



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 12:40 am BST

PDB ID : 3LFL  
Title : Crystal Structure of human Glutathione Transferase Omega 1, delta 155  
Authors : Brock, J.  
Deposited on : 2010-01-18  
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

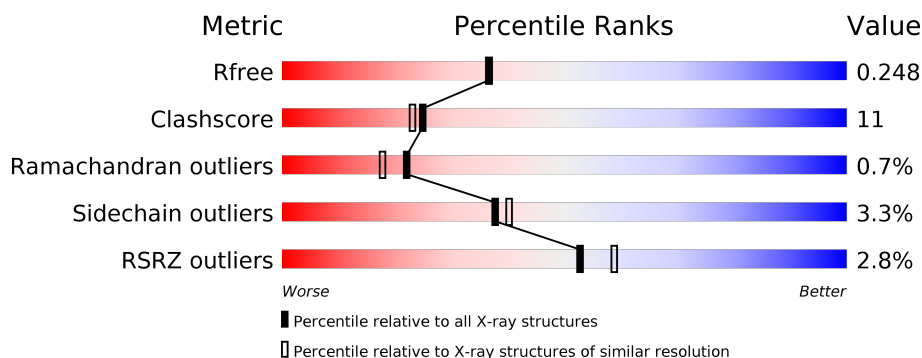
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	240	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 82%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>82%</span> <span>15%</span> <span>••</span> </div> </div>
1	B	240	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 20%, green 72%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>72%</span> <span>20%</span> <span>• 6%</span> </div> </div>
1	C	240	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 21%, green 70%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>70%</span> <span>21%</span> <span>• 7%</span> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5959 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.

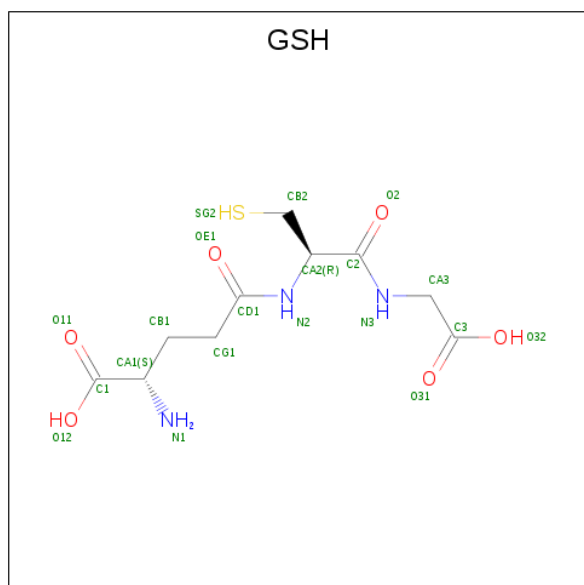
- Molecule 1 is a protein called Glutathione S-transferase omega-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	9	0	0
			1904	1233	311	349	11			
1	B	226	Total	C	N	O	S	17	0	0
			1830	1189	300	331	10			
1	C	224	Total	C	N	O	S	19	0	0
			1813	1178	297	328	10			

There are 3 discrepancies between the modelled and reference sequences:

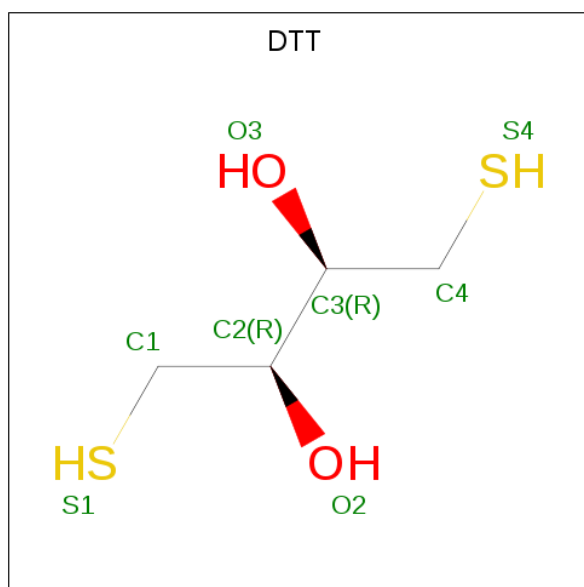
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	DELETION	UNP P78417
B	?	-	GLU	DELETION	UNP P78417
C	?	-	GLU	DELETION	UNP P78417

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



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		
2	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula:  $C_4H_{10}O_2S_2$ ).



