



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:56 pm BST

PDB ID : 5YWX  
Title : Crystal structure of hematopoietic prostaglandin D synthase in complex with F092  
Authors : Kamo, M.; Furubayashi, N.; Inaka, K.; Aritake, K.; Omura, A.; Tanaka, A.  
Deposited on : 2017-11-30  
Resolution : 1.74 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	:	2.11
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

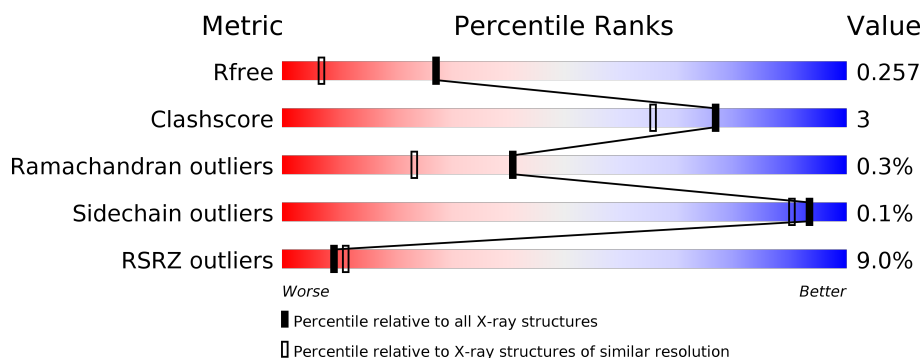
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	198	<div> <div> <div></div> <div>88%</div> <div>12%</div> </div> </div>
1	B	198	<div> <div>17%</div> <div>92%</div> <div>7%</div> </div>
1	C	198	<div> <div>17%</div> <div>92%</div> <div>8%</div> </div>
1	D	198	<div> <div>2%</div> <div>94%</div> <div>6%</div> </div>

## 2 Entry composition [i](#)

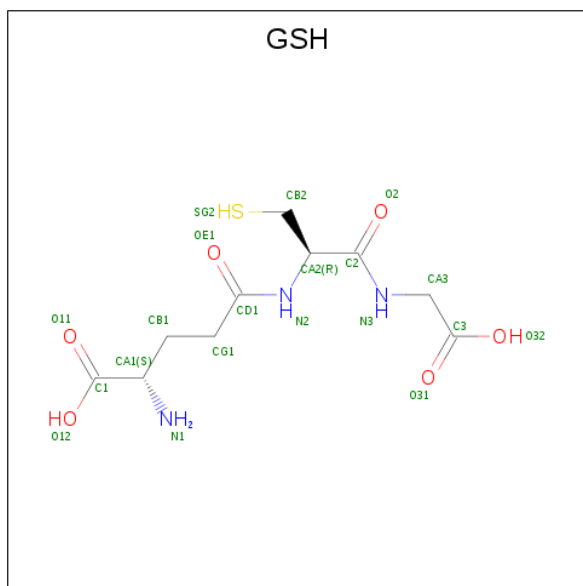
There are 6 unique types of molecules in this entry. The entry contains 7343 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hematopoietic prostaglandin D synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1638	1057	274	299	8			
1	B	198	Total	C	N	O	S	0	0	0
			1638	1057	274	299	8			
1	C	198	Total	C	N	O	S	0	0	0
			1638	1057	274	299	8			
1	D	198	Total	C	N	O	S	0	0	0
			1638	1057	274	299	8			

- 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).



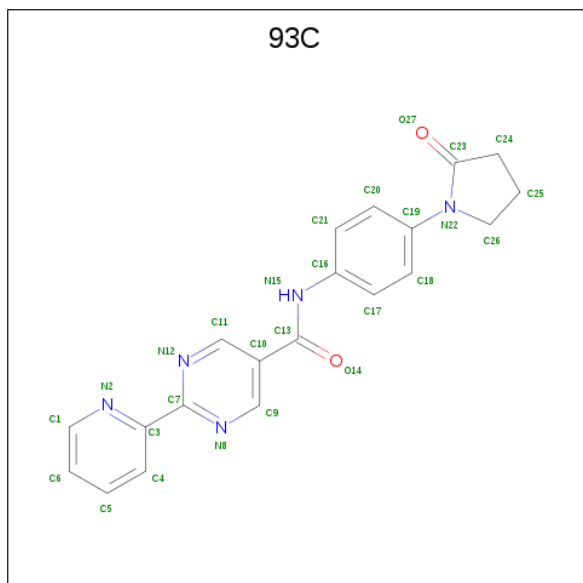
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

*Continued on next page...*

Continued from previous page...

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

- Molecule 3 is N-[4-(2-oxopyrrolidin-1-yl)phenyl]-2-(pyridin-2-yl)pyrimidine-5-carboxamide (three-letter code: 93C) (formula: C<sub>20</sub>H<sub>17</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			27	20	5	2			
3	B	1	Total	C	N	O		0	0
			27	20	5	2			
3	C	1	Total	C	N	O		0	0
			27	20	5	2			
3	D	1	Total	C	N	O		0	0
			27	20	5	2			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

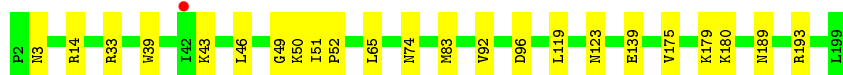
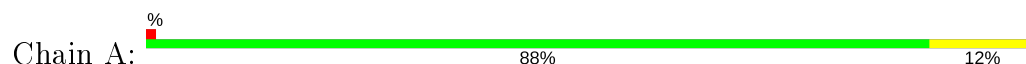
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	205	Total	O	0	0
			205	205		
6	B	89	Total	O	0	0
			89	89		
6	C	83	Total	O	0	0
			83	83		
6	D	206	Total	O	0	0
			206	206		

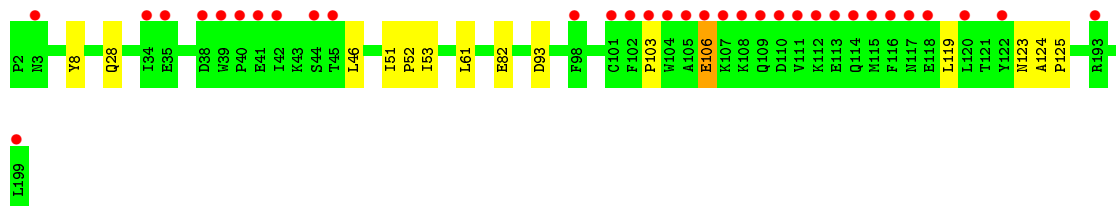
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

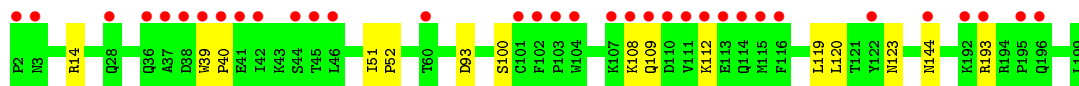
- Molecule 1: Hematopoietic prostaglandin D synthase



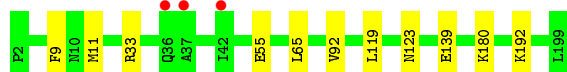
- Molecule 1: Hematopoietic prostaglandin D synthase



- Molecule 1: Hematopoietic prostaglandin D synthase



- Molecule 1: Hematopoietic prostaglandin D synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.04Å 48.17Å 92.11Å 98.97° 92.34° 90.01°	Depositor
Resolution (Å)	47.04 – 1.74 45.45 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.04-1.74) 97.1 (45.45-1.74)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.203 , 0.253 0.212 , 0.257	Depositor DCC
$R_{free}$ test set	3992 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.088 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% 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: 93C, GOL, MG, 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	0.66	0/1681	0.78	2/2284 (0.1%)
1	B	0.52	0/1681	0.68	1/2284 (0.0%)
1	C	0.51	0/1681	0.70	2/2284 (0.1%)
1	D	0.68	0/1681	0.76	1/2284 (0.0%)
All	All	0.59	0/6724	0.73	6/9136 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	33	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	93	ASP	CB-CG-OD2	6.06	123.76	118.30
1	D	33	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	93	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	120	LEU	CB-CG-CD2	5.56	120.45	111.00

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	1638	0	1619	18	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1638	0	1619	11	0
1	C	1638	0	1619	8	0
1	D	1638	0	1619	6	0
2	A	20	0	15	1	0
2	B	20	0	15	0	0
2	C	20	0	15	0	0
2	D	20	0	15	0	0
3	A	27	0	0	0	0
3	B	27	0	0	0	0
3	C	27	0	0	0	0
3	D	27	0	0	0	0
4	A	12	0	16	0	0
4	D	6	0	8	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	205	0	0	1	0
6	B	89	0	0	1	0
6	C	83	0	0	2	0
6	D	206	0	0	2	0
All	All	7343	0	6560	40	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 3.

