



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 07:16 AM UTC

PDB ID : 10PW / pdb_000010pw
Title : Crystal structure of Glutathione Transferase from Shrimp *Litopenaeus vannamei* in complex with silver ions and a molecules of Glutathione binding in G-site and H-site
Authors : Escudero-Garcia, A.; Miranda-Blancas, R.; Rudino-Pinera, E.
Deposited on : 2026-01-31
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

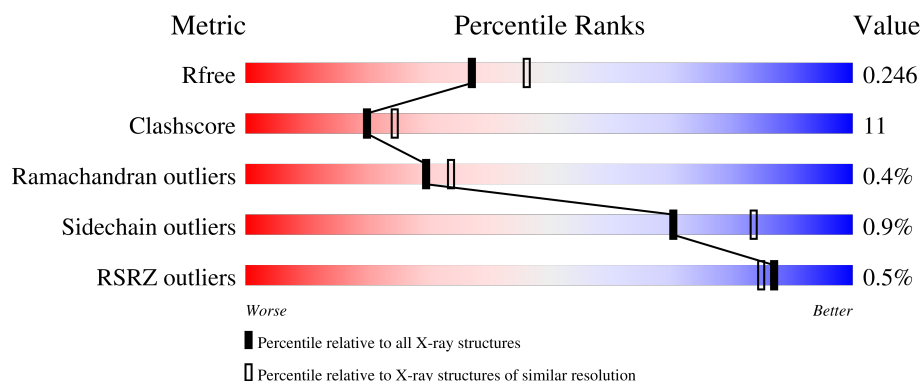
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	219	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>.</div> </div> </div>
1	B	219	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>.</div> </div> </div>
1	C	219	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
1	D	219	<div> <div></div> <div> <div></div> <div>79%</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	E	219	 81% 17% .
1	F	219	 86% 14%
1	G	219	 79% 19% .
1	H	219	 82% 16% .

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
2	GSH	A	301	-	X	X	-
2	GSH	H	301	-	-	X	-
3	TAM	A	302	-	X	X	-
5	GOL	D	303	-	-	X	-
5	GOL	D	304	-	-	X	-
6	1PE	G	303	-	-	X	-

2 Entry composition

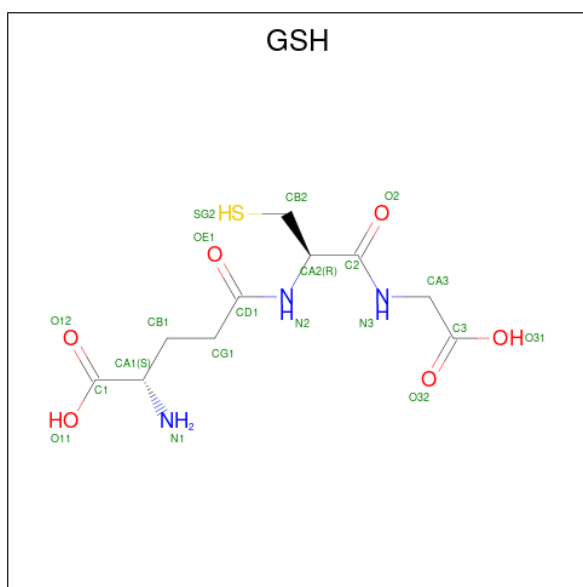
There are 7 unique types of molecules in this entry. The entry contains 16079 atoms, of which 16 are hydrogens and 0 are deuteriums.

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 transferase.

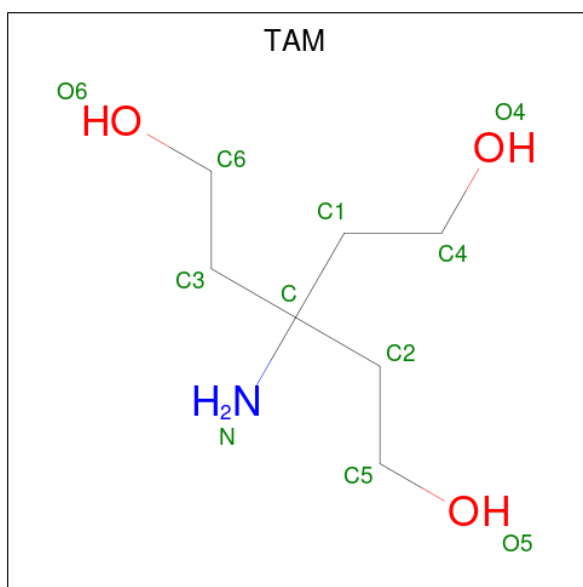
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1784	1163	288	323	10			
1	B	218	Total	C	N	O	S	0	0	0
			1792	1167	289	326	10			
1	C	219	Total	C	N	O	S	0	0	0
			1800	1172	290	327	11			
1	D	218	Total	C	N	O	S	0	1	0
			1803	1173	293	327	10			
1	E	219	Total	C	N	O	S	0	3	0
			1826	1187	294	334	11			
1	F	218	Total	C	N	O	S	0	2	0
			1810	1179	293	328	10			
1	G	219	Total	C	N	O	S	0	2	0
			1817	1182	293	331	11			
1	H	218	Total	C	N	O	S	0	1	0
			1801	1173	291	327	10			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	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	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		
2	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	G	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	H	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 4 is SILVER ION (CCD ID: AG) (formula: Ag) (labeled as "Ligand of Interest" by depositor).

