



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2022 – 10:44 AM EDT

PDB ID : 7M8H  
Title : Structure of Memo1 C244S metal binding site mutant at 1.75Å  
Authors : Boniecki, M.T.; Uhlemann, E.E.; Dmitriev, O.Y.  
Deposited on : 2021-03-29  
Resolution : 1.75 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.

---

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 : 2.27  
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) : 2.27

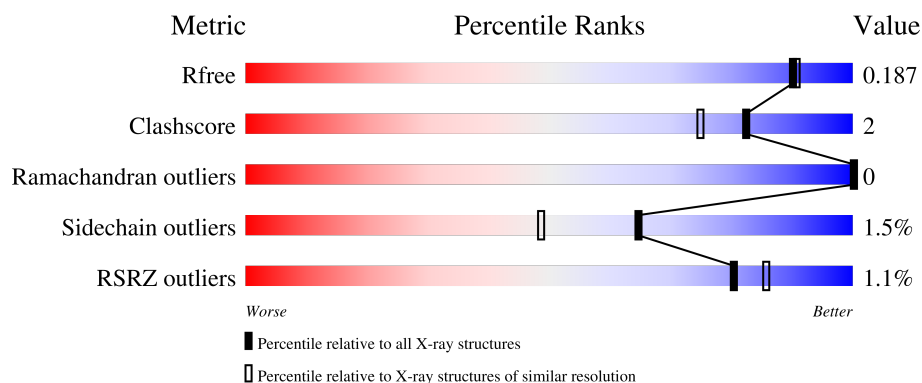
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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  $\geq 3$ , 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	294	<div> <div>94%</div> <div>6%</div> </div>
1	B	294	<div> <div>96%</div> <div>.</div> </div>
1	C	294	<div> <div>93%</div> <div>6%</div> </div>
1	D	294	<div> <div>98%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	310	-	-	X	-
3	EDO	C	503	-	-	X	-
3	EDO	C	506	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11239 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.

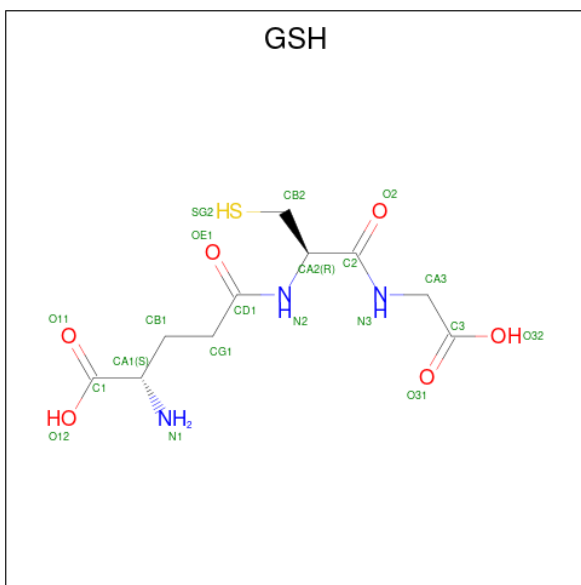
- Molecule 1 is a protein called Protein MEMO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	15	0
			2412	1529	413	455	15			
1	B	294	Total	C	N	O	S	0	10	0
			2385	1513	408	449	15			
1	C	294	Total	C	N	O	S	0	11	0
			2389	1515	408	451	15			
1	D	294	Total	C	N	O	S	0	8	0
			2362	1498	401	448	15			

There are 4 discrepancies between the modelled and reference sequences:

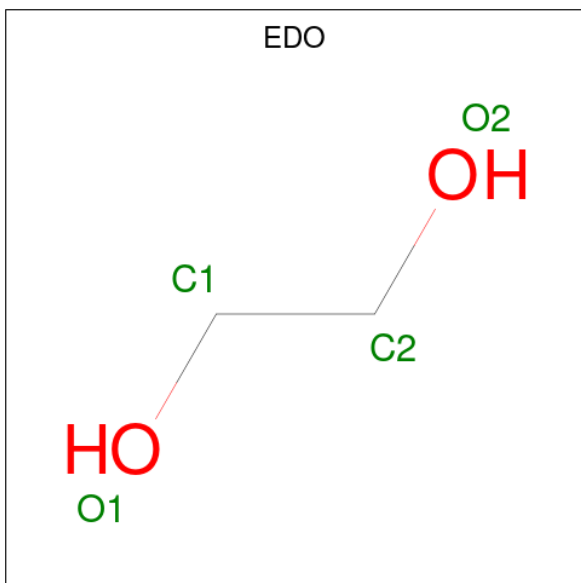
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	SER	CYS	engineered mutation	UNP Q9Y316
B	244	SER	CYS	engineered mutation	UNP Q9Y316
C	244	SER	CYS	engineered mutation	UNP Q9Y316
D	244	SER	CYS	engineered mutation	UNP Q9Y316

- 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) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			40	20	6	12	2		
2	B	1	Total	C	N	O	S	0	1
			20	10	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	D	1	Total	C	N	O	S	0	1
			40	20	6	12	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



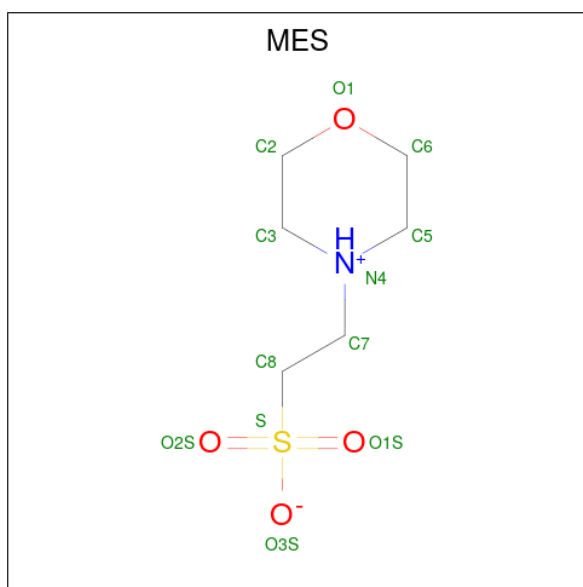
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



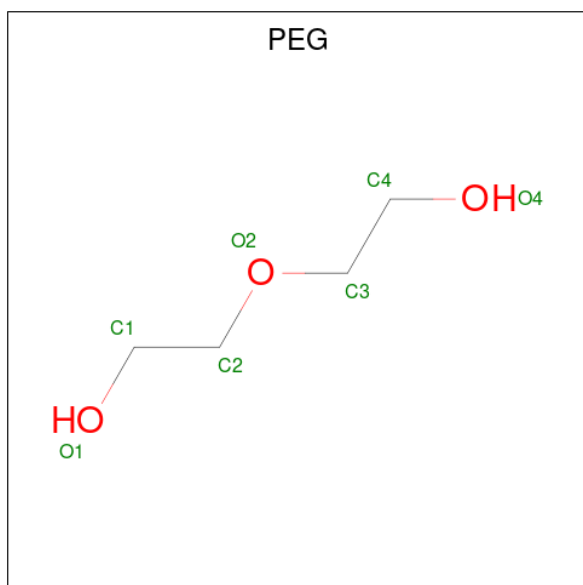
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	365	Total	O	0	0
			365	365		
7	B	327	Total	O	0	0
			327	327		
7	C	337	Total	O	0	0
			337	337		
7	D	339	Total	O	0	0
			339	339		