All (40) 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:119:LEU:HD23	1:B:123:ASN:HD22	1.43	0.81
1:A:189:ASN:HD21	1:A:193:ARG:HE	1.29	0.81
1:A:83:MET:SD	1:B:61:LEU:HD21	2.27	0.72
1:D:55:GLU:OE2	6:D:401:HOH:O	2.12	0.68
1:A:175:VAL:HG12	1:A:179:LYS:HE2	1.79	0.62
1:A:189:ASN:ND2	1:A:193:ARG:HE	1.97	0.62
1:C:144:ASN:HB2	6:C:370:HOH:O	2.02	0.60
1:D:119:LEU:HA	1:D:123:ASN:HD22	1.68	0.58
1:A:189:ASN:HD21	1:A:193:ARG:NE	2.00	0.57
1:A:119:LEU:HA	1:A:123:ASN:HD22	1.70	0.56
1:A:14:ARG:HH22	1:A:96:ASP:CG	2.09	0.56
1:B:46:LEU:HD22	1:B:53:ILE:HD13	1.88	0.55
1:B:46:LEU:CD2	1:B:53:ILE:HD13	2.37	0.54
1:A:139:GLU:HG2	1:A:180:LYS:HE2	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HD13	1:A:92:VAL:HG12	1.90	0.52
1:B:28:GLN:HA	6:B:359:HOH:O	2.10	0.50
1:A:83:MET:SD	1:B:61:LEU:CD2	2.98	0.49
1:D:65:LEU:HD13	1:D:92:VAL:HG12	1.94	0.49
1:C:109:GLN:HA	1:C:112:LYS:CB	2.42	0.49
1:A:39:TRP:CZ2	1:A:43:LYS:HD2	2.47	0.49
1:B:51:ILE:HB	1:B:52:PRO:HA	1.95	0.48
1:C:109:GLN:HA	1:C:112:LYS:HB2	1.95	0.48
1:C:119:LEU:HD23	1:C:123:ASN:OD1	2.14	0.48
1:D:139:GLU:HG2	1:D:180:LYS:HE2	1.95	0.48
1:A:14:ARG:NE	2:A:301:GSH:O12	2.43	0.46
1:D:9:PHE:HB2	1:D:11:MET:HG2	1.98	0.45
1:C:51:ILE:HB	1:C:52:PRO:HA	1.97	0.45
1:B:103:PRO:HB2	1:B:106:GLU:HB3	1.99	0.45
1:A:51:ILE:HB	1:A:52:PRO:HA	1.98	0.44
1:A:119:LEU:HD23	1:A:123:ASN:HD22	1.83	0.43
1:A:193:ARG:NH1	6:A:409:HOH:O	2.51	0.42
1:A:43:LYS:HA	1:A:46:LEU:HD12	2.01	0.42
1:A:74:ASN:ND2	1:B:82:GLU:OE1	2.53	0.42
1:C:39:TRP:HB3	1:C:40:PRO:HD3	2.01	0.42
1:A:49:GLY:O	1:A:50:LYS:HD3	2.20	0.41
1:C:193:ARG:NH2	6:C:306:HOH:O	2.53	0.41
1:B:124:ALA:N	1:B:125:PRO:CD	2.84	0.41
1:D:192:LYS:HE2	6:D:438:HOH:O	2.21	0.41
1:C:14:ARG:NH2	1:C:100:SER:OG	2.55	0.40
1:B:8:TYR:HA	1:B:51:ILE:HD12	2.02	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	196/198 (99%)	193 (98%)	3 (2%)	0	100	100
1	B	196/198 (99%)	192 (98%)	3 (2%)	1 (0%)	29	12
1	C	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	29	12
1	D	196/198 (99%)	194 (99%)	2 (1%)	0	100	100
All	All	784/792 (99%)	768 (98%)	14 (2%)	2 (0%)	41	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	108	LYS
1	B	106	GLU

### 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	178/178 (100%)	177 (99%)	1 (1%)	86	79
1	B	178/178 (100%)	178 (100%)	0	100	100
1	C	178/178 (100%)	178 (100%)	0	100	100
1	D	178/178 (100%)	178 (100%)	0	100	100
All	All	712/712 (100%)	711 (100%)	1 (0%)	93	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	28	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	85	GLN
1	A	117	ASN
1	A	123	ASN
1	A	170	ASN
1	A	189	ASN
1	B	117	ASN
1	B	123	ASN
1	B	170	ASN
1	C	74	ASN
1	C	85	GLN
1	D	28	GLN
1	D	123	ASN
1	D	170	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z  > 2$
4	GOL	A	304	-	5,5,5	0.45	0	5,5,5	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	93C	D	302	-	30,30,30	0.73	1 (3%)	40,41,41	2.76	17 (42%)
3	93C	A	302	-	30,30,30	0.76	0	40,41,41	2.68	14 (35%)
2	GSH	B	202	-	12,19,19	0.82	1 (8%)	15,24,24	1.71	6 (40%)
3	93C	B	203	-	30,30,30	0.66	1 (3%)	40,41,41	3.03	16 (40%)
4	GOL	A	303	-	5,5,5	0.37	0	5,5,5	0.24	0
2	GSH	D	301	-	12,19,19	0.39	0	15,24,24	1.61	4 (26%)
4	GOL	D	303	-	5,5,5	0.40	0	5,5,5	0.82	0
2	GSH	A	301	-	12,19,19	0.62	0	15,24,24	1.58	4 (26%)
3	93C	C	203	-	30,30,30	0.78	1 (3%)	40,41,41	2.89	15 (37%)
2	GSH	C	202	-	12,19,19	0.56	0	15,24,24	0.98	1 (6%)

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
4	GOL	A	304	-	-	0/4/4/4	-
3	93C	D	302	-	-	0/16/26/26	0/4/4/4
3	93C	A	302	-	-	2/16/26/26	0/4/4/4
2	GSH	B	202	-	-	0/18/24/24	-
3	93C	B	203	-	-	2/16/26/26	0/4/4/4
4	GOL	A	303	-	-	0/4/4/4	-
2	GSH	D	301	-	-	1/18/24/24	-
4	GOL	D	303	-	-	2/4/4/4	-
2	GSH	A	301	-	-	0/18/24/24	-
3	93C	C	203	-	-	0/16/26/26	0/4/4/4
2	GSH	C	202	-	-	0/18/24/24	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	GSH	CB2-CA2	2.22	1.55	1.53
3	B	203	93C	C16-N15	-2.18	1.37	1.41
3	C	203	93C	C16-N15	-2.18	1.37	1.41
3	D	302	93C	C16-N15	-2.16	1.37	1.41