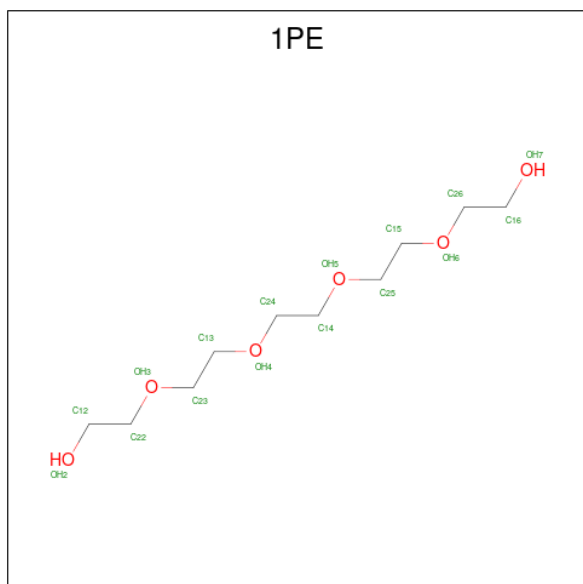
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Ag	0	0
			1	1		
4	E	1	Total	Ag	0	0
			1	1		
4	G	1	Total	Ag	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			16	10	6		

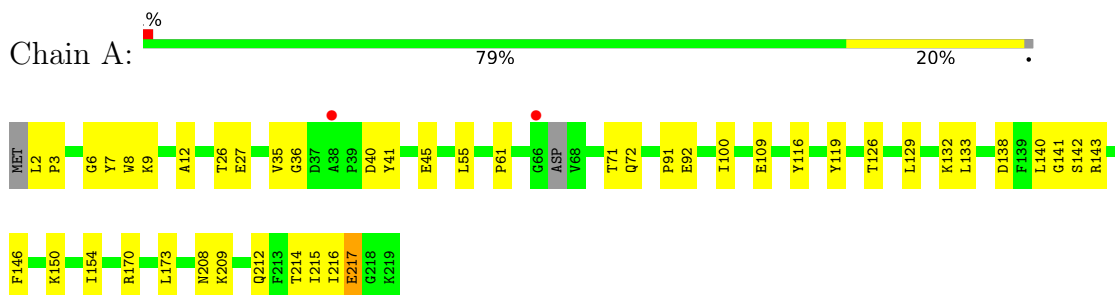
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	158	Total 158	O 158	0	0
7	B	151	Total 151	O 151	0	0
7	C	195	Total 195	O 195	0	0
7	D	171	Total 171	O 171	0	0
7	E	163	Total 163	O 163	0	0
7	F	178	Total 178	O 178	0	0
7	G	184	Total 184	O 184	0	0
7	H	188	Total 188	O 188	0	0

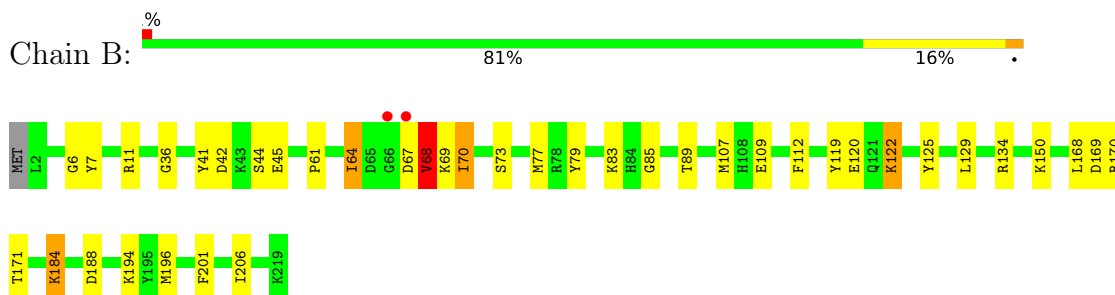
3 Residue-property plots [i](#)

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.