### 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: Protein MEMO1

Chain A: 



- Molecule 1: Protein MEMO1

Chain B: 



- Molecule 1: Protein MEMO1

Chain C: 



- Molecule 1: Protein MEMO1

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.00Å 89.52Å 97.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.63 – 1.75 48.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.63-1.75) 94.8 (48.00-1.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.154 , 0.187 0.155 , 0.187	Depositor DCC
$R_{free}$ test set	6187 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11239	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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 40.15 % 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 2.8547e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PEG, MES, GOL, GSH, EDO

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	0.40	0/2519	0.61	0/3406
1	B	0.37	0/2477	0.60	0/3355
1	C	0.40	0/2484	0.61	0/3362
1	D	0.38	0/2448	0.58	0/3316
All	All	0.39	0/9928	0.60	0/13439

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	2412	0	2366	14	0
1	B	2385	0	2311	10	0
1	C	2389	0	2316	19	0
1	D	2362	0	2270	5	0
2	A	40	0	30	1	0
2	B	20	0	15	1	0
2	C	20	0	15	1	0
2	D	40	0	30	1	0
3	A	28	0	42	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	40	0	60	7	0
3	C	36	0	54	7	0
3	D	24	0	36	1	0
4	A	12	0	12	0	0
4	D	24	0	24	0	0
5	A	7	0	10	0	0
5	C	7	0	10	0	0
5	D	7	0	10	0	0
6	B	6	0	8	1	0
6	C	6	0	8	3	0
6	D	6	0	8	0	0
7	A	365	0	0	5	0
7	B	327	0	0	0	0
7	C	337	0	0	3	0
7	D	339	0	0	4	0
All	All	11239	0	9635	48	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 2.

All (48) 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:C:53:THR:HB	3:C:503:EDO:H11	1.69	0.75
1:C:167:GLN:HE21	6:C:501:GOL:H32	1.52	0.73
1:A:226:GLN:HA	1:D:180:PRO:HG3	1.72	0.72
1:A:285:SER:H	3:A:307:EDO:H12	1.56	0.69
1:B:53:THR:HB	3:B:310:EDO:H22	1.76	0.68
1:C:51:GLY:HA3	3:C:503:EDO:H12	1.80	0.64
1:C:254:ASN:HD21	6:C:501:GOL:H31	1.65	0.62
1:A:266:MET:HG3	1:A:296:VAL:HG22	1.82	0.61
1:B:240:HIS:HD2	3:B:308:EDO:H12	1.66	0.61
1:A:148:LYS:NZ	7:A:404:HOH:O	2.33	0.60
1:C:18[A]:THR:HG22	1:C:20:SER:H	1.66	0.59
1:A:118[A]:MET:SD	1:A:172:LEU:HD12	2.44	0.58
1:D:196:ARG:NH2	7:D:404:HOH:O	2.34	0.58
1:A:69[A]:SER:OG	1:B:40[A]:ARG:NH1	2.37	0.57
1:C:25:ASN:HD22	1:C:100:LEU:HD22	1.71	0.56
1:C:53:THR:CB	3:C:503:EDO:H11	2.36	0.55
1:C:92[A]:SER:HB2	3:C:510:EDO:H21	1.90	0.54
1:B:51:GLY:HA3	3:B:310:EDO:H21	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:HIS:HB2	3:B:304:EDO:H22	1.91	0.53
1:B:240:HIS:CD2	3:B:308:EDO:H12	2.43	0.53
1:C:29[A]:GLU:HG3	1:C:142:LYS:HZ1	1.74	0.52
2:B:301[A]:GSH:HN12	3:B:310:EDO:H12	1.75	0.52
1:C:29[A]:GLU:OE2	1:C:142:LYS:NZ	2.44	0.51
1:C:167:GLN:NE2	6:C:501:GOL:H32	2.24	0.51
1:A:266:MET:CG	1:A:296:VAL:HG22	2.40	0.51
1:C:104[B]:ARG:NE	7:C:611:HOH:O	2.44	0.51
2:D:301[A]:GSH:SG2	7:D:406:HOH:O	2.43	0.50
1:B:233:SER:HB2	6:B:303:GOL:H32	1.93	0.50
1:C:29[A]:GLU:HG3	1:C:142:LYS:CE	2.43	0.48
1:C:149:ASP:OD2	7:C:601:HOH:O	2.20	0.48
1:B:211:ARG:NH1	1:B:214:GLU:OE1	2.46	0.48
1:D:61:HIS:HD2	7:D:694:HOH:O	1.96	0.47
1:C:29[A]:GLU:OE2	7:C:602:HOH:O	2.21	0.47
1:A:266:MET:HG2	1:A:294:LEU:HD11	1.95	0.46
1:C:6:VAL:H	3:C:507:EDO:H12	1.80	0.46
3:C:503:EDO:HO2	2:C:511:GSH:HN12	1.58	0.46
1:C:92[B]:SER:HB3	3:C:510:EDO:H21	1.97	0.46
1:B:265:ASN:HB2	1:C:72[A]:ARG:CZ	2.46	0.46
1:A:16:TRP:CE2	2:A:301[A]:GSH:HA1	2.51	0.46
1:A:196:ARG:NH2	7:A:412:HOH:O	2.49	0.45
1:D:196:ARG:NH1	7:D:412:HOH:O	2.47	0.45
1:D:244:SER:HA	3:D:305:EDO:H11	1.99	0.45
1:A:87:ARG:NH2	1:A:120[B]:GLU:HG2	2.32	0.44
1:A:148:LYS:HE2	7:A:567:HOH:O	2.20	0.42
1:B:53:THR:CB	3:B:310:EDO:H22	2.49	0.42
1:C:29[A]:GLU:HG3	1:C:142:LYS:HE2	2.02	0.41
1:A:104[A]:ARG:HD3	7:A:585:HOH:O	2.19	0.41
1:A:297:HIS:HB3	7:A:518:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/294 (104%)	302 (98%)	5 (2%)	0	100	100
1	B	302/294 (103%)	297 (98%)	5 (2%)	0	100	100
1	C	303/294 (103%)	299 (99%)	4 (1%)	0	100	100
1	D	300/294 (102%)	295 (98%)	5 (2%)	0	100	100
All	All	1212/1176 (103%)	1193 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/256 (106%)	267 (98%)	4 (2%)	65	49
1	B	262/256 (102%)	260 (99%)	2 (1%)	81	72
1	C	263/256 (103%)	257 (98%)	6 (2%)	50	28
1	D	258/256 (101%)	255 (99%)	3 (1%)	71	56
All	All	1054/1024 (103%)	1039 (99%)	15 (1%)	65	52