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	93C	C26-N22-C23	-10.78	102.89	112.95
3	B	203	93C	C24-C23-N22	10.30	115.14	108.23
3	C	203	93C	C26-N22-C23	-8.70	104.83	112.95
3	C	203	93C	C24-C23-N22	8.67	114.05	108.23
3	D	302	93C	C26-N22-C23	-8.49	105.03	112.95
3	A	302	93C	C24-C23-N22	7.15	113.03	108.23
3	B	203	93C	C26-N22-C23	-6.94	106.48	112.95
3	B	203	93C	C26-N22-C19	-6.78	111.02	120.76
3	C	203	93C	C26-N22-C19	-6.76	111.04	120.76
3	D	302	93C	C24-C23-N22	6.47	112.57	108.23
3	D	302	93C	C20-C19-N22	5.89	128.79	120.18
3	B	203	93C	C25-C26-N22	4.95	108.74	103.42
3	B	203	93C	O27-C23-N22	-4.74	122.37	125.40
3	D	302	93C	C18-C19-N22	-4.66	113.37	120.18
3	B	203	93C	C11-N12-C7	4.41	122.05	116.22
3	D	302	93C	C9-N8-C7	4.27	121.86	116.22
3	C	203	93C	C20-C19-N22	4.04	126.09	120.18
3	C	203	93C	C11-N12-C7	3.74	121.17	116.22
3	B	203	93C	C9-N8-C7	3.55	120.91	116.22
3	B	203	93C	C7-C3-N2	3.55	120.81	116.75
3	C	203	93C	C9-N8-C7	3.54	120.90	116.22
2	A	301	GSH	CA3-N3-C2	3.52	127.39	122.34
3	D	302	93C	C11-N12-C7	3.48	120.81	116.22
3	D	302	93C	C26-N22-C19	-3.41	115.86	120.76
3	B	203	93C	C1-N2-C3	3.36	121.94	117.23
3	C	203	93C	C1-N2-C3	3.33	121.90	117.23
3	A	302	93C	C9-N8-C7	3.31	120.59	116.22
3	C	203	93C	C7-C3-N2	3.27	120.49	116.75
3	A	302	93C	C10-C9-N8	-3.17	119.25	123.67
3	D	302	93C	C10-C9-N8	-3.15	119.27	123.67
3	B	203	93C	C10-C11-N12	-3.06	119.39	123.67
2	B	202	GSH	C3-CA3-N3	3.02	116.26	110.43
3	B	203	93C	N12-C7-N8	-2.93	119.25	125.57
3	A	302	93C	C11-N12-C7	2.91	120.07	116.22
3	A	302	93C	O14-C13-C10	-2.88	115.80	120.94
3	C	203	93C	C25-C26-N22	2.84	106.47	103.42
3	C	203	93C	C18-C19-N22	-2.82	116.06	120.18
2	D	301	GSH	CA3-N3-C2	2.78	126.34	122.34
3	A	302	93C	C1-N2-C3	2.76	121.11	117.23
3	C	203	93C	N12-C7-N8	-2.76	119.60	125.57
3	A	302	93C	C11-C10-C9	2.76	119.04	115.43
3	D	302	93C	C1-N2-C3	2.76	121.10	117.23
3	A	302	93C	C18-C19-N22	2.75	124.20	120.18

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	93C	O27-C23-N22	-2.72	123.66	125.40
3	D	302	93C	N12-C7-N8	-2.71	119.71	125.57
3	D	302	93C	C21-C16-N15	2.68	129.41	120.40
3	D	302	93C	C3-C7-N8	2.61	121.03	117.49
3	D	302	93C	C10-C11-N12	-2.58	120.07	123.67
2	B	202	GSH	CA3-N3-C2	-2.53	118.69	122.34
2	D	301	GSH	CA2-CB2-SG2	-2.53	111.35	114.19
2	D	301	GSH	CB2-CA2-C2	-2.49	104.63	109.76
3	C	203	93C	C3-C7-N8	2.47	120.85	117.49
3	B	203	93C	C10-C9-N8	-2.47	120.22	123.67
3	C	203	93C	C10-C9-N8	-2.44	120.26	123.67
2	A	301	GSH	CA2-CB2-SG2	-2.44	111.45	114.19
3	D	302	93C	C7-C3-N2	2.43	119.53	116.75
3	C	203	93C	C10-C11-N12	-2.43	120.28	123.67
3	A	302	93C	C26-N22-C19	-2.43	117.27	120.76
3	B	203	93C	O14-C13-C10	-2.39	116.68	120.94
3	A	302	93C	C10-C11-N12	-2.37	120.36	123.67
3	D	302	93C	C17-C16-N15	-2.30	112.66	120.40
3	B	203	93C	C3-C7-N12	2.29	120.60	117.49
3	A	302	93C	N12-C7-N8	-2.26	120.69	125.57
3	C	203	93C	O27-C23-C24	-2.25	121.33	127.08
3	A	302	93C	O27-C23-N22	-2.22	123.98	125.40
2	B	202	GSH	CA2-CB2-SG2	2.22	116.69	114.19
2	B	202	GSH	CA2-C2-N3	2.21	120.99	116.54
2	B	202	GSH	OE1-CD1-CG1	-2.19	118.01	122.02
3	B	203	93C	C4-C3-N2	-2.19	119.00	122.26
2	A	301	GSH	CB2-CA2-C2	-2.18	105.26	109.76
2	D	301	GSH	OE1-CD1-CG1	-2.18	118.04	122.02
3	D	302	93C	C11-C10-C9	2.15	118.25	115.43
3	B	203	93C	C11-C10-C9	2.10	118.18	115.43
2	C	202	GSH	CB2-CA2-N2	-2.09	108.31	111.28
2	A	301	GSH	O2-C2-N3	2.08	127.45	122.99
3	A	302	93C	C18-C17-C16	2.05	122.67	120.30
2	B	202	GSH	CB1-CG1-CD1	-2.04	108.49	113.04

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	93C	C18-C19-N22-C23
3	A	302	93C	C20-C19-N22-C23
4	D	303	GOL	O1-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	203	93C	C18-C19-N22-C23
4	D	303	GOL	O1-C1-C2-O2
2	D	301	GSH	C2-CA2-CB2-SG2
3	B	203	93C	C20-C19-N22-C23

There are no ring outliers.

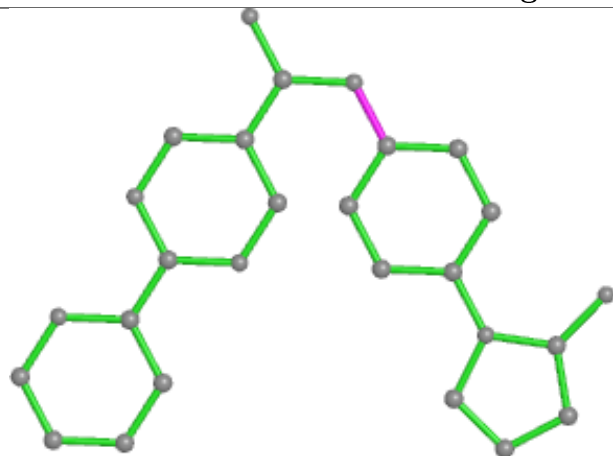
1 monomer is involved in 1 short contact:

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

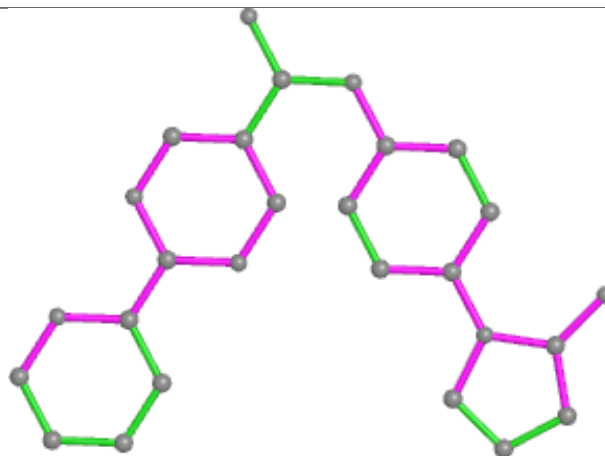
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