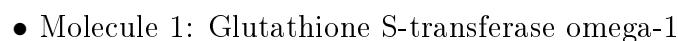
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		
3	B	1	Total	C	O	S	0	0
			8	4	2	2		
3	C	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total	O	0	0
			137	137		
4	B	92	Total	O	0	0
			92	92		
4	C	99	Total	O	0	0
			99	99		



- Molecule 1: Glutathione S-transferase omega-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.01Å 201.94Å 53.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.51 – 2.10 36.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	72.1 (36.51-2.10) 72.1 (36.50-2.10)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.94 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.199 , 0.255 0.192 , 0.248	Depositor DCC
$R_{free}$ test set	1731 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GSH, DTT

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	0.41	0/1953	0.51	0/2636
1	B	0.36	0/1877	0.49	0/2533
1	C	0.38	0/1860	0.51	0/2510
All	All	0.39	0/5690	0.50	0/7679

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	1904	0	1913	27	0
1	B	1830	0	1852	45	0
1	C	1813	0	1833	50	0
2	A	20	0	15	1	0
2	B	20	0	15	1	0
2	C	20	0	15	3	0
3	A	8	0	10	1	0
3	B	8	0	10	3	0
3	C	8	0	10	2	0
4	A	137	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	92	0	0	2	0
4	C	99	0	0	7	0
All	All	5959	0	5673	121	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 11.