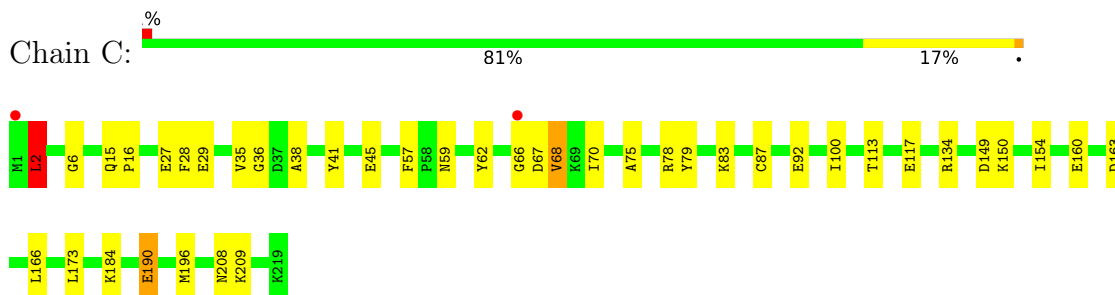
- Molecule 1: Glutathione transferase



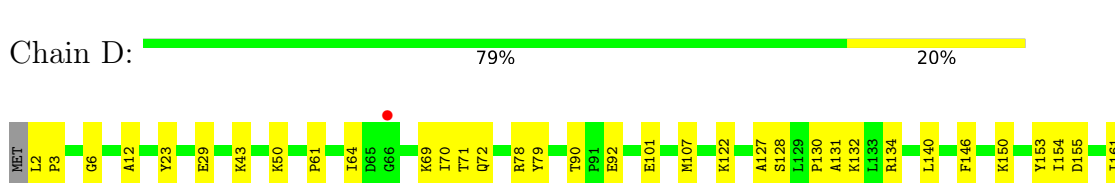
- Molecule 1: Glutathione transferase

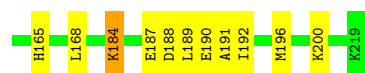


- Molecule 1: Glutathione transferase



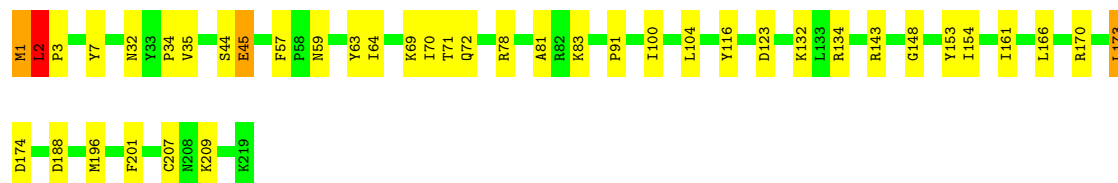
- Molecule 1: Glutathione transferase





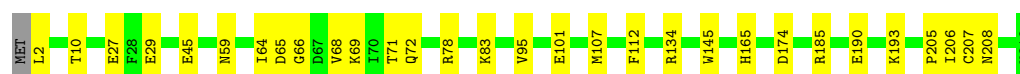
- Molecule 1: Glutathione transferase

Chain E: 81% 17% .



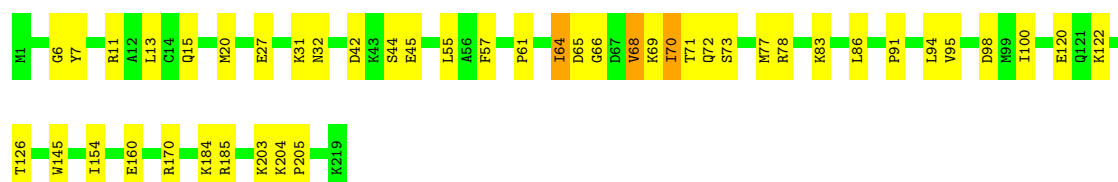
- Molecule 1: Glutathione transferase

Chain F: 86% 14% .



- Molecule 1: Glutathione transferase

Chain G: 79% 19% .



- Molecule 1: Glutathione transferase

Chain H: 82% 16% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.39Å 93.02Å 169.11Å 90.00° 90.75° 90.00°	Depositor
Resolution (Å)	56.37 – 2.20 56.37 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (56.37-2.20) 98.2 (56.37-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874)	Depositor
R, R_{free}	0.192 , 0.243 0.193 , 0.246	Depositor DCC
R_{free} test set	4472 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16079	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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 28.09 % 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 1.9581e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AG, GSH, GOL, TAM, 1PE

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	0.46	1/1832 (0.1%)	0.56	1/2472 (0.0%)
1	B	0.43	0/1841	0.64	3/2486 (0.1%)
1	C	0.49	2/1849 (0.1%)	0.61	0/2496
1	D	0.42	1/1852 (0.1%)	0.54	0/2500
1	E	0.53	1/1875 (0.1%)	0.58	0/2530
1	F	0.40	2/1859 (0.1%)	0.54	0/2508
1	G	0.60	5/1866 (0.3%)	0.64	2/2518 (0.1%)
1	H	0.38	0/1850	0.55	0/2497
All	All	0.47	12/14824 (0.1%)	0.58	6/20007 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
All	All	0	2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	70	ILE	C-O	-7.70	1.15	1.24
1	G	66	GLY	C-O	-7.66	1.15	1.24
1	D	184	LYS	C-O	-6.68	1.16	1.24
1	E	2	LEU	C-O	-6.02	1.16	1.24
1	A	217	GLU	C-O	-6.01	1.16	1.24

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	70	ILE	N-CA-C	7.55	118.77	107.75
1	B	122	LYS	N-CA-C	6.50	118.02	111.07
1	G	68	VAL	N-CA-C	6.34	117.30	108.23
1	B	67	ASP	CB-CA-C	5.77	120.54	112.11
1	A	217	GLU	N-CA-C	5.52	120.12	112.45

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	66	GLY	Mainchain
1	E	173	LEU	Mainchain

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	1784	0	1765	49	0
1	B	1792	0	1770	31	0
1	C	1800	0	1782	42	0
1	D	1803	0	1782	49	0
1	E	1826	0	1802	34	0
1	F	1810	0	1794	29	0
1	G	1817	0	1797	44	0
1	H	1801	0	1782	42	0
2	A	20	0	15	15	0
2	B	40	0	30	3	0
2	C	20	0	15	2	0
2	D	20	0	15	1	0
2	E	20	0	15	0	0
2	F	40	0	30	6	0
2	G	20	0	15	0	0
2	H	20	0	15	7	0
3	A	11	0	17	14	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	D	12	16	15	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	16	0	22	8	0
7	A	158	0	0	13	0
7	B	151	0	0	10	0
7	C	195	0	0	19	1
7	D	171	0	0	20	3
7	E	163	0	0	16	3
7	F	178	0	0	15	1
7	G	184	0	0	17	1
7	H	188	0	0	22	1
All	All	16063	16	14478	333	5

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.