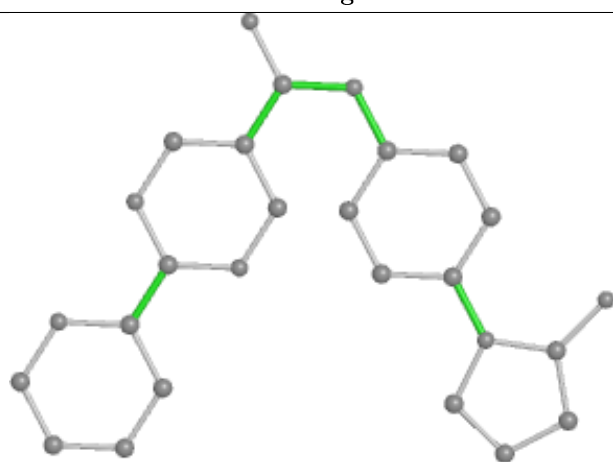
## Ligand 93C D 302



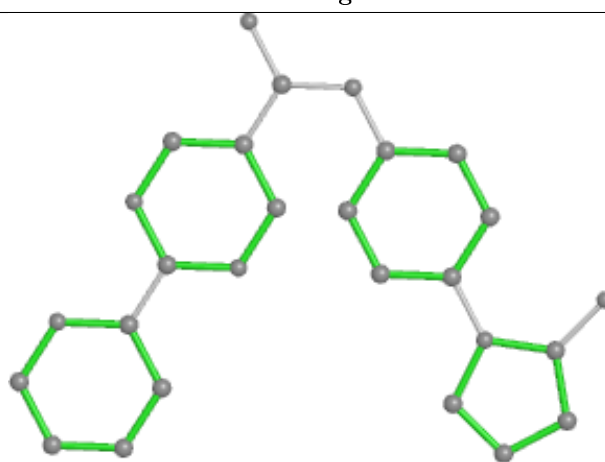
Bond lengths



Bond angles

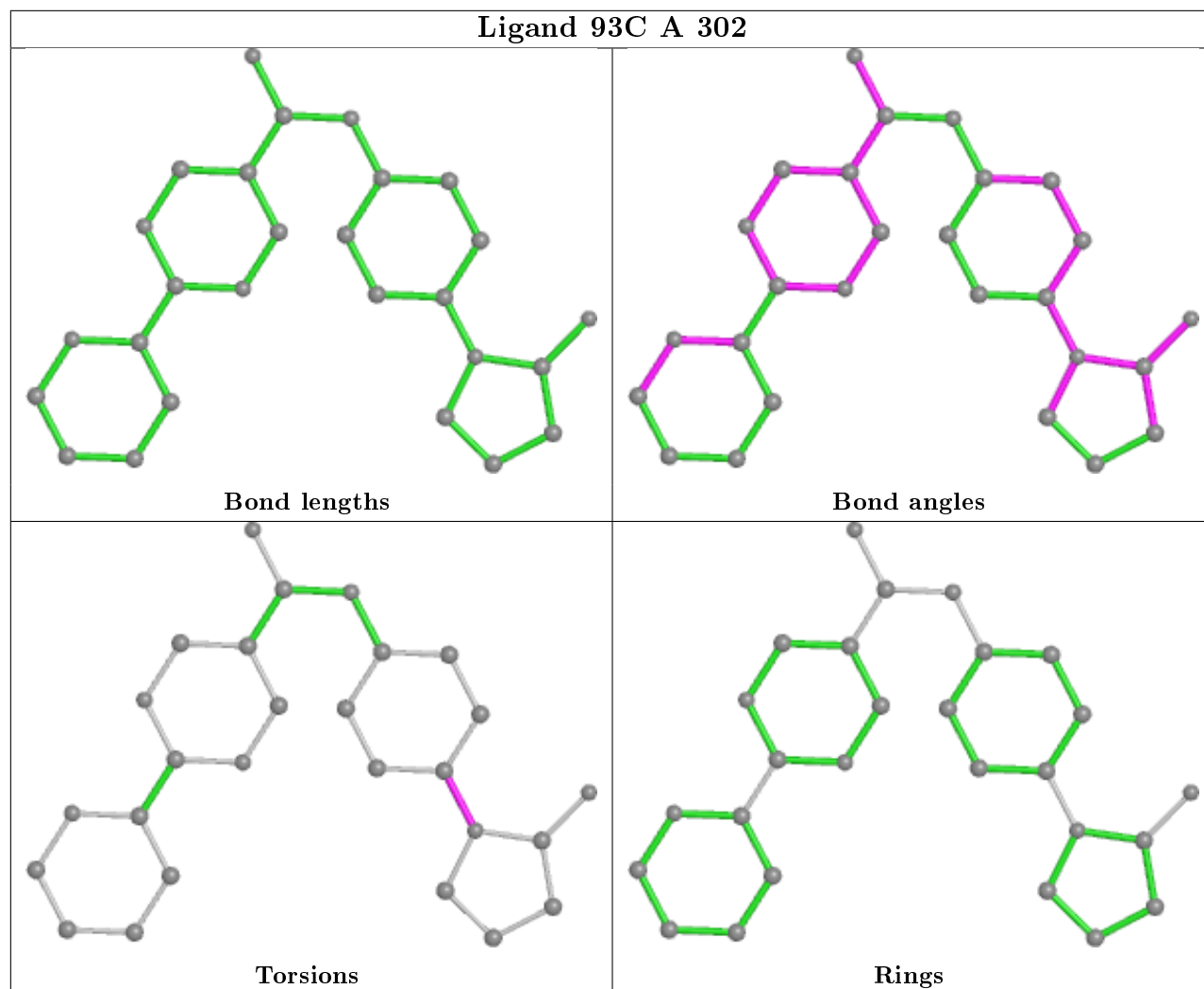


Torsions

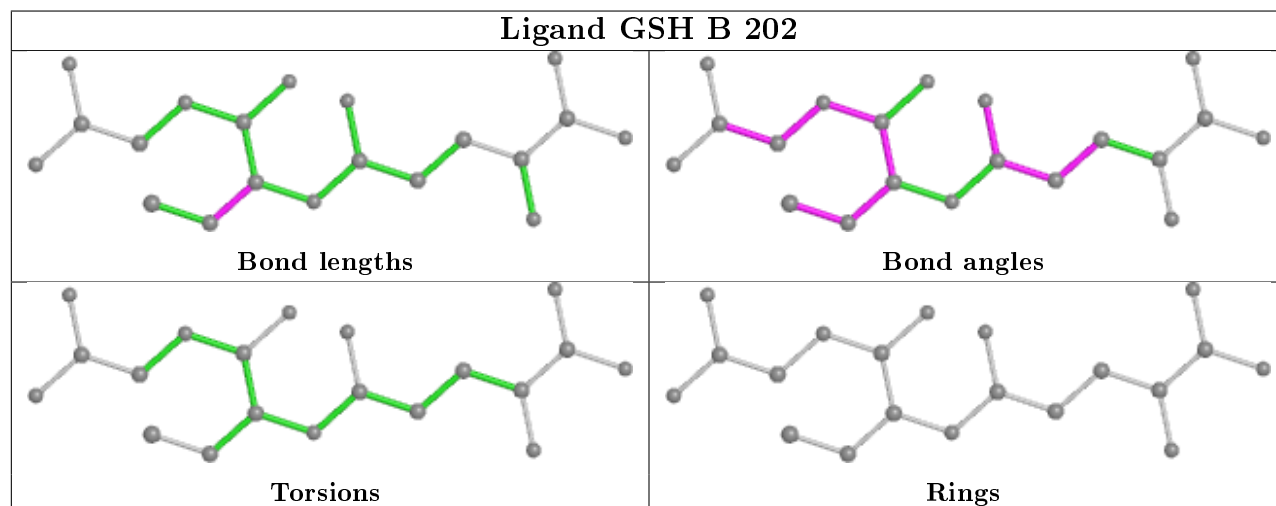


Rings

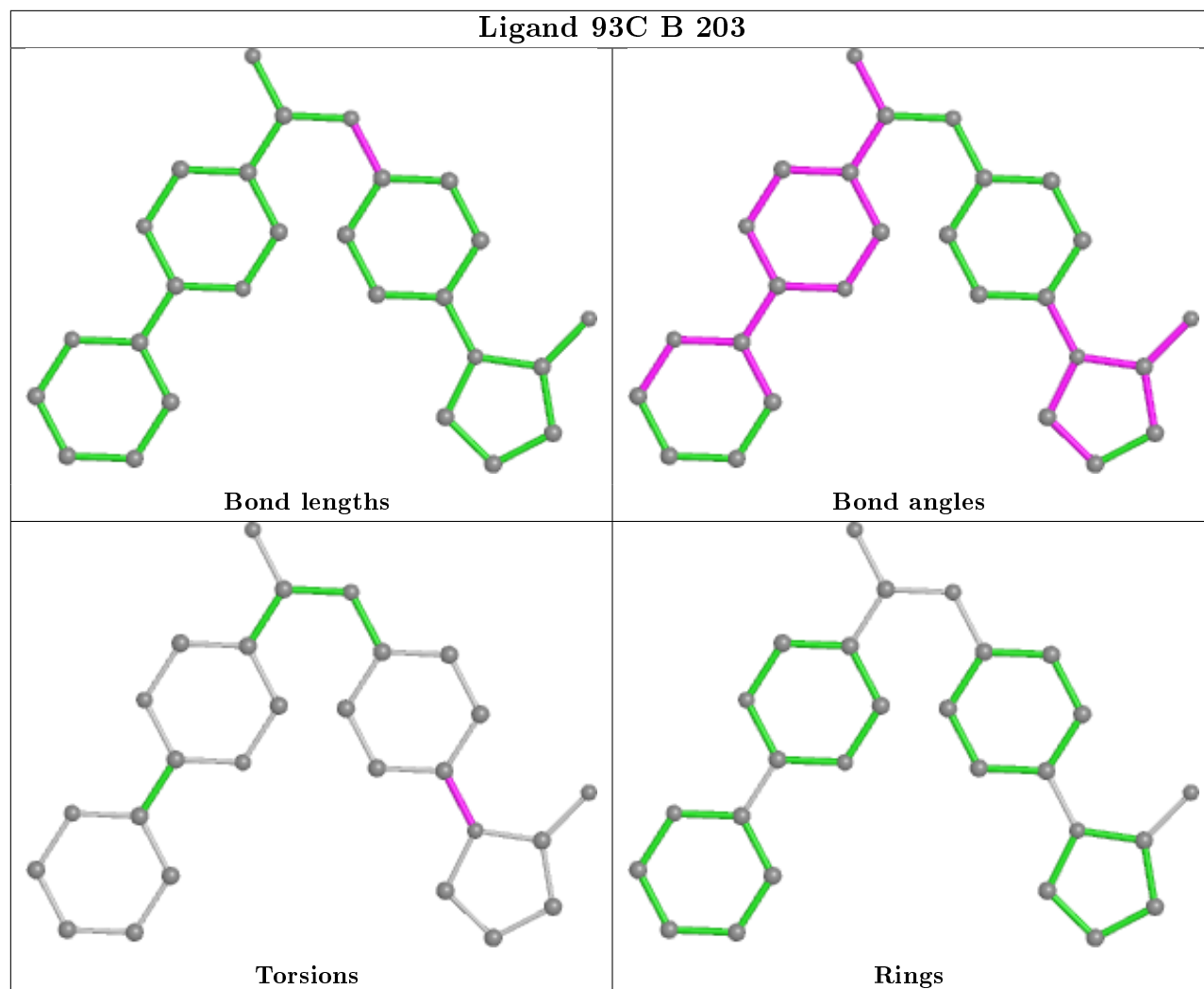
## Ligand 93C A 302



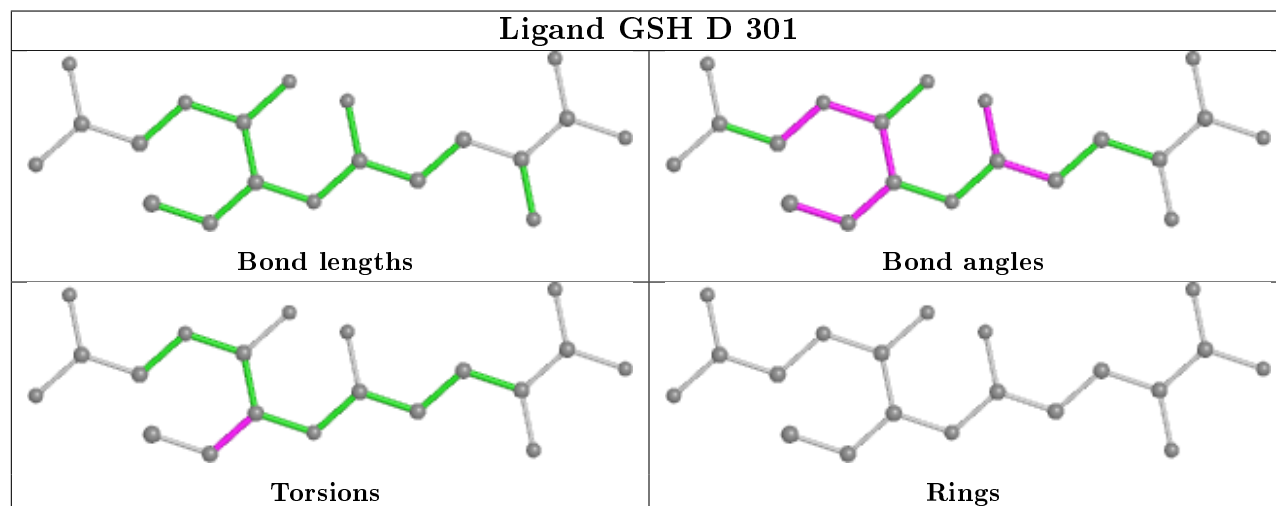
## Ligand GSH B 202

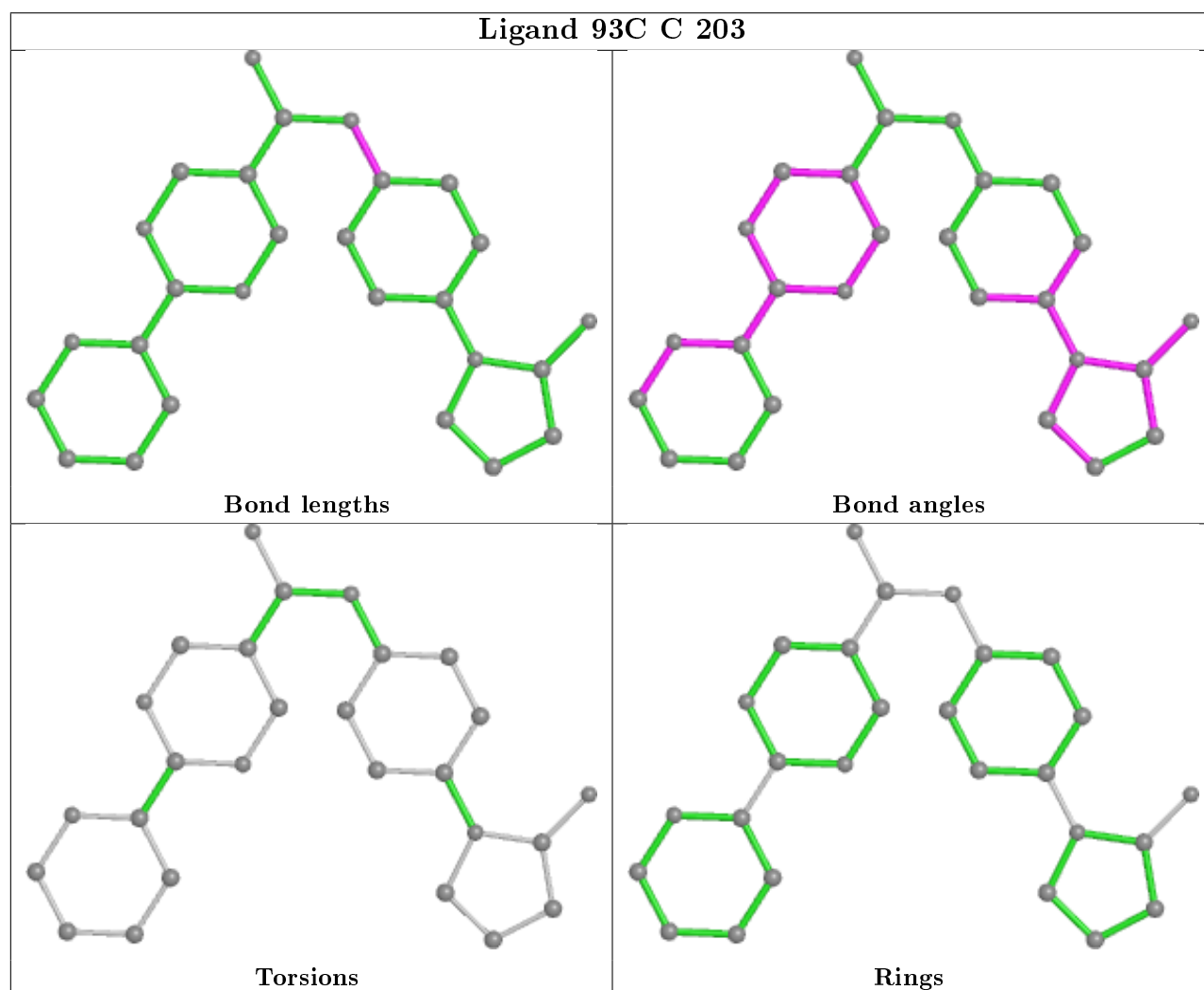
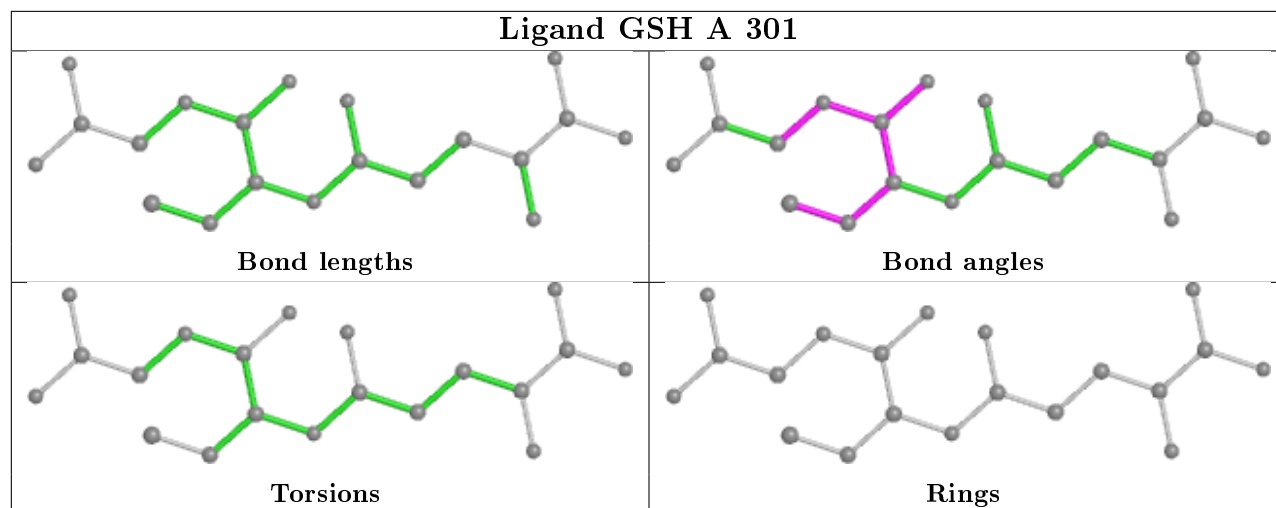


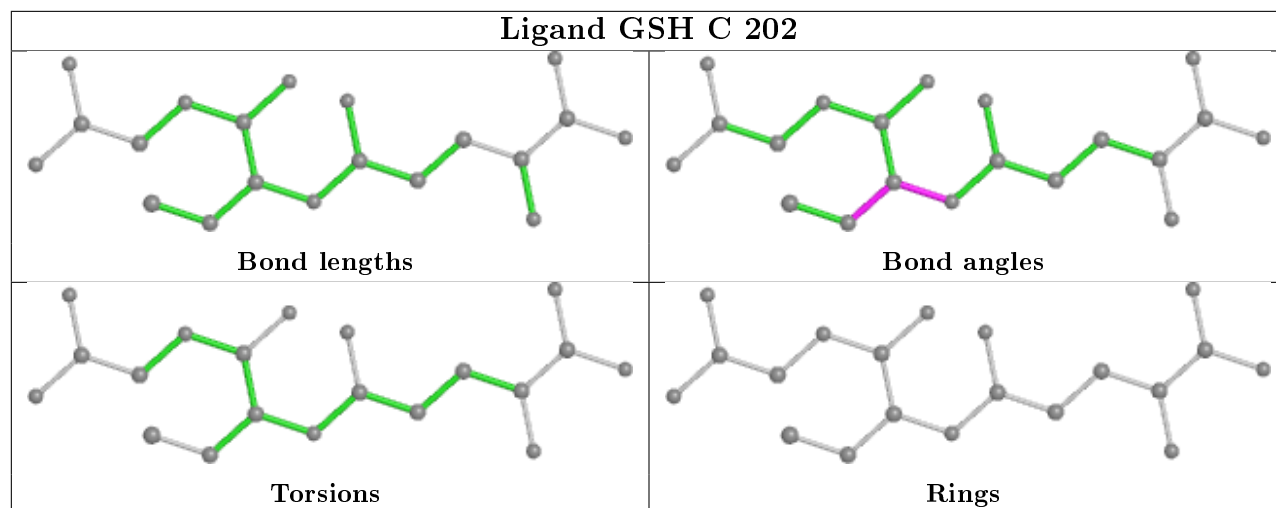
## Ligand 93C B 203



## Ligand GSH D 301







## 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, 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	198/198 (100%)	0.28	1 (0%) 91 93	6, 13, 30, 39	0
1	B	198/198 (100%)	0.98	33 (16%) 1 2	9, 22, 60, 94	0
1	C	198/198 (100%)	1.12	34 (17%) 1 2	9, 24, 58, 103	0
1	D	198/198 (100%)	0.33	3 (1%) 73 80	6, 13, 33, 40	0
All	All	792/792 (100%)	0.68	71 (8%) 9 11	6, 18, 47, 103	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	111	VAL	20.0