All (121) 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:158:ASN:HB2	1:B:159:LYS:HA	1.26	1.13
1:B:35:ALA:HA	1:B:73:PRO:HG3	1.50	0.93
1:B:158:ASN:CB	1:B:159:LYS:HA	2.07	0.85
1:C:35:ALA:HA	1:C:73:PRO:HG3	1.56	0.84
1:A:32:CYS:SG	2:A:241:GSH:SG2	2.44	0.81
1:C:32:CYS:HG	2:C:242:GSH:HSG	0.92	0.79
1:B:191:CYS:HG	3:B:242:DTT:HS2	1.30	0.78
1:C:21:GLU:H	1:C:21:GLU:CD	1.90	0.74
1:B:191:CYS:SG	3:B:242:DTT:S4	2.86	0.73
1:A:11:LYS:HB2	4:A:350:HOH:O	1.90	0.72
1:C:191:CYS:SG	3:C:241:DTT:S1	2.65	0.71
1:C:32:CYS:SG	2:C:242:GSH:SG2	2.71	0.71
1:A:191:CYS:SG	3:A:242:DTT:S1	2.67	0.66
1:A:147:ARG:O	1:A:151:THR:HG23	1.95	0.66
1:C:110:LYS:HG3	4:C:328:HOH:O	1.96	0.66
1:B:32:CYS:SG	2:B:241:GSH:SG2	2.45	0.65
1:B:39:ARG:HH11	1:B:39:ARG:HA	1.63	0.64
1:B:204:ALA:O	1:B:207:GLU:HG2	1.98	0.63
1:C:222:GLN:OE1	1:C:222:GLN:HA	1.98	0.62
1:C:226:GLU:HB2	1:C:227:LEU:HD22	1.82	0.60
1:C:152:LYS:HA	1:C:156:LEU:HD13	1.85	0.59
1:C:5:SER:O	1:C:6:ALA:HB2	2.03	0.59
1:B:144:GLU:O	1:B:148:LYS:HG2	2.04	0.57
1:B:61:GLU:H	1:B:61:GLU:CD	2.08	0.57
1:C:184:GLU:HG3	4:C:256:HOH:O	2.05	0.57
1:C:101:LYS:HG2	1:C:103:LEU:O	2.05	0.57
1:B:39:ARG:NH1	4:B:287:HOH:O	2.38	0.56
1:C:154:GLU:OE2	1:C:195:THR:HB	2.07	0.55
3:C:241:DTT:S1	3:C:241:DTT:O3	2.63	0.55
1:A:109:GLU:HG2	4:A:272:HOH:O	2.07	0.54
1:C:156:LEU:HD12	1:C:156:LEU:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:HB2	1:B:159:LYS:NZ	2.23	0.54
1:C:21:GLU:HG3	4:C:331:HOH:O	2.06	0.54
1:C:85:GLU:HB2	1:C:88:ILE:HD12	1.90	0.54
1:A:102:LEU:O	1:A:170:SER:HB2	2.09	0.53
1:A:104:PRO:HG2	1:A:109:GLU:HB3	1.91	0.53
1:C:127:VAL:HG13	1:C:186:MET:SD	2.48	0.53
1:A:157:THR:HG21	1:A:164:PHE:CD2	2.43	0.53
1:C:103:LEU:HD22	4:C:328:HOH:O	2.08	0.52
1:C:29:MET:HG2	1:C:56:LEU:CD1	2.40	0.51
1:B:84:TYR:O	1:B:85:GLU:HB2	2.10	0.51
1:C:127:VAL:HG13	1:C:186:MET:HE1	1.93	0.51
1:B:207:GLU:HG3	4:B:332:HOH:O	2.09	0.50
1:C:222:GLN:HG3	1:C:226:GLU:OE1	2.10	0.50
1:C:84:TYR:O	1:C:85:GLU:HB2	2.11	0.50
1:A:85:GLU:HB2	1:A:88:ILE:HD12	1.93	0.50
1:A:189:ASN:O	1:A:192:VAL:HG22	2.12	0.49
1:C:132:ARG:O	1:C:133:SER:C	2.50	0.49
1:B:157:THR:O	1:B:158:ASN:C	2.51	0.49
1:A:234:GLU:OE2	1:A:234:GLU:HA	2.13	0.48
1:A:120:PHE:O	1:A:120:PHE:CG	2.67	0.48
1:B:193:ASP:OD2	1:B:199:LYS:HE2	2.14	0.48
1:C:32:CYS:HG	2:C:242:GSH:CB2	2.23	0.48
1:A:151:THR:HG22	1:A:194:HIS:CD2	2.49	0.48
1:C:130:PHE:CZ	1:C:188:LEU:HD21	2.48	0.48
1:C:145:GLU:HG3	4:C:337:HOH:O	2.13	0.47
1:C:193:ASP:OD2	1:C:199:LYS:HE3	2.14	0.47
1:C:66:LYS:HA	1:C:82:LEU:HD13	1.96	0.47
1:B:106:ASP:OD1	1:B:109:GLU:HG3	2.14	0.47
1:C:11:LYS:NZ	1:C:61:GLU:HB2	2.30	0.47
1:B:9:LEU:HD23	1:B:62:TRP:HZ2	1.79	0.47
1:C:77:ASN:HB2	4:C:272:HOH:O	2.15	0.47
1:B:9:LEU:HD23	1:B:62:TRP:CZ2	2.50	0.47
1:A:223:GLY:HA3	1:A:238:TYR:CZ	2.50	0.47
1:C:227:LEU:HD22	1:C:227:LEU:H	1.80	0.47
1:B:158:ASN:CB	1:B:159:LYS:CA	2.86	0.46
1:C:185:ALA:HB1	1:C:225:LEU:HD21	1.97	0.46
