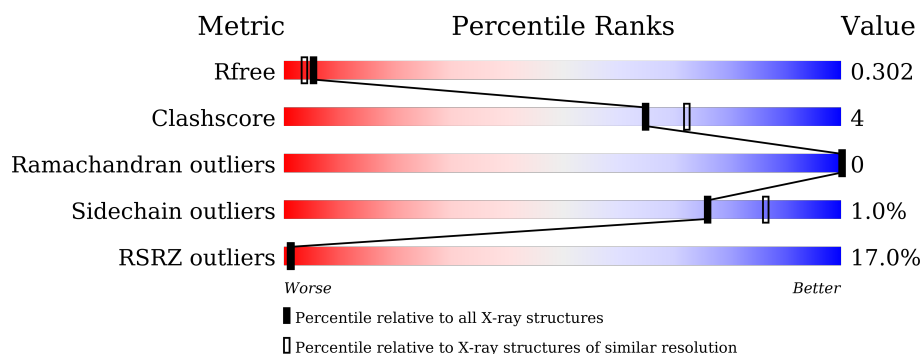
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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	<div> <div>15%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
1	B	237	<div> <div>22%</div> <div>81%</div> <div>14%</div> <div>5%</div> </div>
1	C	237	<div> <div>13%</div> <div>84%</div> <div>11%</div> <div>6%</div> </div>
1	D	237	<div> <div>14%</div> <div>86%</div> <div>8%</div> <div>7%</div> </div>

2 Entry composition [i](#)

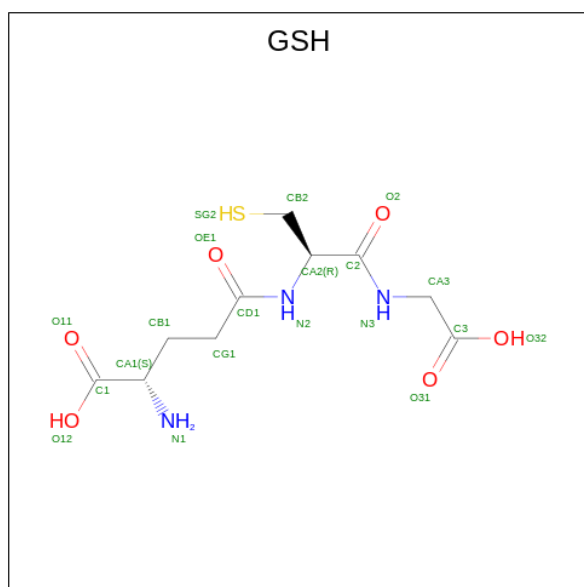
There are 3 unique types of molecules in this entry. The entry contains 14837 atoms, of which 7327 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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		

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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		

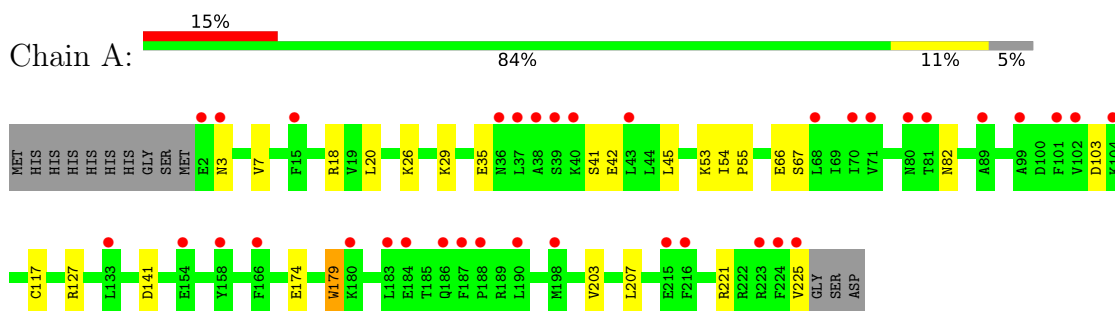
- Molecule 3 is water.