The worst 5 of 333 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:209:LYS:HE3	7:C:403:HOH:O	1.16	1.25
1:A:143:ARG:NH1	3:A:302:TAM:H21	1.55	1.21
1:H:78:ARG:NH1	7:H:403:HOH:O	1.75	1.18
1:H:68:VAL:HG23	7:H:410:HOH:O	1.46	1.16
1:A:208:ASN:ND2	2:A:301:GSH:HA32	1.58	1.15

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:489:HOH:O	7:E:515:HOH:O[1_445]	1.62	0.58
7:D:507:HOH:O	7:H:455:HOH:O[2_545]	2.04	0.16
7:C:569:HOH:O	7:G:575:HOH:O[2_645]	2.09	0.11
7:D:539:HOH:O	7:E:558:HOH:O[1_545]	2.15	0.05
7:E:511:HOH:O	7:F:449:HOH:O[1_455]	2.16	0.04

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	213/219 (97%)	206 (97%)	6 (3%)	1 (0%)	24	27
1	B	216/219 (99%)	207 (96%)	8 (4%)	1 (0%)	24	27
1	C	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
1	D	217/219 (99%)	210 (97%)	6 (3%)	1 (0%)	24	27
1	E	220/219 (100%)	211 (96%)	6 (3%)	3 (1%)	9	7
1	F	218/219 (100%)	211 (97%)	7 (3%)	0	100	100
1	G	219/219 (100%)	211 (96%)	8 (4%)	0	100	100
1	H	217/219 (99%)	209 (96%)	6 (3%)	2 (1%)	14	14
All	All	1737/1752 (99%)	1674 (96%)	55 (3%)	8 (0%)	30	27

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	VAL
1	E	174[A]	ASP
1	E	174[B]	ASP
1	H	67	ASP
1	D	12	ALA

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	189/191 (99%)	188 (100%)	1 (0%)	81	90
1	B	190/191 (100%)	186 (98%)	4 (2%)	47	63
1	C	191/191 (100%)	188 (98%)	3 (2%)	55	71
1	D	191/191 (100%)	190 (100%)	1 (0%)	81	90
1	E	194/191 (102%)	190 (98%)	4 (2%)	47	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	192/191 (100%)	192 (100%)	0	100	100
1	G	193/191 (101%)	192 (100%)	1 (0%)	81	90
1	H	191/191 (100%)	190 (100%)	1 (0%)	81	90
All	All	1531/1528 (100%)	1516 (99%)	15 (1%)	70	81

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	190	GLU
1	G	86	LEU
1	D	184	LYS
1	H	78	ARG
1	E	45[A]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	118	HIS
1	H	180	GLN
1	C	135	GLN
1	E	118	HIS
1	E	121	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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
5	GOL	D	303	-	5,5,5	0.25	0	5,5,5	0.27	0
2	GSH	H	301	-	18,19,19	0.77	0	21,24,24	0.97	2 (9%)
2	GSH	F	302	-	18,19,19	0.94	1 (5%)	21,24,24	1.43	3 (14%)
2	GSH	B	302	-	18,19,19	2.09	3 (16%)	21,24,24	2.13	8 (38%)
2	GSH	C	301	-	18,19,19	2.16	4 (22%)	21,24,24	1.25	2 (9%)
2	GSH	E	302	-	18,19,19	2.07	4 (22%)	21,24,24	1.32	2 (9%)
2	GSH	D	302	-	18,19,19	2.06	4 (22%)	21,24,24	1.32	2 (9%)
3	TAM	A	302	-	10,10,10	2.33	2 (20%)	12,12,12	3.82	8 (66%)
6	1PE	G	303	-	15,15,15	0.71	0	14,14,14	1.18	2 (14%)
2	GSH	F	301	-	18,19,19	1.72	5 (27%)	21,24,24	1.85	4 (19%)
2	GSH	G	302	-	18,19,19	0.84	2 (11%)	21,24,24	0.80	0
2	GSH	B	301	-	18,19,19	2.03	3 (16%)	21,24,24	1.32	3 (14%)
5	GOL	D	304	-	5,5,5	1.18	1 (20%)	5,5,5	0.79	0
2	GSH	A	301	-	18,19,19	1.86	5 (27%)	21,24,24	2.16	9 (42%)

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
5	GOL	D	303	-	-	0/4/4/4	-
2	GSH	H	301	-	-	14/24/24/24	-
2	GSH	F	302	-	-	12/24/24/24	-
2	GSH	B	302	-	-	9/24/24/24	-
2	GSH	C	301	-	-	2/24/24/24	-
2	GSH	E	302	-	-	0/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	D	302	-	-	2/24/24/24	-
3	TAM	A	302	-	-	8/12/12/12	-
6	1PE	G	303	-	-	8/13/13/13	-
2	GSH	F	301	-	-	5/24/24/24	-
2	GSH	G	302	-	-	3/24/24/24	-
2	GSH	B	301	-	-	2/24/24/24	-
5	GOL	D	304	-	-	2/4/4/4	-
2	GSH	A	301	-	-	19/24/24/24	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	GSH	CD1-N2	5.91	1.46	1.34
3	A	302	TAM	C2-C	5.72	1.61	1.53
2	D	302	GSH	CD1-N2	5.60	1.45	1.34
2	B	301	GSH	CD1-N2	5.59	1.45	1.34
2	C	301	GSH	C2-N3	5.58	1.46	1.33