1	B	108	LYS	9.9
1	B	111	VAL	8.8
1	B	107	LYS	8.7
1	C	112	LYS	8.2
1	C	110	ASP	6.9
1	B	101	CYS	6.6
1	B	109	GLN	6.4
1	C	108	LYS	6.4
1	C	109	GLN	6.2
1	C	107	LYS	5.7
1	C	39	TRP	5.7
1	B	112	LYS	5.3
1	B	115	MET	5.2
1	C	101	CYS	5.2
1	B	39	TRP	5.2
1	B	102	PHE	5.0
1	B	104	TRP	4.8
1	B	103	PRO	4.7
1	B	113	GLU	4.3
1	B	110	ASP	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	42	ILE	4.2
1	C	45	THR	4.2
1	C	114	GLN	4.1
1	B	42	ILE	4.1
1	C	113	GLU	3.9
1	C	103	PRO	3.8
1	C	115	MET	3.7
1	C	104	TRP	3.7
1	C	3	ASN	3.6
1	C	193	ARG	3.5
1	B	40	PRO	3.5
1	B	106	GLU	3.5
1	B	45	THR	3.5
1	B	38	ASP	3.3
1	C	40	PRO	3.3
1	B	114	GLN	3.2
1	C	46	LEU	3.1
1	C	44	SER	3.1
1	B	116	PHE	3.1
1	B	117	ASN	2.9
1	B	122	TYR	2.9
1	D	37	ALA	2.9
1	B	3	ASN	2.9
1	B	98	PHE	2.8
1	B	35	GLU	2.8
1	C	38	ASP	2.7
1	B	44	SER	2.7
1	B	199	LEU	2.6
1	D	36	GLN	2.5
1	C	196	GLN	2.5
1	C	144	ASN	2.4
1	B	120	LEU	2.4
1	C	2	PRO	2.4