1:B:187:LYS:O	1:B:188:LEU:HD23	2.15	0.46
1:A:157:THR:HG21	1:A:164:PHE:HD2	1.80	0.46
1:B:143:LYS:HD3	3:B:242:DTT:H42	1.97	0.46
1:B:183:LEU:HA	1:B:186:MET:HE2	1.98	0.46
1:B:229:LEU:O	1:B:230:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:LEU:N	1:C:227:LEU:HD22	2.31	0.46
1:C:148:LYS:HB2	1:C:148:LYS:HE2	1.73	0.45
1:A:223:GLY:HA3	1:A:238:TYR:CE2	2.51	0.45
1:B:186:MET:O	1:B:187:LYS:HB2	2.16	0.45
1:C:127:VAL:HG13	1:C:186:MET:CE	2.46	0.45
1:A:138:ASP:O	1:A:142:LEU:HB2	2.17	0.45
1:B:26:ILE:HD13	1:B:39:ARG:HD3	1.97	0.45
1:C:33:PRO:HB2	1:C:179:TRP:CZ2	2.52	0.45
1:C:123:VAL:HB	1:C:124:PRO:HD3	1.98	0.44
1:B:119:LEU:HD23	1:C:69:PHE:HZ	1.82	0.44
1:A:9:LEU:HD23	1:A:62:TRP:HZ2	1.84	0.43
1:C:29:MET:HG2	1:C:56:LEU:HD11	2.01	0.43
1:B:138:ASP:O	1:B:139:TYR:C	2.56	0.43
1:B:35:ALA:O	1:B:39:ARG:HG2	2.19	0.43
1:C:11:LYS:HD2	4:C:255:HOH:O	2.18	0.43
1:A:159:LYS:HD3	1:A:164:PHE:CD2	2.54	0.43
1:C:21:GLU:CD	1:C:21:GLU:N	2.64	0.43
1:C:156:LEU:CD1	1:C:156:LEU:N	2.81	0.42
1:C:218:GLU:HG3	1:C:221:TRP:CZ3	2.54	0.42
1:B:89:THR:O	1:B:93:LEU:HG	2.19	0.42
1:A:123:VAL:HB	1:A:124:PRO:HD3	2.00	0.42
1:A:35:ALA:HA	1:A:73:PRO:HG3	2.00	0.42
1:B:110:LYS:O	1:B:114:LYS:HE3	2.19	0.42
1:B:77:ASN:HD21	1:B:81:GLN:HB2	1.84	0.42
1:B:77:ASN:ND2	1:B:81:GLN:HB2	2.34	0.42
1:A:232:SER:HA	1:A:233:PRO:HD3	1.84	0.42
1:C:6:ALA:O	1:C:7:ARG:HB2	2.19	0.42
1:C:5:SER:O	1:C:6:ALA:CB	2.67	0.42
1:A:133:SER:OG	1:A:138:ASP:HB2	2.20	0.41
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.90	0.41
1:B:15:PRO:HA	1:B:16:PRO:HD3	1.89	0.41
1:C:29:MET:HB3	1:C:72:VAL:HG21	2.01	0.41
1:B:183:LEU:HD12	1:B:186:MET:CE	2.50	0.41
1:C:160:LYS:HE2	1:C:160:LYS:HB2	1.78	0.41
1:B:159:LYS:HZ3	1:B:159:LYS:HB2	1.86	0.41
1:C:29:MET:HG2	1:C:56:LEU:HD12	2.01	0.41
1:B:127:VAL:HG13	1:B:186:MET:SD	2.60	0.41
1:C:152:LYS:O	1:C:156:LEU:HB2	2.21	0.41
1:A:120:PHE:CD2	1:A:120:PHE:O	2.74	0.41
1:B:119:LEU:HD23	1:C:69:PHE:CZ	2.56	0.41
1:B:152:LYS:O	1:B:156:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLY:O	1:A:240:LEU:CB	2.69	0.41
1:B:33:PRO:HB2	1:B:179:TRP:CZ2	2.56	0.41
1:A:240:LEU:HA	1:A:240:LEU:HD22	1.66	0.40
1:B:103:LEU:HA	1:B:104:PRO:HD3	1.94	0.40
1:B:135:ASN:O	1:B:138:ASP:HB2	2.21	0.40
1:B:229:LEU:O	1:B:230:GLN:CB	2.69	0.40
1:B:82:LEU:C	1:B:83:ILE:HG13	2.42	0.40
1:A:158:ASN:CG	1:A:160:LYS:HZ1	2.24	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	234/240 (98%)	230 (98%)	4 (2%)	0	100	100
1	B	224/240 (93%)	216 (96%)	6 (3%)	2 (1%)	17	12
1	C	222/240 (92%)	208 (94%)	11 (5%)	3 (1%)	11	6
All	All	680/720 (94%)	654 (96%)	21 (3%)	5 (1%)	22	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	ALA
1	C	7	ARG
1	C	6	ALA
1	C	133	SER
1	B	158	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	209/212 (99%)	203 (97%)	6 (3%)	42	46
1	B	201/212 (95%)	195 (97%)	6 (3%)	41	44
1	C	199/212 (94%)	191 (96%)	8 (4%)	31	32
All	All	609/636 (96%)	589 (97%)	20 (3%)	38	40