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		

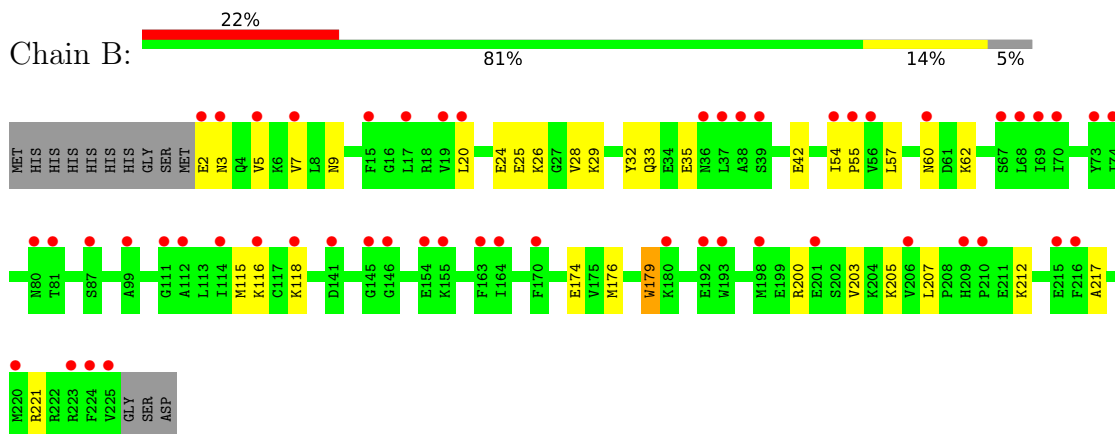
3 Residue-property plots [i](#)

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.

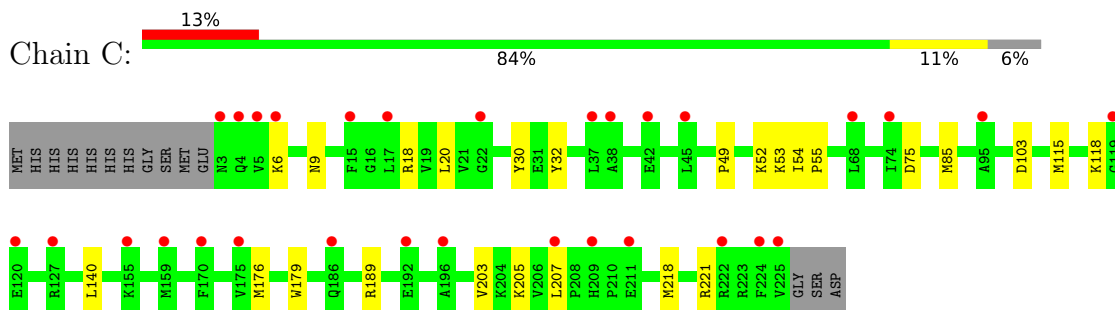
• Molecule 1: PdGSTU1



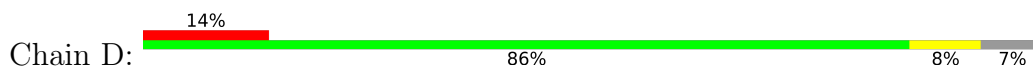
• Molecule 1: PdGSTU1

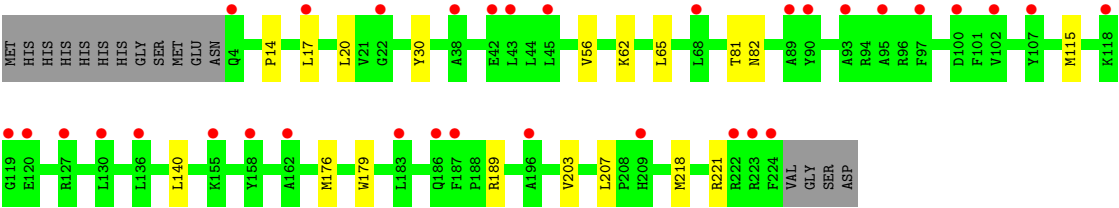


• Molecule 1: PdGSTU1



• 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) 93.5 (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)	Xtrriage
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	1994 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtrriage
Anisotropy	0.463	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.41$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [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	0.39	0/1881	0.58	0/2540
1	B	0.40	0/1881	0.62	0/2540
1	C	0.39	0/1872	0.63	0/2528
1	D	0.40	0/1857	0.62	0/2507
All	All	0.39	0/7491	0.61	0/10115