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	TAM	C5-C2-C	8.53	126.03	115.97
2	B	302	GSH	CA2-CB2-SG2	-4.75	108.81	114.16
2	F	301	GSH	CA2-CB2-SG2	4.64	119.39	114.16
3	A	302	TAM	C3-C-C2	4.52	118.48	110.50
3	A	302	TAM	C2-C-N	4.30	119.02	108.22

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

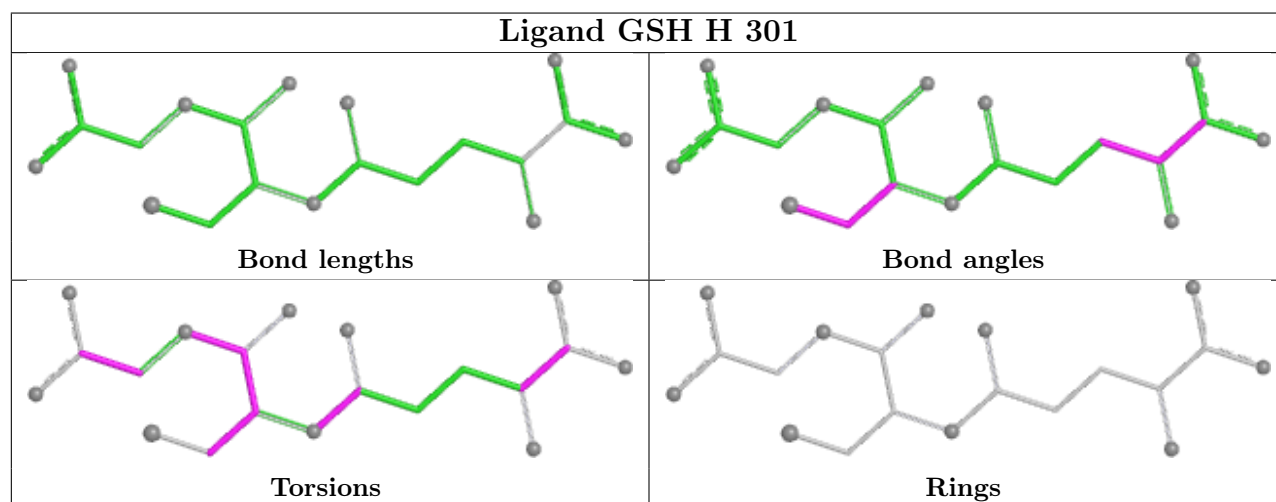
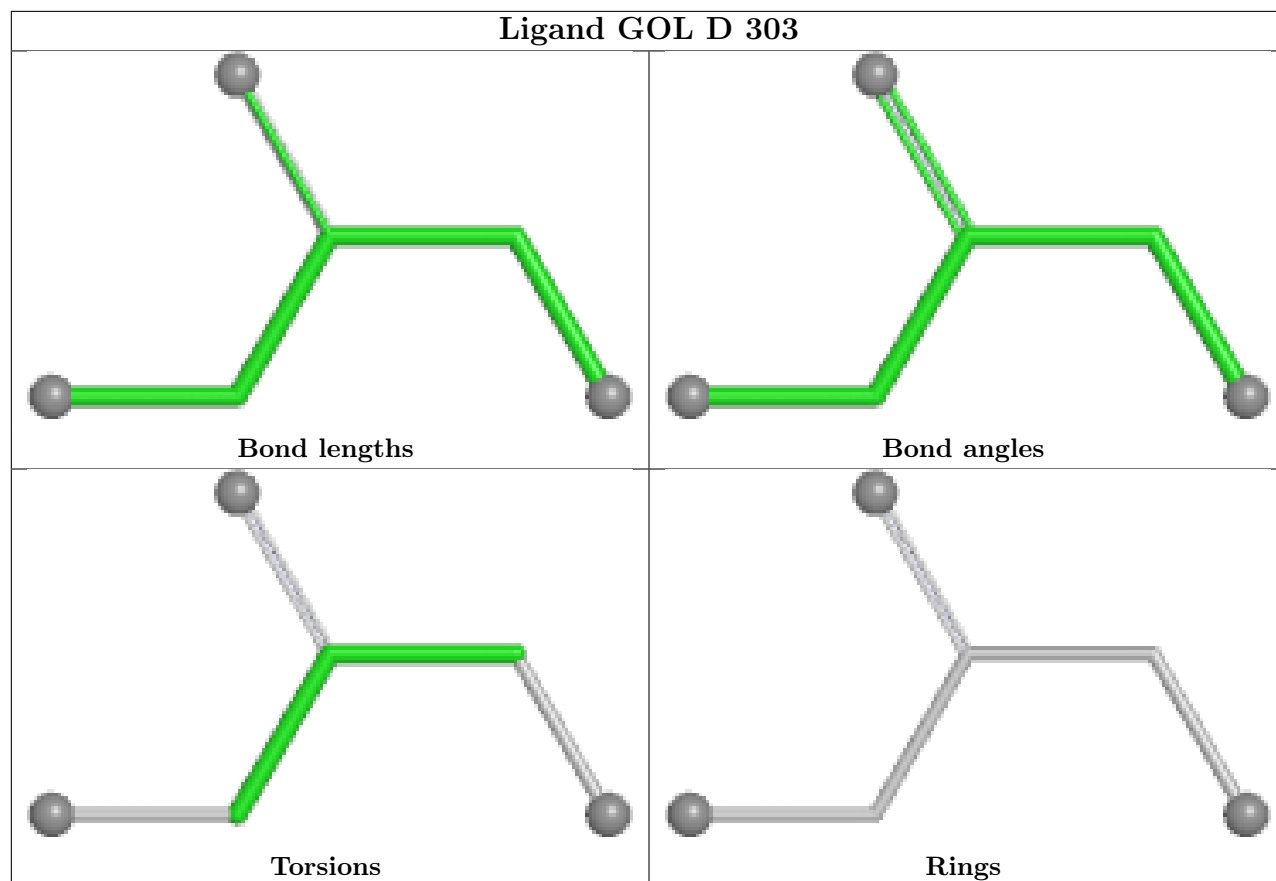
Mol	Chain	Res	Type	Atoms
2	A	301	GSH	N1-CA1-CB1-CG1
2	A	301	GSH	N2-CA2-CB2-SG2
2	A	301	GSH	C2-CA2-CB2-SG2
2	A	301	GSH	CA2-C2-N3-CA3
2	A	301	GSH	O2-C2-N3-CA3