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	134	GLN
1	A	136	LYS
1	A	142	LEU
1	A	158	ASN
1	A	240	LEU
1	B	9	LEU
1	B	137	GLU
1	B	156	LEU
1	B	159	LYS
1	B	183	LEU
1	B	184	GLU
1	C	9	LEU
1	C	61	GLU
1	C	136	LYS
1	C	138	ASP
1	C	139	TYR
1	C	183	LEU
1	C	222	GLN
1	C	228	TYR

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	B	241	-	12,19,19	2.30	2 (16%)	15,24,24	2.59	7 (46%)
3	DTT	C	241	-	7,7,7	0.54	0	4,8,8	0.67	0
2	GSH	C	242	-	12,19,19	2.49	4 (33%)	15,24,24	2.03	6 (40%)
2	GSH	A	241	-	12,19,19	2.40	3 (25%)	15,24,24	1.83	6 (40%)
3	DTT	B	242	-	7,7,7	0.63	0	4,8,8	0.45	0
3	DTT	A	242	-	7,7,7	0.57	0	4,8,8	0.50	0

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	B	241	-	-	0/18/24/24	-
3	DTT	C	241	-	-	4/8/8/8	-
2	GSH	C	242	-	-	1/18/24/24	-

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	A	241	-	-	1/18/24/24	-
3	DTT	B	242	-	-	4/8/8/8	-
3	DTT	A	242	-	-	5/8/8/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	242	GSH	CD1-N2	5.76	1.46	1.34
2	A	241	GSH	C2-N3	5.45	1.45	1.33
2	A	241	GSH	CD1-N2	5.40	1.45	1.34
2	C	242	GSH	C2-N3	5.35	1.45	1.33
2	B	241	GSH	CD1-N2	5.21	1.45	1.34
2	B	241	GSH	C2-N3	5.12	1.44	1.33
2	C	242	GSH	O2-C2	-2.43	1.18	1.23
2	A	241	GSH	OE1-CD1	-2.41	1.18	1.23
2	C	242	GSH	OE1-CD1	-2.09	1.19	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	GSH	CA2-CB2-SG2	-6.43	106.97	114.19
2	B	241	GSH	CB2-CA2-N2	-4.55	104.79	111.28
2	C	242	GSH	CB2-CA2-N2	-3.83	105.82	111.28
2	A	241	GSH	CB2-CA2-N2	-3.63	106.11	111.28
2	B	241	GSH	CA3-N3-C2	-3.37	117.49	122.34
2	C	242	GSH	CA2-CB2-SG2	-3.30	110.48	114.19
2	A	241	GSH	C3-CA3-N3	-3.13	104.39	110.43
2	C	242	GSH	CG1-CD1-N2	2.87	120.81	115.83
2	C	242	GSH	CG1-CB1-CA1	-2.83	107.24	113.84
2	B	241	GSH	CG1-CB1-CA1	-2.74	107.44	113.84
2	C	242	GSH	C3-CA3-N3	-2.73	105.17	110.43
2	B	241	GSH	CA2-N2-CD1	-2.63	114.89	121.65
2	A	241	GSH	OE1-CD1-N2	-2.38	118.93	122.95
2	A	241	GSH	CG1-CD1-N2	2.32	119.85	115.83
2	C	242	GSH	OE1-CD1-N2	-2.24	119.17	122.95
2	B	241	GSH	OE1-CD1-N2	-2.22	119.21	122.95
2	A	241	GSH	CG1-CB1-CA1	-2.15	108.83	113.84
2	A	241	GSH	CA2-N2-CD1	-2.15	116.12	121.65
2	B	241	GSH	CG1-CD1-N2	2.10	119.47	115.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