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	TYR
1	A	139	TYR
1	A	216	LEU
1	A	266	MET
1	B	110	TYR
1	B	139	TYR
1	C	4	ARG
1	C	25	ASN
1	C	87	ARG
1	C	110	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	115	LYS
1	C	139	TYR
1	D	6	VAL
1	D	110	TYR
1	D	139	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	GLN
1	B	147	HIS
1	B	240	HIS
1	B	262	ASN
1	D	61	HIS
1	D	262	ASN
1	D	265	ASN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

47 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
3	EDO	B	310	-	3,3,3	0.46	0	2,2,2	0.37	0
5	PEG	A	308	-	6,6,6	0.51	0	5,5,5	0.39	0
4	MES	D	307	-	12,12,12	2.13	1 (8%)	14,16,16	2.43	6 (42%)
2	GSH	C	511	-	12,19,19	2.53	4 (33%)	15,24,24	2.05	3 (20%)
2	GSH	B	301[A]	-	12,19,19	2.54	4 (33%)	15,24,24	2.17	4 (26%)
3	EDO	A	310	-	3,3,3	0.46	0	2,2,2	0.32	0
4	MES	A	304	-	12,12,12	2.06	1 (8%)	14,16,16	2.44	5 (35%)
2	GSH	A	301[B]	-	12,19,19	2.48	4 (33%)	15,24,24	1.55	3 (20%)
3	EDO	A	303	-	3,3,3	0.36	0	2,2,2	0.87	0
6	GOL	B	303	-	5,5,5	1.05	0	5,5,5	1.47	1 (20%)
6	GOL	D	309	-	5,5,5	1.03	0	5,5,5	1.01	0
3	EDO	B	309	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	D	311	-	3,3,3	0.48	0	2,2,2	0.29	0
4	MES	D	306	-	12,12,12	2.07	1 (8%)	14,16,16	2.28	5 (35%)
2	GSH	A	301[A]	-	12,19,19	2.49	4 (33%)	15,24,24	2.19	4 (26%)
3	EDO	B	306	-	3,3,3	0.40	0	2,2,2	0.53	0
3	EDO	B	302	-	3,3,3	0.28	0	2,2,2	0.52	0
3	EDO	C	507	-	3,3,3	0.43	0	2,2,2	0.62	0
3	EDO	B	307	-	3,3,3	0.25	0	2,2,2	0.06	0
3	EDO	B	305	-	3,3,3	0.44	0	2,2,2	0.50	0
3	EDO	A	307	-	3,3,3	0.51	0	2,2,2	0.27	0
3	EDO	C	503	-	3,3,3	0.40	0	2,2,2	0.49	0
3	EDO	A	309	-	3,3,3	0.49	0	2,2,2	0.20	0
3	EDO	C	502	-	3,3,3	0.43	0	2,2,2	0.57	0
3	EDO	A	302	-	3,3,3	0.38	0	2,2,2	0.50	0
3	EDO	A	306	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	B	311	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	D	302	-	3,3,3	0.44	0	2,2,2	0.39	0
5	PEG	C	504	-	6,6,6	0.49	0	5,5,5	0.30	0
3	EDO	A	305	-	3,3,3	0.49	0	2,2,2	0.29	0
5	PEG	D	303	-	6,6,6	0.49	0	5,5,5	0.28	0
6	GOL	C	501	-	5,5,5	1.30	1 (20%)	5,5,5	0.97	0
3	EDO	D	305	-	3,3,3	0.44	0	2,2,2	0.50	0
3	EDO	C	508	-	3,3,3	0.40	0	2,2,2	0.48	0
3	EDO	B	304	-	3,3,3	0.55	0	2,2,2	0.38	0
2	GSH	D	301[B]	-	12,19,19	2.47	3 (25%)	15,24,24	1.86	2 (13%)
3	EDO	C	509	-	3,3,3	0.47	0	2,2,2	0.71	0
3	EDO	C	505	-	3,3,3	0.46	0	2,2,2	0.26	0
3	EDO	D	304	-	3,3,3	0.44	0	2,2,2	0.62	0
3	EDO	D	308	-	3,3,3	0.51	0	2,2,2	0.22	0
3	EDO	C	510	-	3,3,3	0.45	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	C	506	-	3,3,3	0.41	0	2,2,2	0.34	0
2	GSH	D	301[A]	-	12,19,19	2.51	3 (25%)	15,24,24	1.59	4 (26%)
3	EDO	D	310	-	3,3,3	0.46	0	2,2,2	0.38	0
3	EDO	C	512	-	3,3,3	0.46	0	2,2,2	0.38	0
3	EDO	B	308	-	3,3,3	0.49	0	2,2,2	0.19	0
3	EDO	B	312	-	3,3,3	0.45	0	2,2,2	0.39	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
3	EDO	B	310	-	-	1/1/1/1	-
5	PEG	A	308	-	-	2/4/4/4	-
4	MES	D	307	-	-	5/6/14/14	0/1/1/1
2	GSH	C	511	-	-	1/18/24/24	-
2	GSH	B	301[A]	-	-	1/18/24/24	-
3	EDO	A	310	-	-	1/1/1/1	-
4	MES	A	304	-	-	4/6/14/14	0/1/1/1
2	GSH	A	301[B]	-	-	0/18/24/24	-
3	EDO	A	303	-	-	1/1/1/1	-
6	GOL	B	303	-	-	2/4/4/4	-
6	GOL	D	309	-	-	0/4/4/4	-
3	EDO	B	309	-	-	0/1/1/1	-
3	EDO	D	311	-	-	0/1/1/1	-
4	MES	D	306	-	-	4/6/14/14	0/1/1/1
2	GSH	A	301[A]	-	-	0/18/24/24	-
3	EDO	B	306	-	-	0/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
3	EDO	C	507	-	-	1/1/1/1	-
3	EDO	B	307	-	-	1/1/1/1	-
3	EDO	B	305	-	-	0/1/1/1	-
3	EDO	A	307	-	-	0/1/1/1	-
3	EDO	C	503	-	-	0/1/1/1	-
3	EDO	A	309	-	-	0/1/1/1	-
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	A	306	-	-	0/1/1/1	-
3	EDO	B	311	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	C	504	-	-	2/4/4/4	-
3	EDO	A	305	-	-	0/1/1/1	-
5	PEG	D	303	-	-	1/4/4/4	-
6	GOL	C	501	-	-	0/4/4/4	-
3	EDO	D	305	-	-	0/1/1/1	-
3	EDO	C	508	-	-	1/1/1/1	-
3	EDO	B	304	-	-	0/1/1/1	-
2	GSH	D	301[B]	-	-	1/18/24/24	-
3	EDO	C	509	-	-	1/1/1/1	-
3	EDO	C	505	-	-	0/1/1/1	-
3	EDO	D	304	-	-	1/1/1/1	-
3	EDO	D	308	-	-	1/1/1/1	-
3	EDO	C	510	-	-	1/1/1/1	-
3	EDO	C	506	-	-	1/1/1/1	-
2	GSH	D	301[A]	-	-	0/18/24/24	-
3	EDO	D	310	-	-	1/1/1/1	-
3	EDO	C	512	-	-	1/1/1/1	-
3	EDO	B	308	-	-	1/1/1/1	-
3	EDO	B	312	-	-	1/1/1/1	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	307	MES	C8-S	-7.04	1.67	1.77
4	A	304	MES	C8-S	-6.85	1.67	1.77
4	D	306	MES	C8-S	-6.84	1.67	1.77
2	C	511	GSH	CD1-N2	5.81	1.46	1.34
2	D	301[A]	GSH	C2-N3	5.73	1.46	1.33
2	B	301[A]	GSH	C2-N3	5.73	1.46	1.33
2	D	301[B]	GSH	C2-N3	5.68	1.46	1.33
2	A	301[B]	GSH	C2-N3	5.66	1.46	1.33
2	B	301[A]	GSH	CD1-N2	5.66	1.46	1.34
2	D	301[A]	GSH	CD1-N2	5.62	1.46	1.34
2	C	511	GSH	C2-N3	5.61	1.45	1.33
2	A	301[A]	GSH	C2-N3	5.58	1.45	1.33
2	A	301[B]	GSH	CD1-N2	5.56	1.45	1.34
2	D	301[B]	GSH	CD1-N2	5.54	1.45	1.34
2	A	301[A]	GSH	CD1-N2	5.51	1.45	1.34
2	A	301[A]	GSH	OE1-CD1	-2.39	1.18	1.23
2	B	301[A]	GSH	O2-C2	-2.33	1.18	1.23
2	A	301[A]	GSH	O2-C2	-2.23	1.19	1.23
2	D	301[A]	GSH	O2-C2	-2.23	1.19	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301[A]	GSH	OE1-CD1	-2.20	1.18	1.23
6	C	501	GOL	C1-C2	2.19	1.60	1.51
2	D	301[B]	GSH	O2-C2	-2.15	1.19	1.23
2	C	511	GSH	OE1-CD1	-2.14	1.18	1.23
2	A	301[B]	GSH	OE1-CD1	-2.14	1.18	1.23
2	C	511	GSH	O2-C2	-2.08	1.19	1.23
2	A	301[B]	GSH	O2-C2	-2.01	1.19	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	511	GSH	CA2-CB2-SG2	-6.01	107.44	114.19
2	A	301[A]	GSH	CA2-CB2-SG2	-5.42	108.11	114.19
2	D	301[B]	GSH	CA2-CB2-SG2	-5.26	108.28	114.19
2	B	301[A]	GSH	CA2-CB2-SG2	-5.21	108.34	114.19
4	A	304	MES	O2S-S-C8	4.87	112.78	106.92
4	D	307	MES	C5-N4-C3	4.74	119.49	108.83
4	A	304	MES	C5-N4-C3	4.73	119.47	108.83
4	D	306	MES	C5-N4-C3	4.50	118.95	108.83
4	D	306	MES	O2S-S-C8	4.34	112.14	106.92
2	D	301[A]	GSH	CA2-CB2-SG2	-3.53	110.22	114.19
4	D	306	MES	C7-N4-C3	3.53	120.27	111.23
4	D	307	MES	O1S-S-C8	3.46	111.08	106.92
2	A	301[B]	GSH	CA2-CB2-SG2	-3.42	110.35	114.19
2	B	301[A]	GSH	CA2-C2-N3	3.37	123.34	116.54
4	A	304	MES	C7-N4-C5	3.33	119.75	111.23
4	D	307	MES	C2-C3-N4	-3.22	105.22	110.10
4	D	307	MES	C7-N4-C3	3.17	119.35	111.23
2	A	301[A]	GSH	CA2-C2-N3	3.15	122.90	116.54
4	D	307	MES	C7-N4-C5	3.11	119.18	111.23
2	A	301[A]	GSH	CG1-CD1-N2	3.04	121.11	115.83
4	A	304	MES	C7-N4-C3	2.81	118.42	111.23
4	A	304	MES	C2-C3-N4	-2.79	105.87	110.10
6	B	303	GOL	C3-C2-C1	-2.71	101.18	111.70
2	A	301[A]	GSH	OE1-CD1-N2	-2.50	118.73	122.95
2	D	301[A]	GSH	CA2-C2-N3	2.49	121.57	116.54
2	D	301[B]	GSH	CA2-C2-N3	2.48	121.54	116.54
2	B	301[A]	GSH	CG1-CD1-N2	2.45	120.08	115.83
4	D	306	MES	C6-C5-N4	-2.40	106.46	110.10
2	C	511	GSH	C3-CA3-N3	2.36	114.98	110.43
2	B	301[A]	GSH	O2-C2-N3	-2.34	117.96	122.99
4	D	306	MES	C7-N4-C5	2.34	117.21	111.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	511	GSH	CA2-C2-N3	2.30	121.18	116.54
2	A	301[B]	GSH	CA2-C2-N3	2.26	121.11	116.54
2	D	301[A]	GSH	C3-CA3-N3	2.18	114.63	110.43
2	A	301[B]	GSH	CG1-CD1-N2	2.13	119.53	115.83
2	D	301[A]	GSH	CG1-CD1-N2	2.07	119.42	115.83
4	D	307	MES	O3S-S-C8	2.05	109.09	105.77