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1831	1824	1823	16	0
1	B	1831	1824	1823	20	0
1	C	1822	1817	1817	15	0
1	D	1807	1802	1802	10	0
2	A	20	15	15	4	0
2	B	20	15	15	0	0
2	C	20	15	15	1	0
2	D	20	15	15	0	0
3	A	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	0	0	4	0
3	C	47	0	0	4	0
3	D	37	0	0	1	0
All	All	7510	7327	7325	60	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 (60) 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:D:62:LYS:NZ	3:D:401:HOH:O	2.22	0.72
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:6:LYS:NZ	3:C: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: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:A:127:ARG:NH1	3:A:402:HOH:O	2.40	0.54
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:C:205:LYS:NZ	3:C:404:HOH:O	2.38	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:26:LYS:HZ3	1:A:82:ASN:C	2.21	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
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 ⓘ

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%)	76	86
1	B	193/204 (95%)	190 (98%)	3 (2%)	62	76
1	C	192/204 (94%)	190 (99%)	2 (1%)	76	86
1	D	190/204 (93%)	189 (100%)	1 (0%)	88	94
All	All	768/816 (94%)	760 (99%)	8 (1%)	76	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	179	TRP
1	B	60	ASN
1	B	118	LYS
1	B	179	TRP
1	C	118	LYS
1	C	179	TRP
1	D	179	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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 monosaccharides 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	A	301	-	18,19,19	1.70	3 (16%)	23,24,24	1.82	6 (26%)
2	GSH	C	301	-	18,19,19	1.65	2 (11%)	23,24,24	1.74	6 (26%)
2	GSH	D	301	-	18,19,19	1.66	2 (11%)	23,24,24	1.58	6 (26%)
2	GSH	B	301	-	18,19,19	1.66	2 (11%)	23,24,24	1.68	6 (26%)

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	-	-	5/24/24/24	-
2	GSH	C	301	-	-	7/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	D	301	-	-	9/24/24/24	-
2	GSH	B	301	-	-	8/24/24/24	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	GSH	C2-N3	4.22	1.42	1.33
2	A	301	GSH	CD1-N2	4.17	1.42	1.34
2	D	301	GSH	C2-N3	4.11	1.42	1.33
2	C	301	GSH	CD1-N2	3.97	1.42	1.34
2	B	301	GSH	C2-N3	3.89	1.42	1.33
2	B	301	GSH	CD1-N2	3.87	1.42	1.34
2	D	301	GSH	CD1-N2	3.86	1.42	1.34
2	A	301	GSH	C2-N3	3.84	1.42	1.33
2	A	301	GSH	CB2-SG2	-2.24	1.76	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	GSH	CA2-CB2-SG2	-4.76	108.84	114.19
2	A	301	GSH	CA2-CB2-SG2	-4.21	109.46	114.19
2	A	301	GSH	CG1-CB1-CA1	-3.66	105.31	113.84
2	D	301	GSH	CB2-CA2-N2	-3.61	106.14	111.28
2	B	301	GSH	CA2-CB2-SG2	-3.39	110.39	114.19
2	B	301	GSH	C2-CA2-N2	-3.24	102.33	111.16
2	D	301	GSH	CG1-CB1-CA1	-3.21	106.35	113.84
2	B	301	GSH	CA2-C2-N3	3.20	123.00	116.54
2	B	301	GSH	CG1-CB1-CA1	-3.10	106.61	113.84
2	A	301	GSH	CG1-CD1-N2	2.81	120.70	115.83
2	A	301	GSH	O12-C1-CA1	2.67	122.49	113.38
2	C	301	GSH	O12-C1-CA1	2.63	122.34	113.38
2	C	301	GSH	CG1-CD1-N2	2.59	120.33	115.83
2	D	301	GSH	CA2-C2-N3	2.37	121.32	116.54
2	D	301	GSH	CA2-CB2-SG2	-2.26	111.66	114.19
2	B	301	GSH	O32-C3-CA3	2.26	120.58	112.74
2	C	301	GSH	O32-C3-CA3	2.16	120.25	112.74
2	A	301	GSH	O32-C3-CA3	2.11	120.08	112.74
2	C	301	GSH	OE1-CD1-N2	-2.11	119.39	122.95
2	C	301	GSH	O12-C1-O11	-2.08	119.36	124.09
2	D	301	GSH	O32-C3-CA3	2.04	119.84	112.74
2	D	301	GSH	O12-C1-CA1	2.02	120.26	113.38
2	B	301	GSH	O2-C2-N3	-2.02	118.66	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	GSH	OE1-CD1-N2	-2.00	119.57	122.95

There are no chirality outliers.