1	B	105	ALA	2.4
1	B	34	ILE	2.3
1	C	28	GLN	2.3
1	C	192	LYS	2.3
1	C	36	GLN	2.2
1	C	195	PRO	2.2
1	B	118	GLU	2.2
1	C	122	TYR	2.1
1	D	42	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	41	GLU	2.1
1	B	193	ARG	2.1
1	C	60	THR	2.1
1	C	102	PHE	2.0
1	A	42	ILE	2.0
1	C	37	ALA	2.0
1	B	41	GLU	2.0
1	C	116	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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	93C	B	203	27/27	0.65	0.27	48,63,79,80	0
3	93C	C	203	27/27	0.74	0.28	36,53,92,95	0
4	GOL	D	303	6/6	0.80	0.24	16,19,20,23	0
2	GSH	A	301	20/20	0.81	0.28	15,26,51,52	0
2	GSH	D	301	20/20	0.83	0.23	13,28,52,57	0
2	GSH	B	202	20/20	0.85	0.19	18,32,47,47	0
4	GOL	A	304	6/6	0.86	0.15	18,19,20,20	0
2	GSH	C	202	20/20	0.86	0.20	18,32,49,51	0
4	GOL	A	303	6/6	0.89	0.13	20,21,22,22	0
3	93C	D	302	27/27	0.89	0.16	14,20,40,40	0
3	93C	A	302	27/27	0.89	0.17	12,17,33,35	0
5	MG	B	201	1/1	0.96	0.07	19,19,19,19	0
5	MG	C	201	1/1	0.98	0.03	21,21,21,21	0