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	511	GSH	C2-CA2-CB2-SG2
4	A	304	MES	C8-C7-N4-C5
4	A	304	MES	C7-C8-S-O3S
4	D	306	MES	C8-C7-N4-C3
4	D	307	MES	C8-C7-N4-C3
4	D	307	MES	C7-C8-S-O1S
4	D	307	MES	C7-C8-S-O3S
6	B	303	GOL	O1-C1-C2-C3
6	B	303	GOL	O1-C1-C2-O2
4	D	306	MES	C7-C8-S-O3S
2	B	301[A]	GSH	C2-CA2-CB2-SG2
3	A	310	EDO	O1-C1-C2-O2
3	B	307	EDO	O1-C1-C2-O2
3	B	308	EDO	O1-C1-C2-O2
3	C	506	EDO	O1-C1-C2-O2
3	D	308	EDO	O1-C1-C2-O2
3	D	310	EDO	O1-C1-C2-O2
5	A	308	PEG	O2-C3-C4-O4
3	A	302	EDO	O1-C1-C2-O2
3	B	310	EDO	O1-C1-C2-O2
4	D	307	MES	C8-C7-N4-C5
2	D	301[B]	GSH	C2-CA2-CB2-SG2
3	C	508	EDO	O1-C1-C2-O2
3	C	507	EDO	O1-C1-C2-O2
3	C	512	EDO	O1-C1-C2-O2
4	A	304	MES	C7-C8-S-O1S
4	A	304	MES	C7-C8-S-O2S
4	D	306	MES	C7-C8-S-O1S
4	D	306	MES	C7-C8-S-O2S
4	D	307	MES	C7-C8-S-O2S
3	C	502	EDO	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