All (29) 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
2	C	301	GSH	N2-CA2-CB2-SG2
2	C	301	GSH	C2-CA2-CB2-SG2
2	C	301	GSH	O31-C3-CA3-N3
2	C	301	GSH	O32-C3-CA3-N3
2	D	301	GSH	N2-CA2-CB2-SG2
2	D	301	GSH	C2-CA2-CB2-SG2
2	B	301	GSH	O12-C1-CA1-N1
2	A	301	GSH	CA1-CB1-CG1-CD1
2	D	301	GSH	O12-C1-CA1-N1
2	A	301	GSH	O12-C1-CA1-N1
2	A	301	GSH	O12-C1-CA1-CB1
2	D	301	GSH	O12-C1-CA1-CB1
2	A	301	GSH	O11-C1-CA1-CB1
2	D	301	GSH	O11-C1-CA1-CB1
2	A	301	GSH	O11-C1-CA1-N1
2	B	301	GSH	O11-C1-CA1-N1
2	D	301	GSH	O11-C1-CA1-N1
2	C	301	GSH	O2-C2-CA2-N2
2	C	301	GSH	N1-CA1-CB1-CG1
2	B	301	GSH	CA1-CB1-CG1-CD1
2	B	301	GSH	O12-C1-CA1-CB1
2	C	301	GSH	N3-C2-CA2-N2
2	D	301	GSH	O31-C3-CA3-N3
2	B	301	GSH	O11-C1-CA1-CB1
2	D	301	GSH	O32-C3-CA3-N3
2	B	301	GSH	N1-CA1-CB1-CG1
2	D	301	GSH	N1-CA1-CB1-CG1

There are no ring outliers.

2 monomers are involved in 5 short contacts:

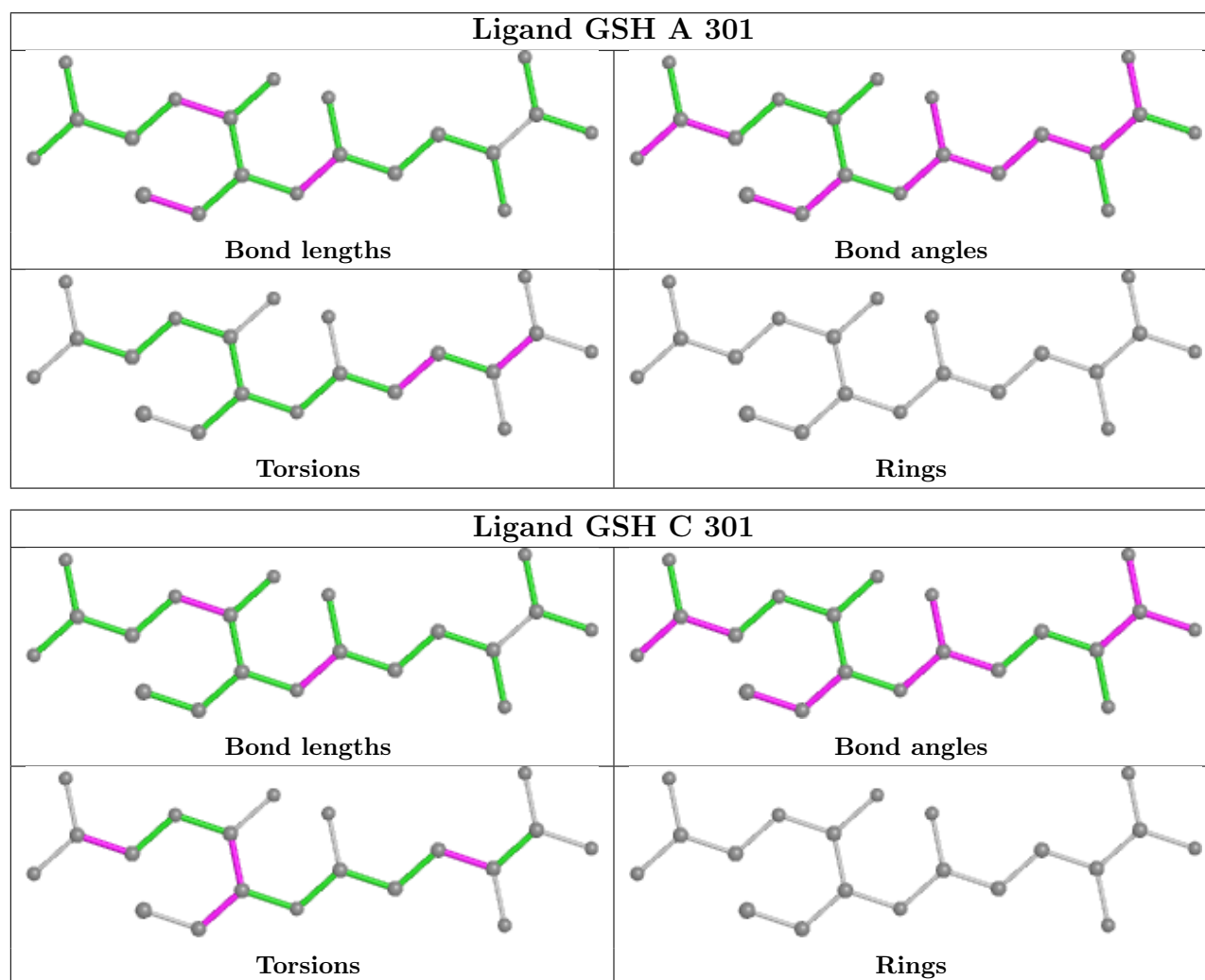
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GSH	4	0