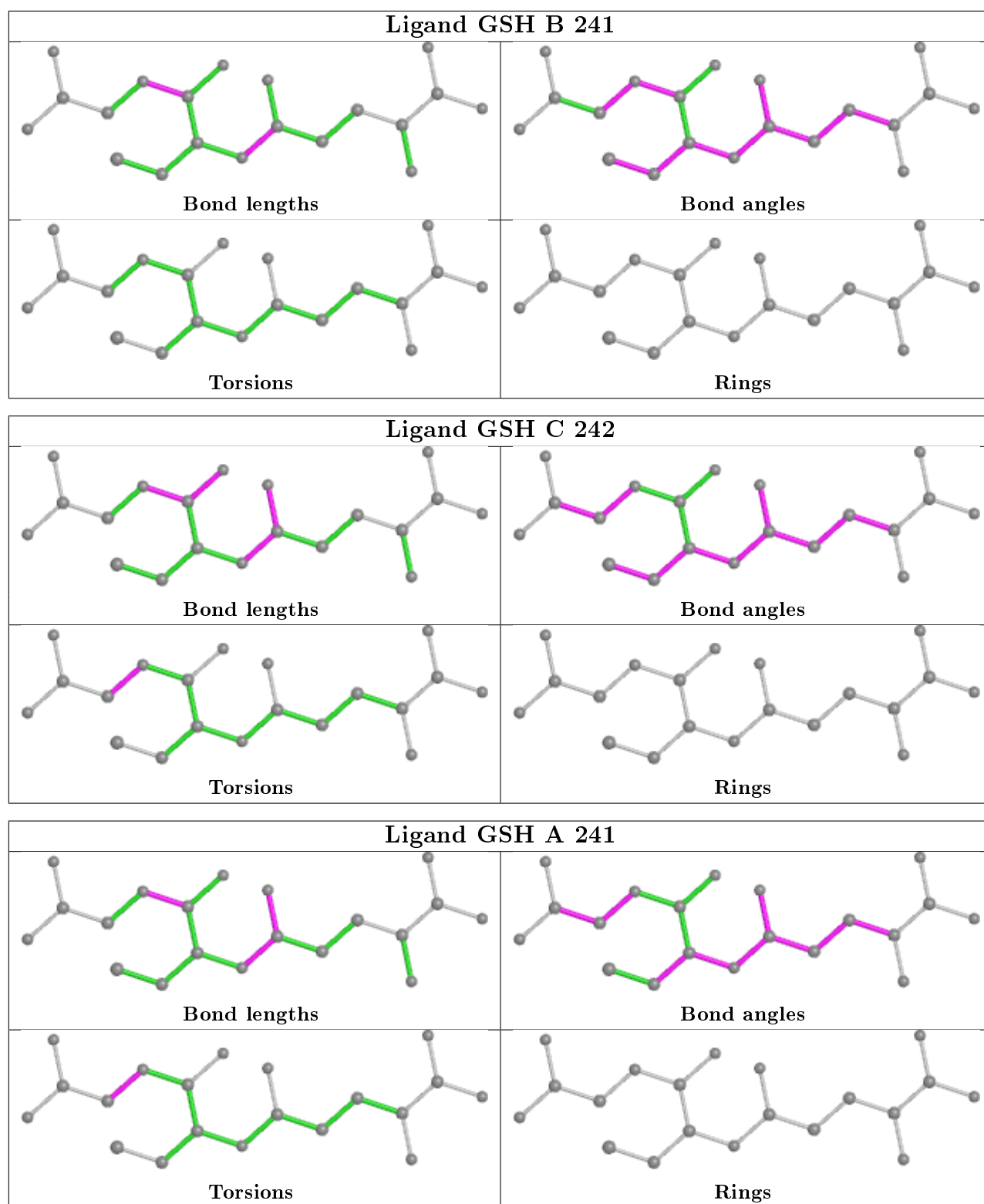
Mol	Chain	Res	Type	Atoms
3	C	241	DTT	C1-C2-C3-O3
3	C	241	DTT	C1-C2-C3-C4
3	C	241	DTT	O2-C2-C3-C4
3	B	242	DTT	S1-C1-C2-C3
3	B	242	DTT	C1-C2-C3-O3
3	B	242	DTT	O2-C2-C3-O3
3	B	242	DTT	O2-C2-C3-C4
3	A	242	DTT	C1-C2-C3-O3
3	A	242	DTT	C1-C2-C3-C4
3	A	242	DTT	O2-C2-C3-C4
3	C	241	DTT	O2-C2-C3-O3
3	A	242	DTT	O2-C2-C3-O3
3	A	242	DTT	S1-C1-C2-O2
2	A	241	GSH	C3-CA3-N3-C2
2	C	242	GSH	C3-CA3-N3-C2

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	241	GSH	1	0
3	C	241	DTT	2	0
2	C	242	GSH	3	0
2	A	241	GSH	1	0
3	B	242	DTT	3	0
3	A	242	DTT	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 ⓘ