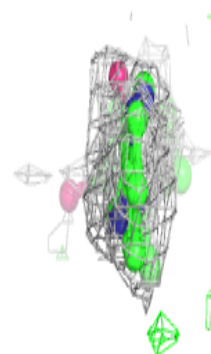
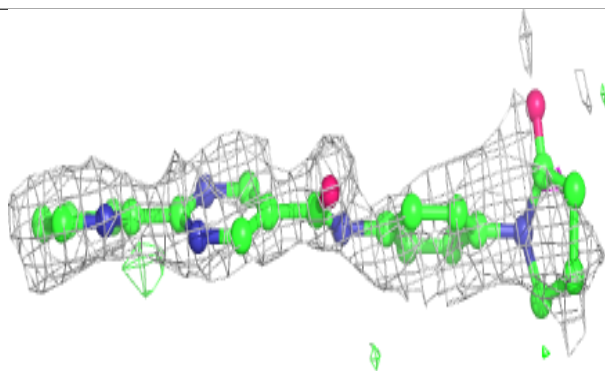
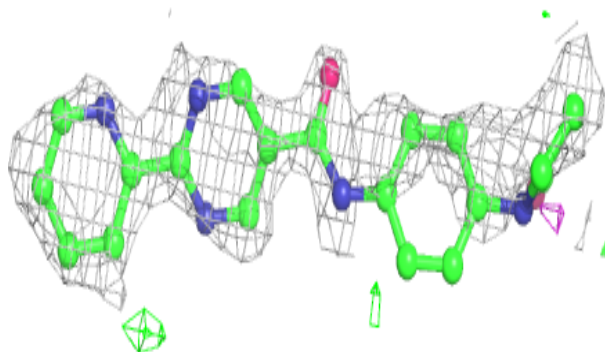
The following is a graphical depiction of the model fit to experimental electron density of all



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.

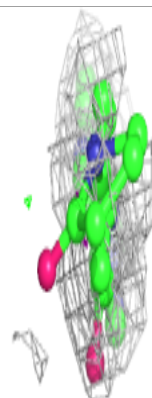
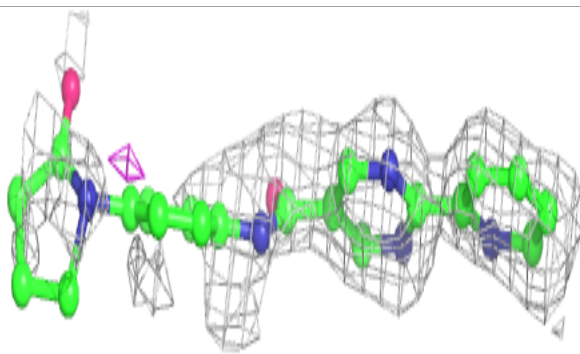
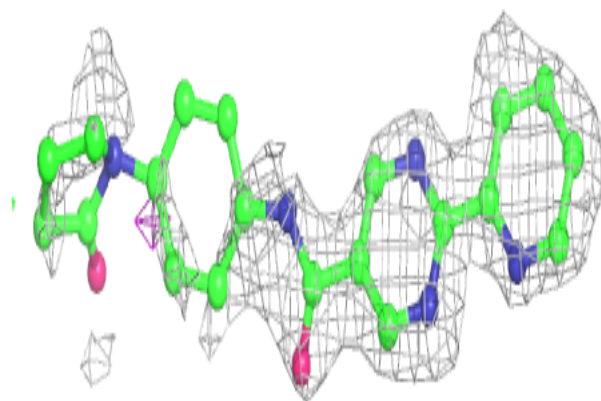
**Electron density around 93C B 203:**

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

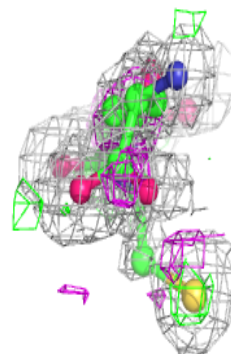
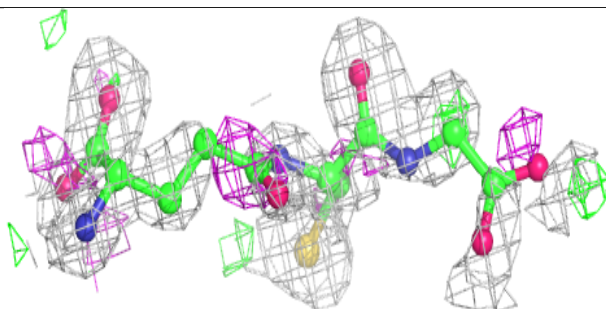
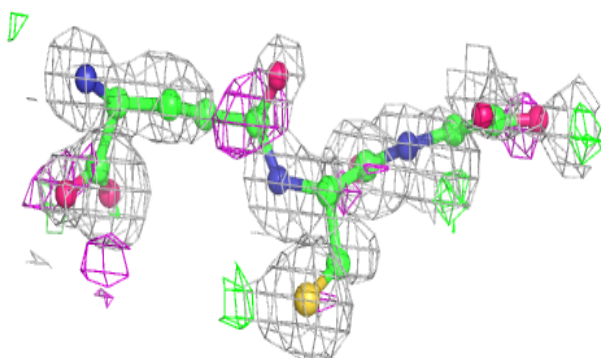


**Electron density around 93C C 203:**

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

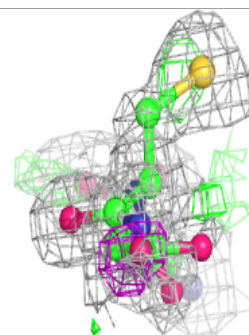
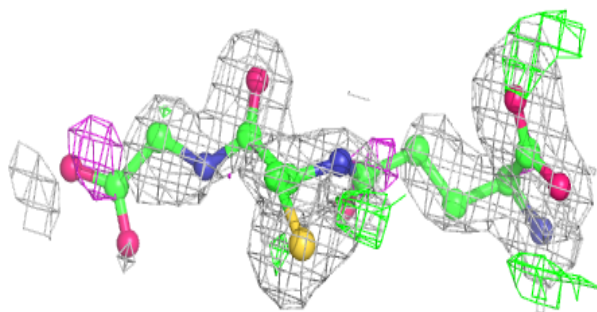
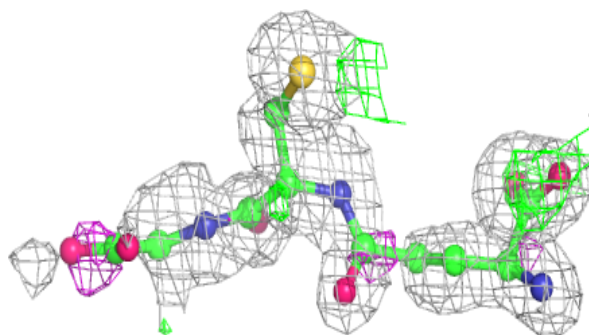
**Electron density around GSH A 301:**