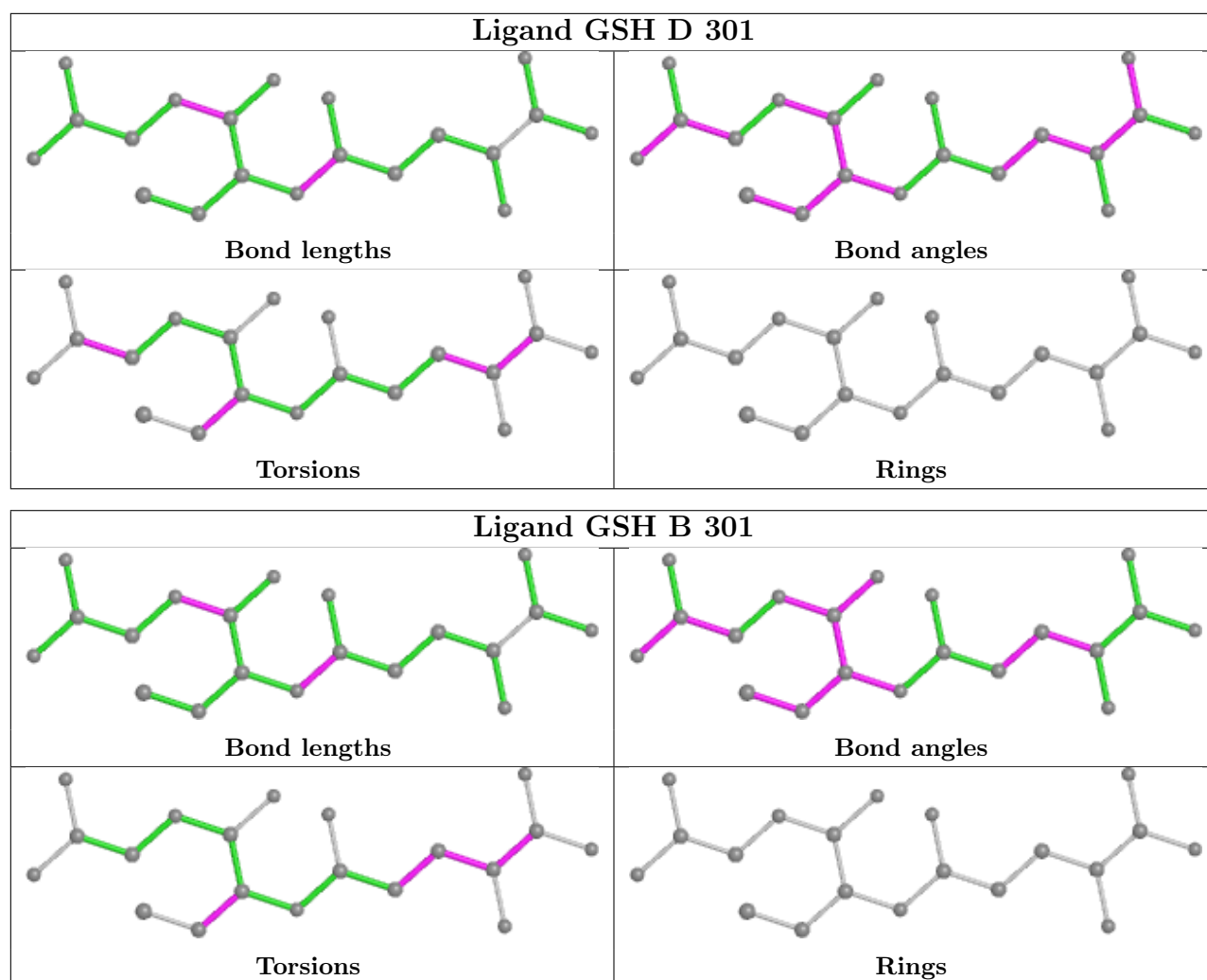
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	GSH	1	0