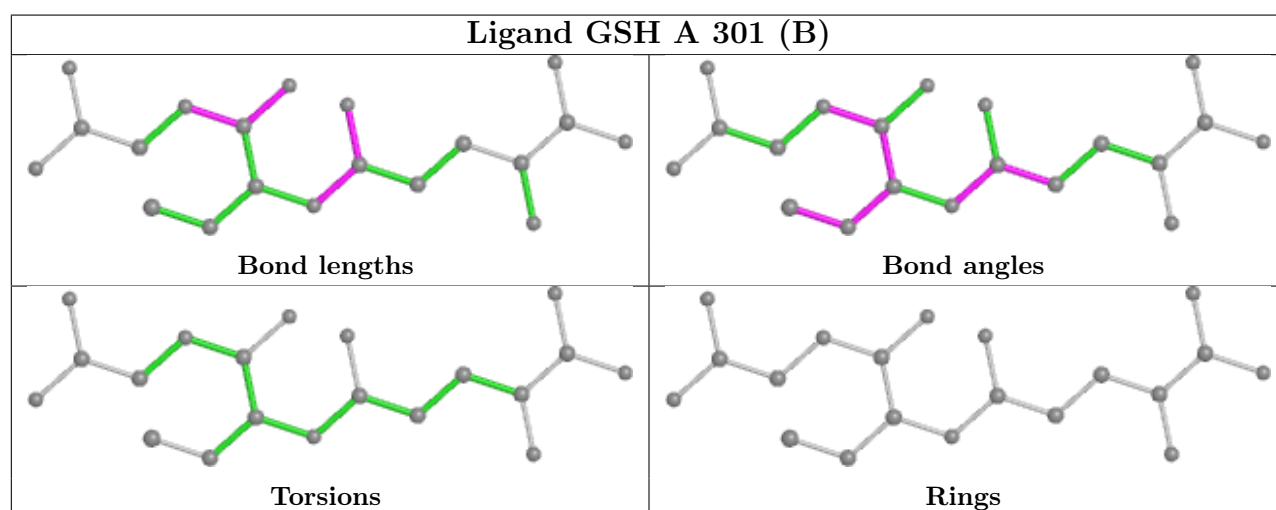
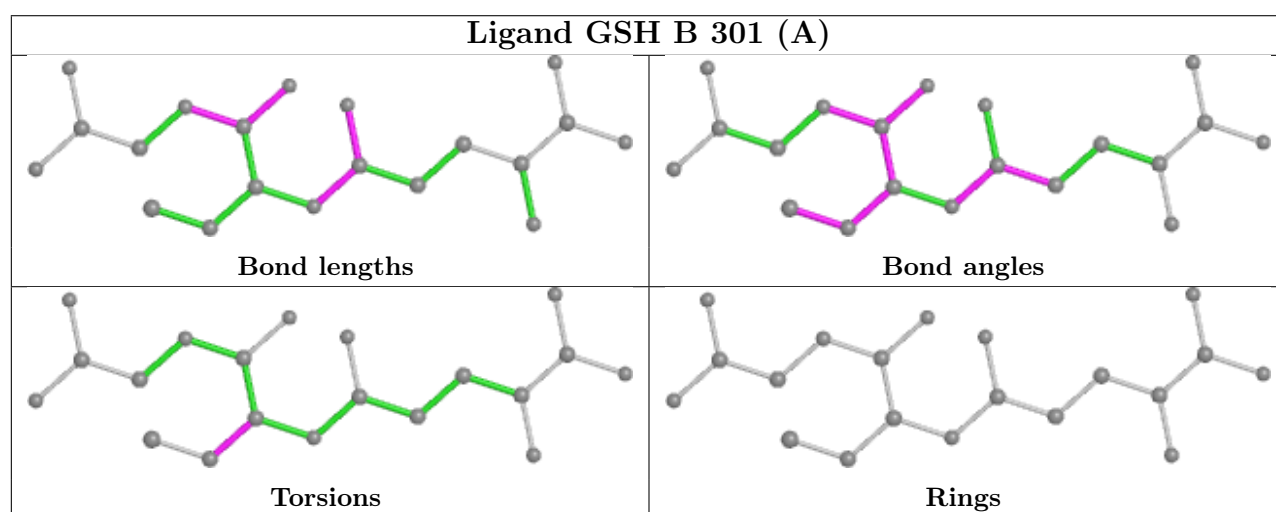
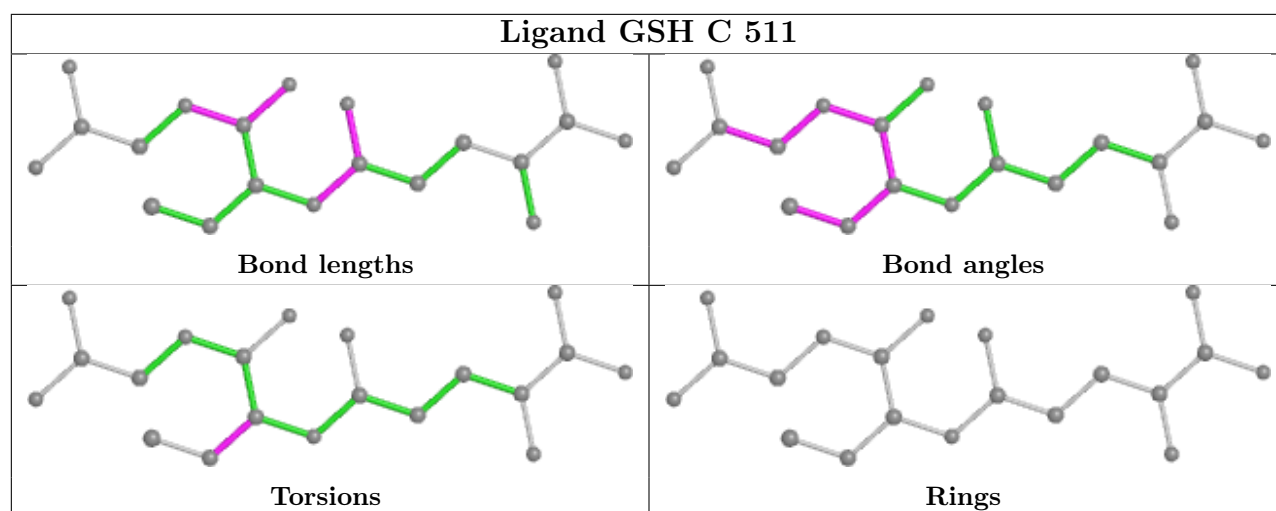
Mol	Chain	Res	Type	Atoms
5	C	504	PEG	C4-C3-O2-C2
3	B	312	EDO	O1-C1-C2-O2
5	A	308	PEG	O1-C1-C2-O2
5	D	303	PEG	O1-C1-C2-O2
3	C	509	EDO	O1-C1-C2-O2
5	C	504	PEG	O1-C1-C2-O2
3	A	303	EDO	O1-C1-C2-O2
3	C	510	EDO	O1-C1-C2-O2
3	D	304	EDO	O1-C1-C2-O2