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, 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	236/240 (98%)	-0.39	2 (0%) 86 88	17, 26, 47, 76	3 (1%)
1	B	226/240 (94%)	-0.25	6 (2%) 54 60	19, 29, 59, 72	4 (1%)
1	C	224/240 (93%)	-0.29	11 (4%) 29 35	17, 28, 58, 87	5 (2%)
All	All	686/720 (95%)	-0.31	19 (2%) 53 59	17, 28, 57, 87	12 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	TYR	5.4
1	C	6	ALA	5.1
1	C	134	GLN	4.3
1	C	227	LEU	4.1
1	C	139	TYR	4.0
1	C	135	ASN	3.5
1	C	138	ASP	3.5
1	C	226	GLU	3.3
1	B	6	ALA	3.0
1	C	133	SER	3.0
1	B	230	GLN	2.9
1	C	137	GLU	2.9
1	B	5	SER	2.8
1	A	134	GLN	2.7
1	B	133	SER	2.4
1	B	7	ARG	2.2
1	B	139	TYR	2.2
1	A	137	GLU	2.1
1	C	5	SER	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](#)

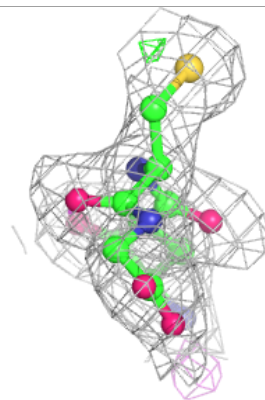
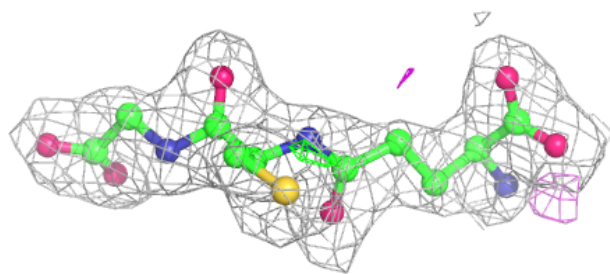
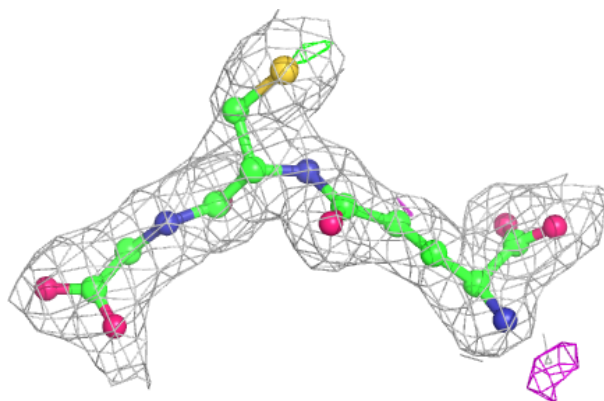
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DTT	B	242	8/8	0.92	0.14	48,54,61,62	0
3	DTT	A	242	8/8	0.92	0.13	42,54,58,64	0
3	DTT	C	241	8/8	0.94	0.10	35,43,53,65	0
2	GSH	B	241	20/20	0.96	0.10	19,23,42,48	0
2	GSH	C	242	20/20	0.96	0.10	18,25,33,34	0
2	GSH	A	241	20/20	0.97	0.09	13,22,32,32	0

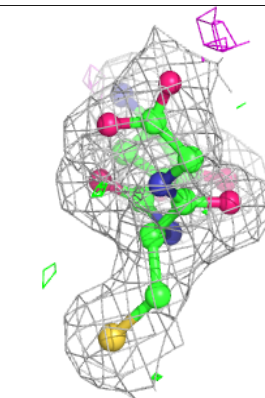
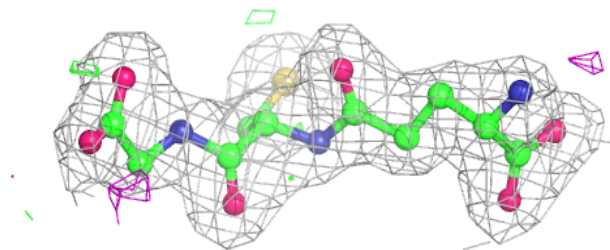
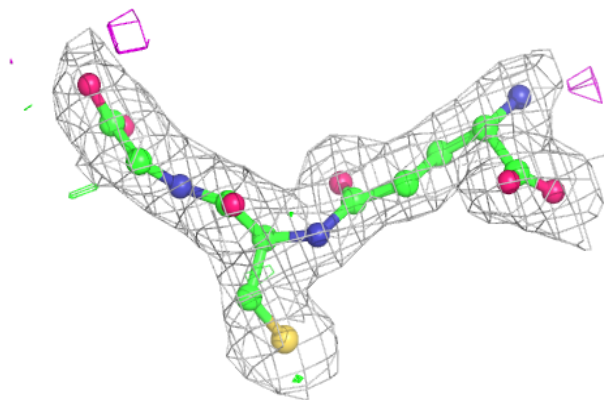
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