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

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%)	1.14	36 (16%) 1 1	31, 47, 68, 89	0
1	B	224/237 (94%)	1.36	53 (23%) 0 0	35, 51, 76, 88	0
1	C	223/237 (94%)	1.09	30 (13%) 3 2	31, 42, 65, 92	0
1	D	221/237 (93%)	1.15	33 (14%) 2 2	30, 43, 66, 114	0
All	All	892/948 (94%)	1.19	152 (17%) 1 1	30, 46, 69, 114	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	ASN	11.2
1	C	38	ALA	10.1
1	C	4	GLN	9.2
1	D	45	LEU	6.1
1	B	37	LEU	6.0
1	D	38	ALA	5.8
1	D	4	GLN	5.6
1	D	186	GLN	5.4
1	B	224	PHE	5.4
1	C	225	VAL	5.0
1	B	68	LEU	5.0
1	B	60	ASN	4.9
1	A	80	ASN	4.8
1	B	15	PHE	4.6
1	A	38	ALA	4.5
1	A	154	GLU	4.2
1	A	68	LEU	4.0
1	A	224	PHE	4.0
1	B	67	SER	3.9
1	D	120	GLU	3.9
1	B	206	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	159	MET	3.8
1	C	45	LEU	3.6
1	B	209	HIS	3.6
1	D	22	GLY	3.6
1	B	5	VAL	3.6
1	A	180	LYS	3.6
1	B	36	ASN	3.5
1	B	69	ILE	3.5
1	B	223	ARG	3.5
1	B	81	THR	3.4
1	C	186	GLN	3.4
1	B	201	GLU	3.4
1	B	70	ILE	3.4
1	D	127	ARG	3.4
1	C	222	ARG	3.4
1	B	154	GLU	3.3
1	D	43	LEU	3.3
1	B	145	GLY	3.3
1	A	187	PHE	3.3
1	D	97	PHE	3.3
1	C	224	PHE	3.3
1	B	192	GLU	3.2
1	A	198	MET	3.2
1	A	89	ALA	3.2
1	A	15	PHE	3.2
1	A	2	GLU	3.1
1	A	184	GLU	3.1
1	B	39	SER	3.1
1	C	42	GLU	3.1
1	B	56	VAL	3.1
1	B	38	ALA	3.1
1	C	22	GLY	3.1
1	B	225	VAL	3.1
1	B	2	GLU	3.1
1	C	120	GLU	3.1
1	A	37	LEU	3.1
1	B	146	GLY	3.0
1	A	81	THR	3.0
1	D	119	GLY	3.0
1	C	196	ALA	3.0
1	A	39	SER	3.0
1	B	3	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	95	ALA	2.9
1	B	220	MET	2.9
1	C	155	LYS	2.9
1	D	102	VAL	2.9
1	A	223	ARG	2.9
1	D	100	ASP	2.8
1	C	211	GLU	2.8
1	A	166	PHE	2.8
1	A	43	LEU	2.8
1	B	111	GLY	2.8
1	B	20	LEU	2.8
1	C	207	LEU	2.8
1	D	136	LEU	2.8
1	C	74	ILE	2.7
1	B	99	ALA	2.7
1	C	5	VAL	2.7
1	B	216	PHE	2.7
1	A	71	VAL	2.7
1	C	6	LYS	2.7
1	A	36	ASN	2.7
1	B	55	PRO	2.6
1	A	216	PHE	2.6
1	C	192	GLU	2.6
1	B	116	LYS	2.6
1	B	80	ASN	2.6
1	D	68	LEU	2.6
1	C	175	VAL	2.6
1	B	118	LYS	2.6
1	B	180	LYS	2.5
1	C	15	PHE	2.5
1	D	42	GLU	2.5
1	D	93	ALA	2.5
1	D	130	LEU	2.5
1	D	162	ALA	2.5
1	D	90	TYR	2.5
1	D	187	PHE	2.5
1	B	7	VAL	2.5
1	C	127	ARG	2.4
1	B	155	LYS	2.4
1	B	114	ILE	2.4
1	A	133	LEU	2.4
1	D	158	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	101	PHE	2.4
1	B	17	LEU	2.4
1	D	183	LEU	2.4
1	C	68	LEU	2.4
1	B	215	GLU	2.4
1	D	209	HIS	2.4
1	A	99	ALA	2.4
1	D	17	LEU	2.3
1	D	222	ARG	2.3
1	B	74	ILE	2.3
1	A	102	VAL	2.3
1	B	19	VAL	2.3
1	B	141	ASP	2.3
1	A	158	TYR	2.2
1	B	112	ALA	2.2
1	A	70	ILE	2.2
1	C	209	HIS	2.2
1	B	193	TRP	2.2
1	A	215	GLU	2.2
1	A	40	LYS	2.2
1	A	190	LEU	2.2
1	B	210	PRO	2.2
1	B	170	PHE	2.2
1	C	95	ALA	2.2
1	C	119	GLY	2.2
1	C	37	LEU	2.2
1	B	198	MET	2.2
1	B	54	ILE	2.1
1	B	73	TYR	2.1
1	D	224	PHE	2.1
1	D	118	LYS	2.1
1	B	163	PHE	2.1
1	D	196	ALA	2.1
1	D	155	LYS	2.1
1	A	3	ASN	2.1
1	A	186	GLN	2.1
1	A	183	LEU	2.1
1	C	170	PHE	2.1
1	D	89	ALA	2.1
1	D	107	TYR	2.1
1	B	87	SER	2.1
1	C	17	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	104	LYS	2.0
1	A	188	PRO	2.0
1	B	164	ILE	2.0
1	A	225	VAL	2.0
1	D	223	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