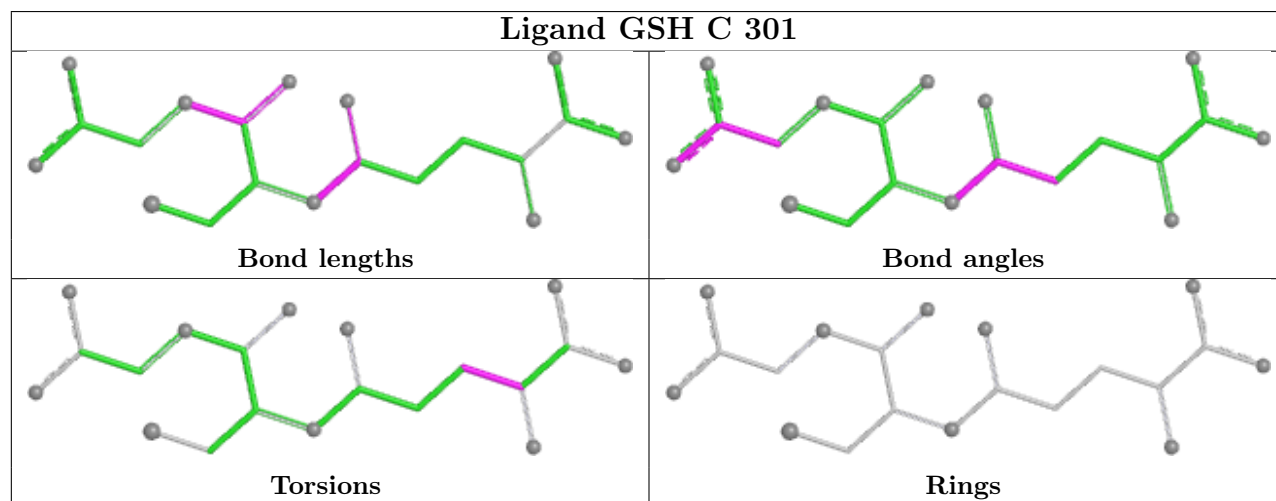
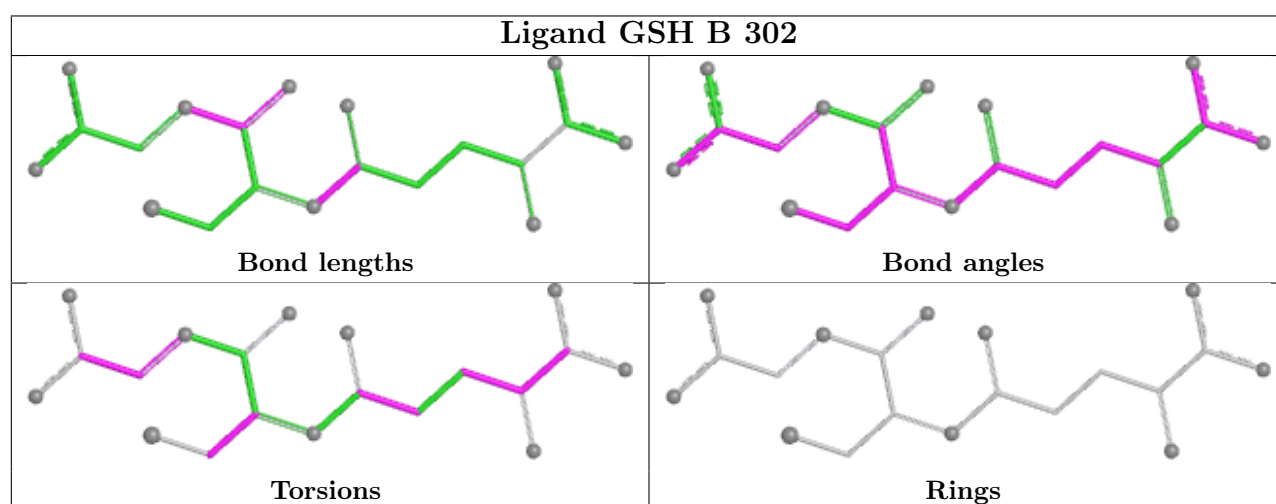
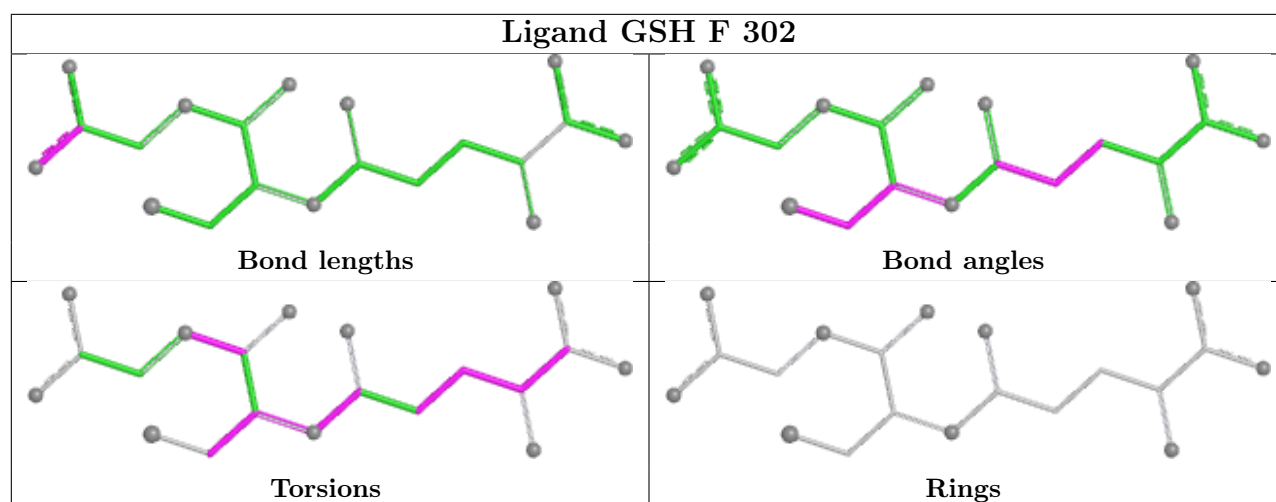
There are no ring outliers.