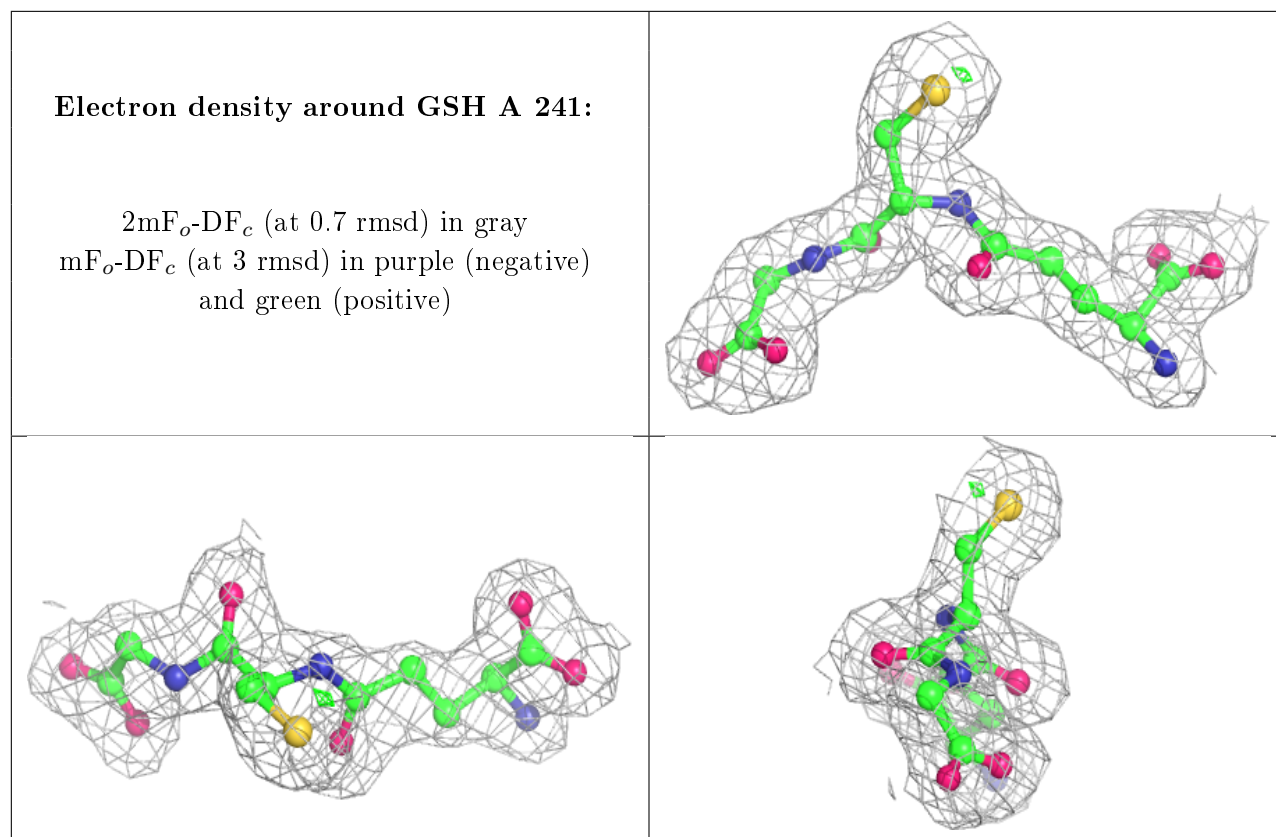
**Electron density around GSH B 241:**

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

**Electron density around GSH C 242:**

$2mF_o-DF_c$  (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.