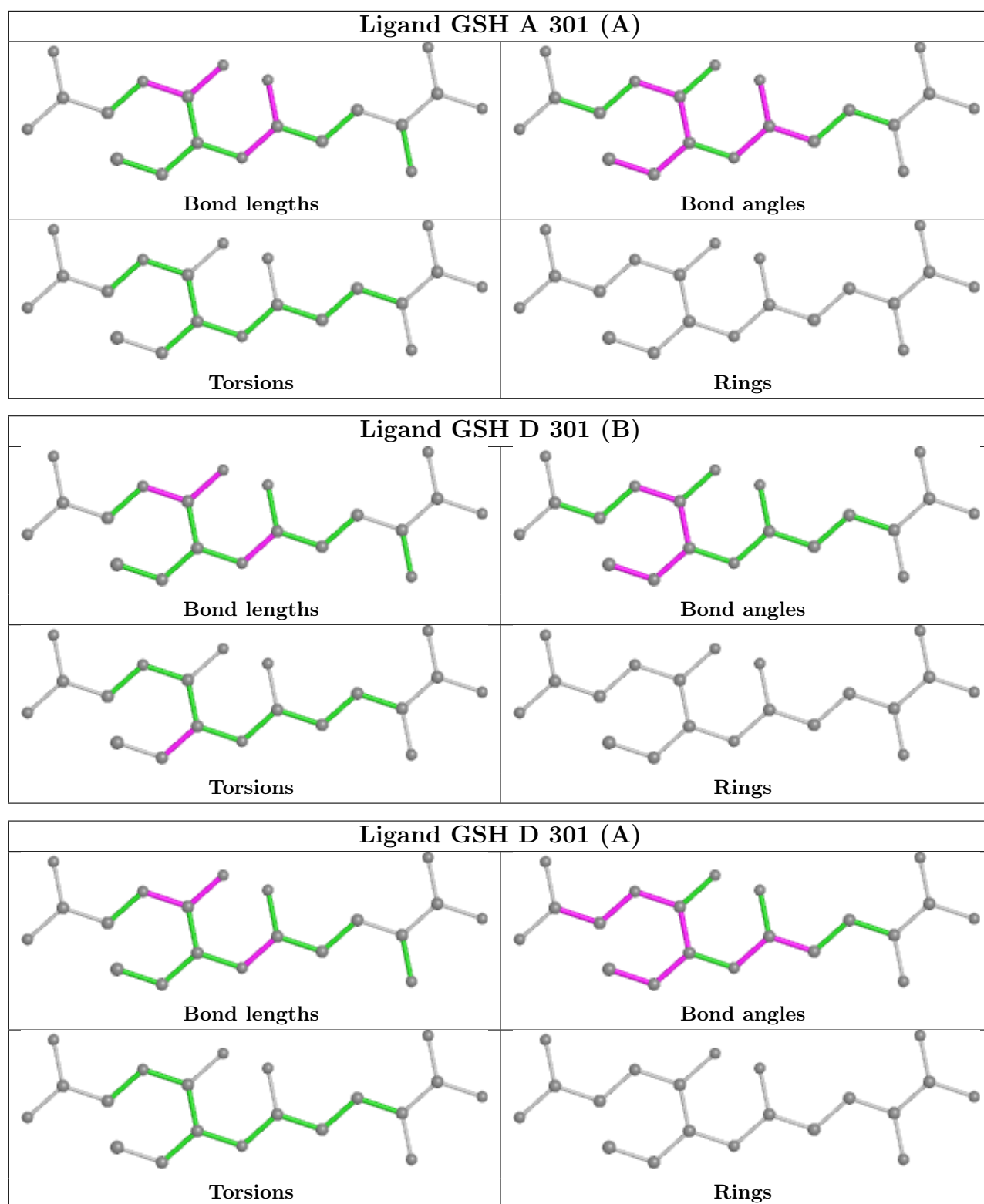
There are no ring outliers.

14 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	310	EDO	4	0
2	C	511	GSH	1	0
2	B	301[A]	GSH	1	0
6	B	303	GOL	1	0
2	A	301[A]	GSH	1	0
3	C	507	EDO	1	0
3	A	307	EDO	1	0
3	C	503	EDO	4	0
6	C	501	GOL	3	0
3	D	305	EDO	1	0
3	B	304	EDO	1	0
3	C	510	EDO	2	0
2	D	301[A]	GSH	1	0
3	B	308	EDO	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 ⓘ

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	294/294 (100%)	0.01	3 (1%) 82 87	12, 17, 33, 52	2 (0%)
1	B	294/294 (100%)	0.04	1 (0%) 94 95	14, 19, 35, 60	4 (1%)
1	C	294/294 (100%)	0.04	3 (1%) 82 87	12, 18, 29, 60	3 (1%)
1	D	294/294 (100%)	0.05	6 (2%) 65 72	14, 20, 35, 67	4 (1%)
All	All	1176/1176 (100%)	0.03	13 (1%) 80 86	12, 19, 33, 67	13 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	84	PRO	4.7
1	A	84	PRO	4.3
1	A	83	VAL	3.6
1	C	84	PRO	3.5
1	A	297	HIS	3.3
1	B	84	PRO	3.2
1	D	5	VAL	2.9
1	C	4	ARG	2.4
1	D	83	VAL	2.4
1	C	282	TRP	2.3
1	D	257	THR	2.1
1	D	4	ARG	2.1
1	D	263	GLY	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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
3	EDO	D	308	4/4	0.54	0.34	47,54,57,57	0
3	EDO	A	309	4/4	0.66	0.17	57,59,59,62	0
3	EDO	B	308	4/4	0.69	0.35	36,42,43,54	0
3	EDO	A	305	4/4	0.69	0.20	35,43,45,52	0
5	PEG	D	303	7/7	0.70	0.16	34,42,51,57	0
2	GSH	D	301[A]	20/20	0.72	0.22	52,54,58,58	20
3	EDO	B	311	4/4	0.72	0.35	38,49,52,53	0
2	GSH	D	301[B]	20/20	0.72	0.22	35,49,52,58	20
5	PEG	A	308	7/7	0.72	0.15	31,43,48,49	0
3	EDO	B	304	4/4	0.72	0.30	26,33,46,50	0
3	EDO	A	307	4/4	0.75	0.24	31,38,50,50	0
3	EDO	A	310	4/4	0.75	0.28	58,59,59,66	0
5	PEG	C	504	7/7	0.76	0.24	37,45,52,61	0
3	EDO	D	311	4/4	0.76	0.18	38,45,48,58	0
3	EDO	C	506	4/4	0.79	0.47	37,46,52,54	0
3	EDO	C	510	4/4	0.79	0.22	42,47,49,54	0
3	EDO	C	512	4/4	0.79	0.23	33,41,44,46	0
2	GSH	C	511	20/20	0.79	0.17	47,49,57,64	0
6	GOL	C	501	6/6	0.80	0.17	19,29,38,44	0
3	EDO	B	312	4/4	0.81	0.20	38,47,49,61	0
3	EDO	C	503	4/4	0.81	0.21	23,26,33,35	0
3	EDO	C	505	4/4	0.81	0.15	41,42,42,53	0
6	GOL	B	303	6/6	0.82	0.17	14,39,43,45	0
3	EDO	B	310	4/4	0.82	0.19	29,30,31,53	0
3	EDO	D	310	4/4	0.84	0.28	41,45,45,54	0
3	EDO	D	304	4/4	0.85	0.28	37,39,47,51	0
2	GSH	B	301[A]	20/20	0.85	0.15	20,31,39,40	20
3	EDO	B	309	4/4	0.85	0.24	39,50,54,60	0
3	EDO	D	305	4/4	0.86	0.29	35,44,48,56	0
3	EDO	C	507	4/4	0.86	0.25	34,34,51,52	0
3	EDO	C	502	4/4	0.86	0.28	31,43,47,50	0
4	MES	D	307	12/12	0.87	0.20	29,47,52,53	12