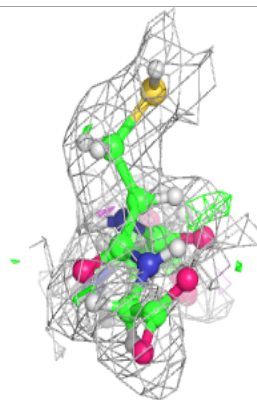
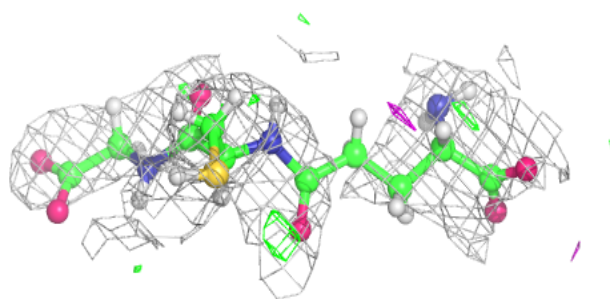
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	301	20/20	0.57	0.39	80,100,131,132	0
2	GSH	C	301	20/20	0.67	0.33	43,63,114,120	0
2	GSH	A	301	20/20	0.69	0.31	42,69,93,94	0
2	GSH	D	301	20/20	0.69	0.26	55,65,74,92	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.

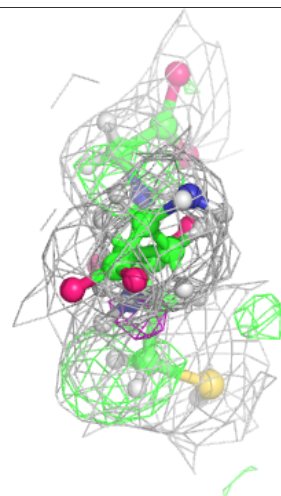
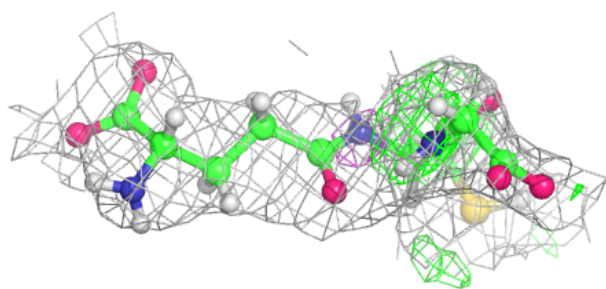
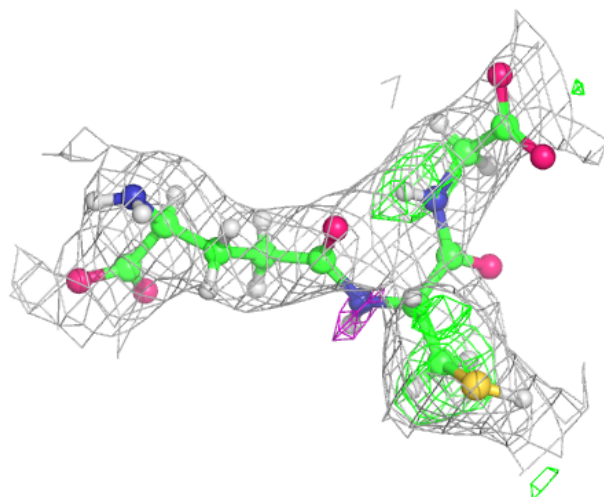
Electron density around GSH B 301:

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



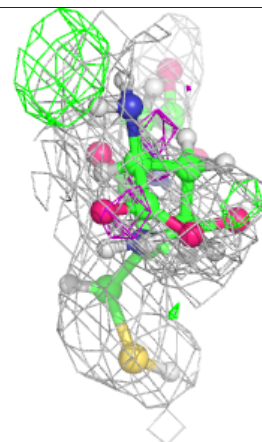
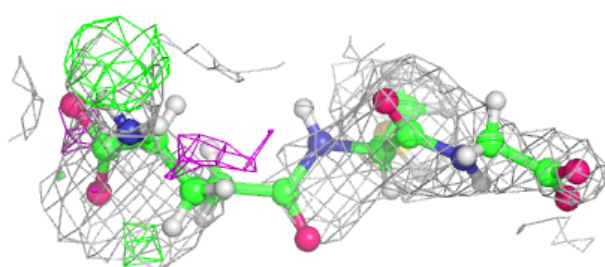
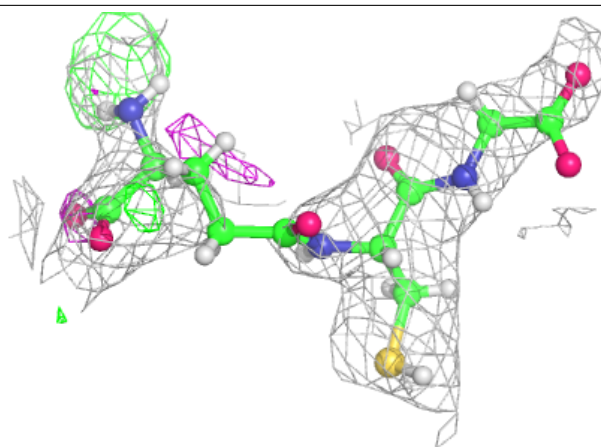
Electron density around GSH C 301:

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

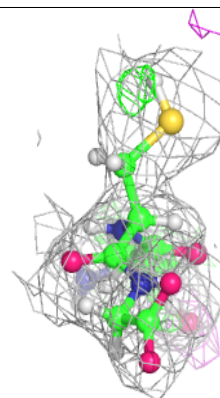
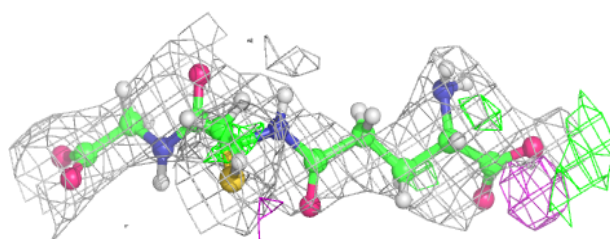
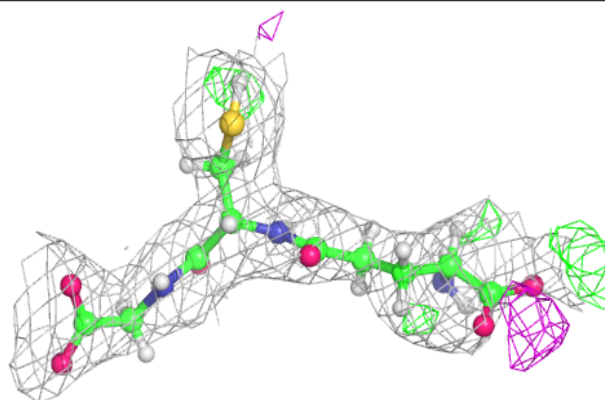


Electron density around GSH A 301:

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

**Electron density around GSH 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.