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

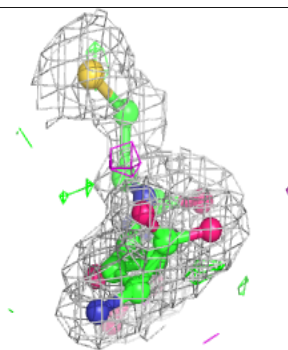
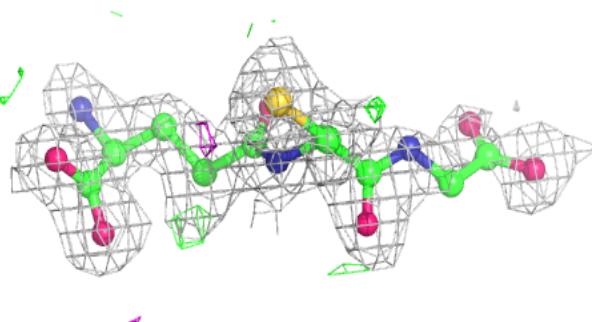
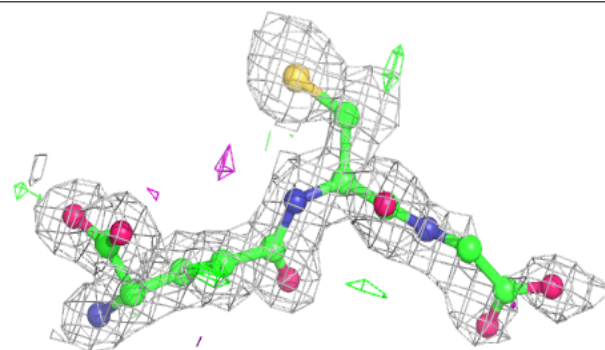


**Electron density around GSH D 301:**

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

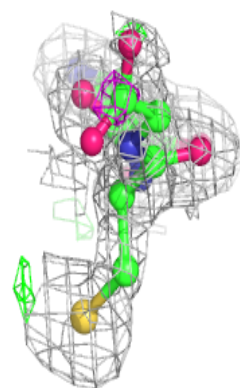
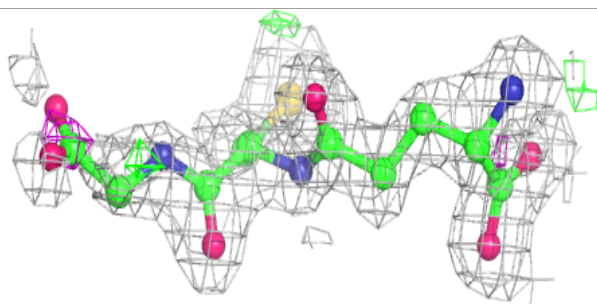
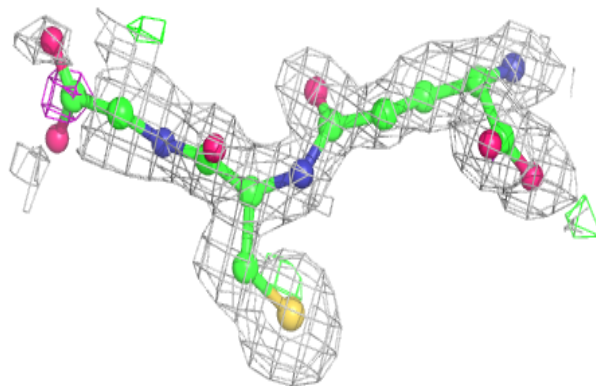
**Electron density around GSH B 202:**

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

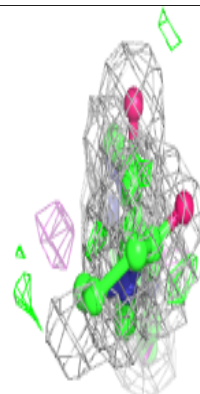
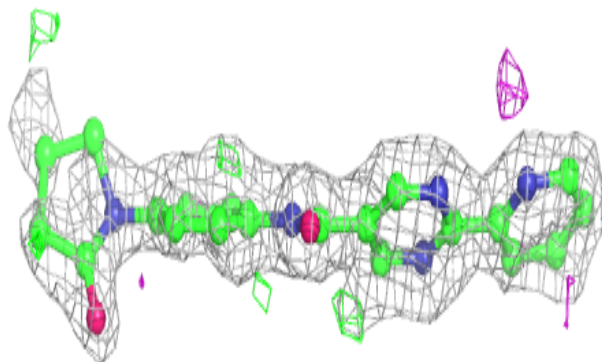
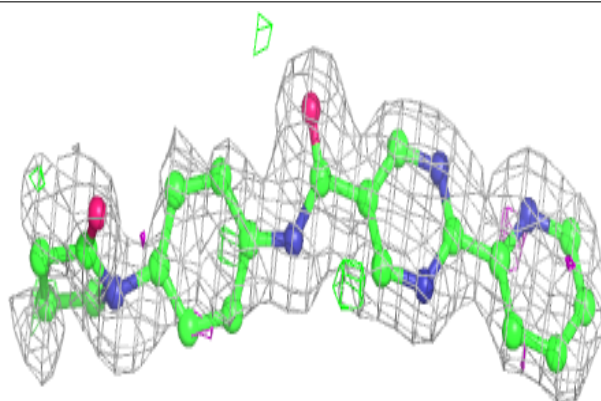


**Electron density around GSH C 202:**

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

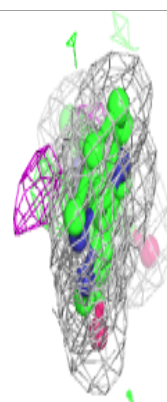
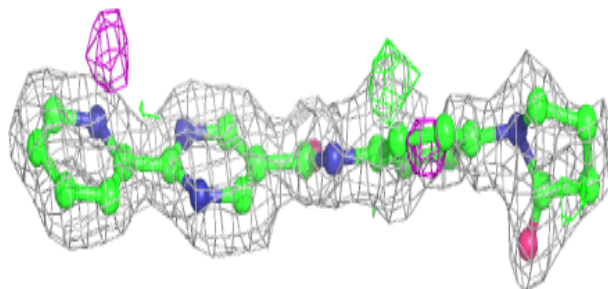
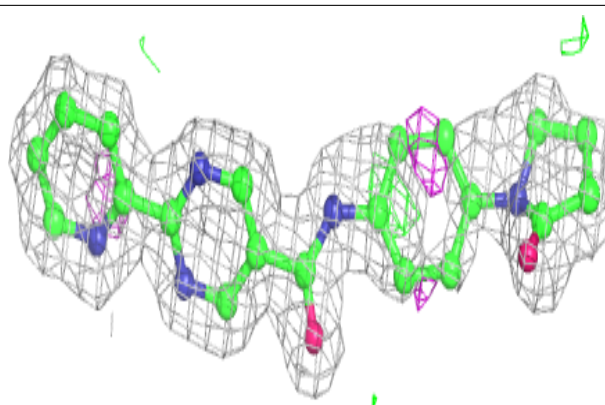
**Electron density around 93C D 302:**

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



**Electron density around 93C A 302:**

$2mF_o-DF_c$  (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.