*Continued on next page...*

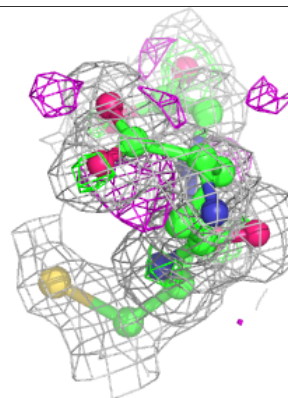
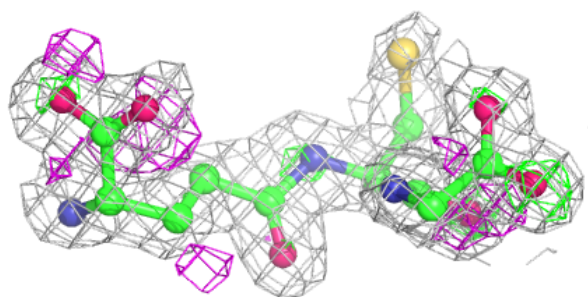
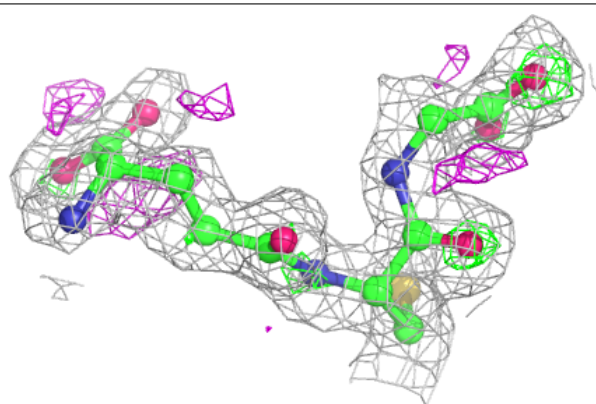
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	307	4/4	0.87	0.20	28,32,43,45	0
6	GOL	D	309	6/6	0.87	0.26	20,36,42,47	0
3	EDO	B	305	4/4	0.88	0.14	34,46,48,58	0
4	MES	D	306	12/12	0.88	0.18	24,41,50,50	12
3	EDO	A	302	4/4	0.88	0.16	25,28,30,37	0
3	EDO	C	509	4/4	0.89	0.18	21,39,39,48	0
3	EDO	B	306	4/4	0.90	0.17	32,34,48,56	0
3	EDO	A	303	4/4	0.90	0.13	25,41,41,41	0
2	GSH	A	301[B]	20/20	0.91	0.12	15,21,24,27	20
3	EDO	C	508	4/4	0.91	0.14	29,36,40,41	0
3	EDO	D	302	4/4	0.91	0.17	25,43,55,56	0
2	GSH	A	301[A]	20/20	0.91	0.12	14,21,28,32	20
4	MES	A	304	12/12	0.92	0.16	19,34,38,40	12
3	EDO	B	302	4/4	0.95	0.22	21,28,33,45	0
3	EDO	A	306	4/4	0.95	0.18	24,24,28,42	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.

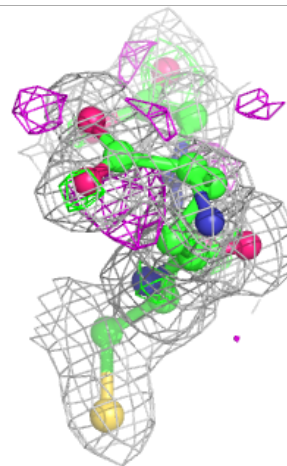
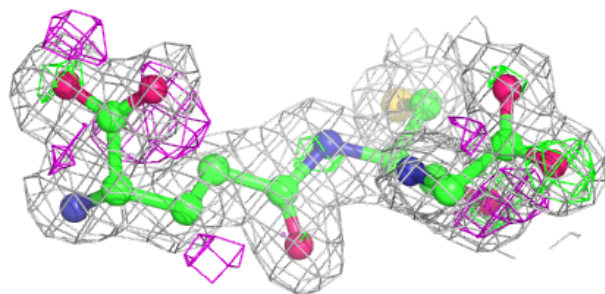
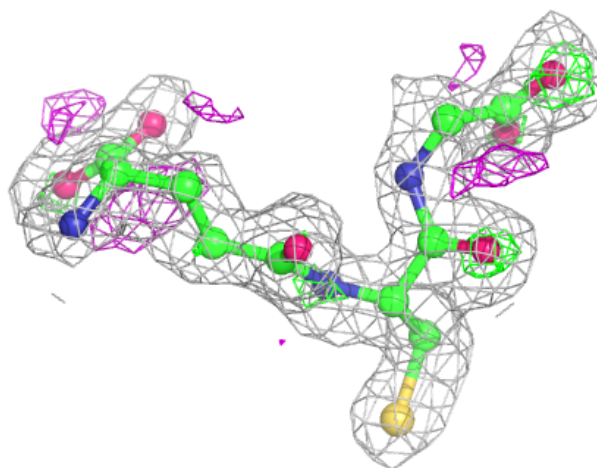
#### Electron density around GSH D 301 (A):

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



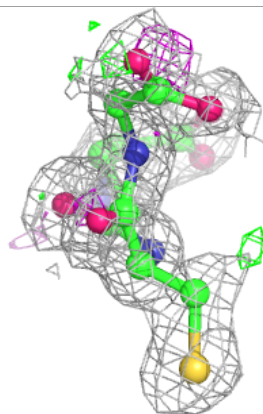
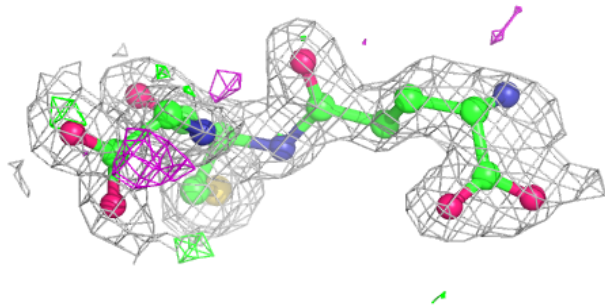
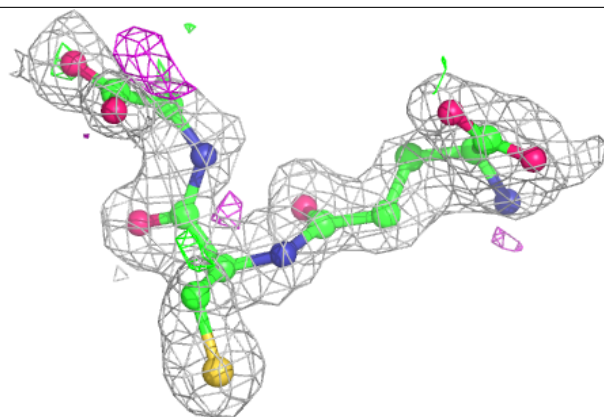
**Electron density around GSH D 301 (B):**

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

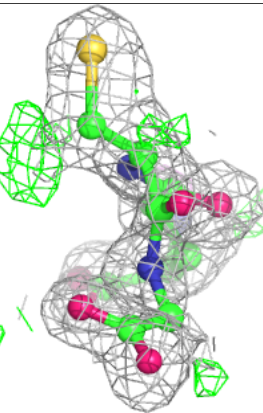
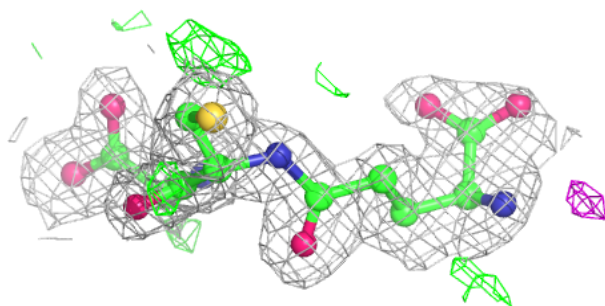
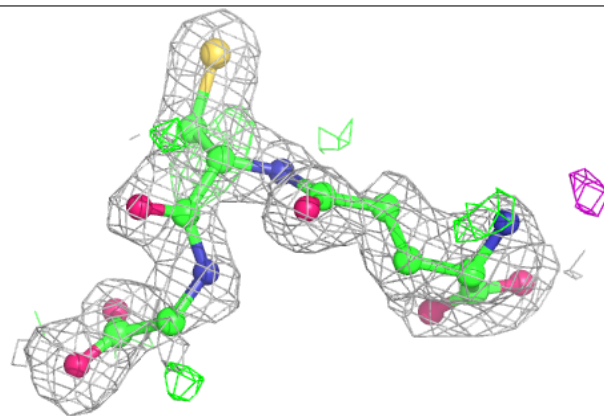


**Electron density around GSH C 511:**

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

**Electron density around GSH B 301 (A):**

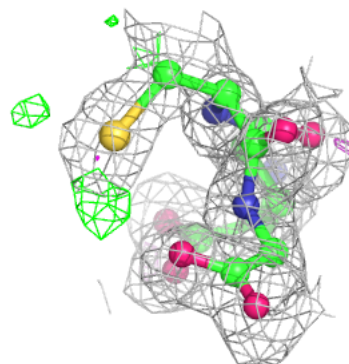
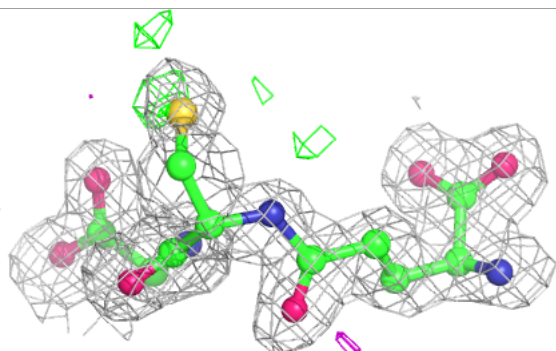
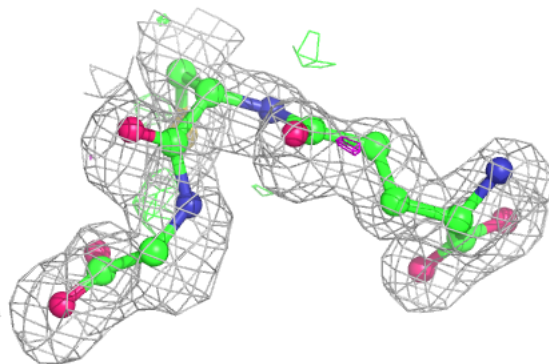
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



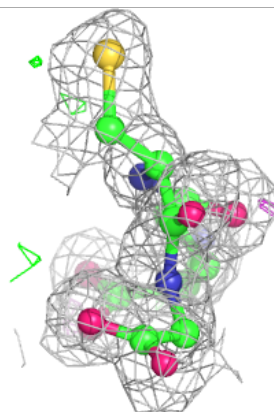
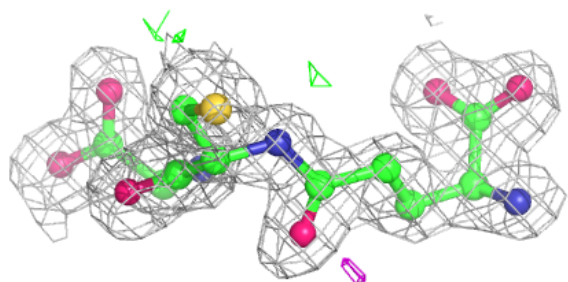
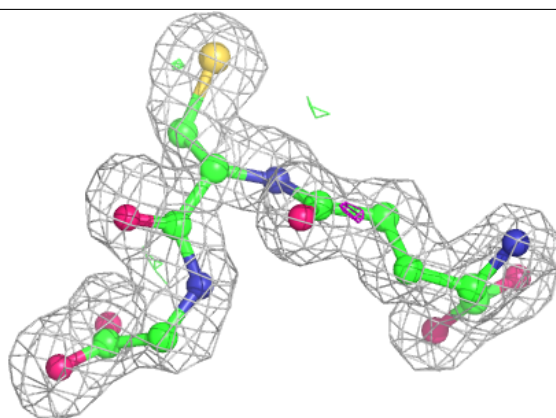


**Electron density around GSH A 301 (B):**

$2mF_o-DF_c$  (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 (A):**

$2mF_o-DF_c$  (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.