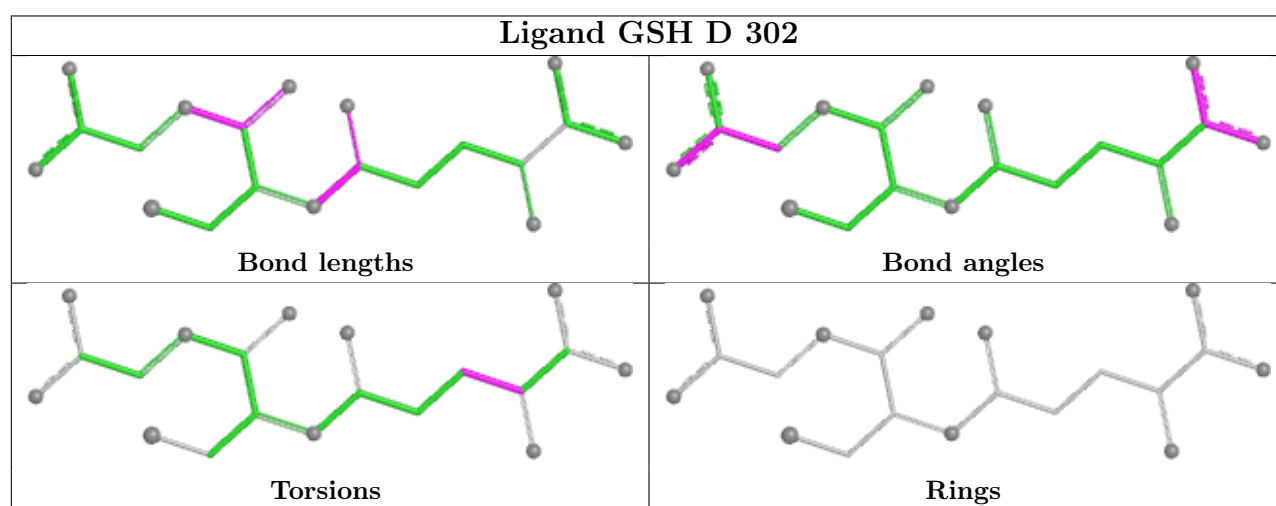
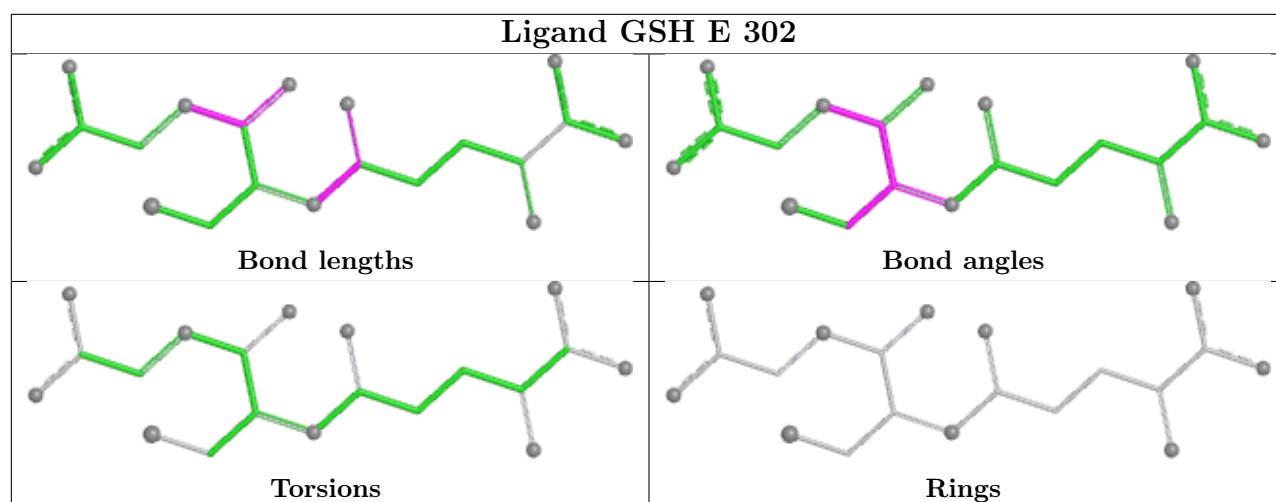
12 monomers are involved in 74 short contacts:

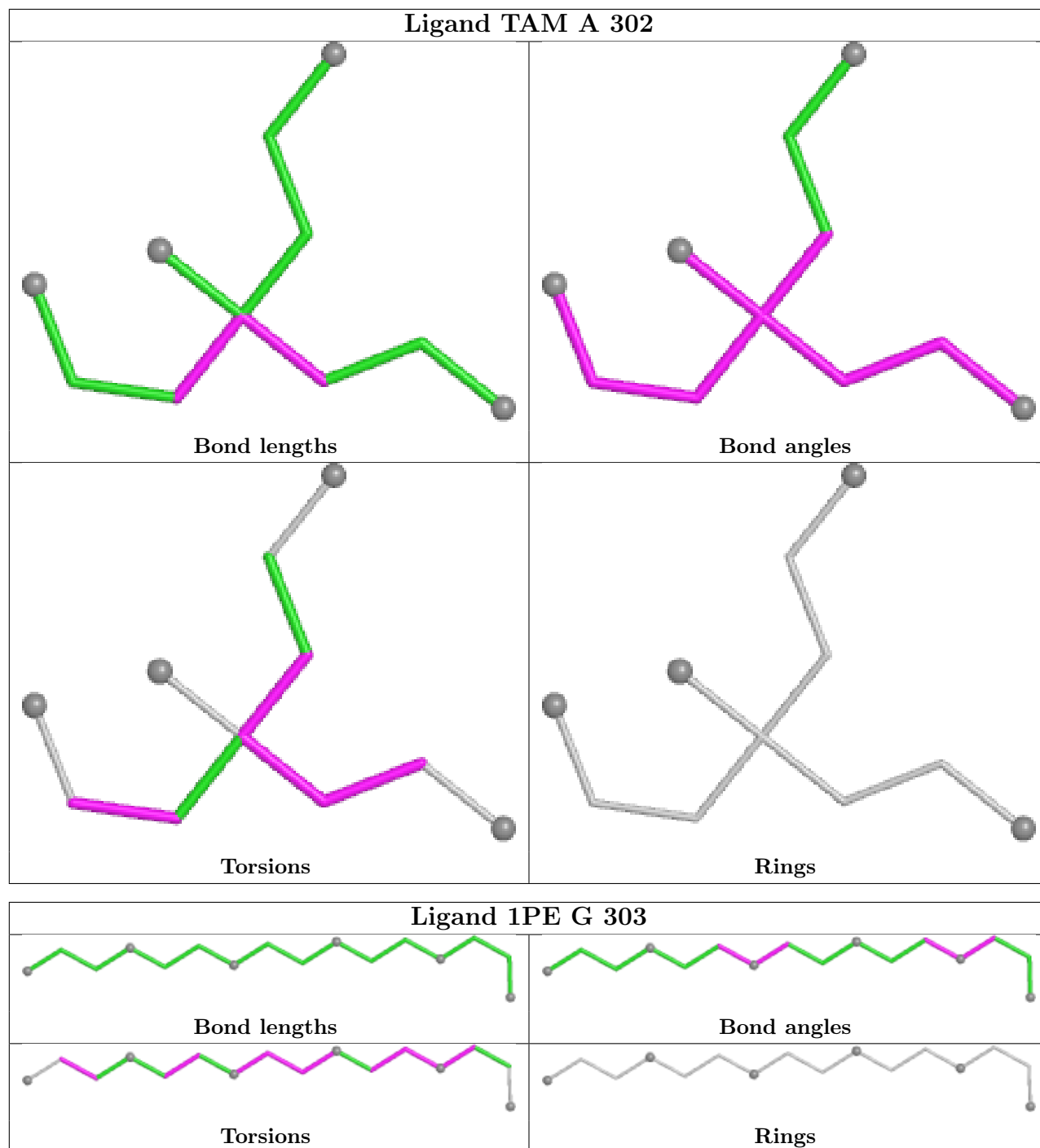
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	303	GOL	12	0
2	H	301	GSH	7	0
2	F	302	GSH	4	0
2	B	302	GSH	2	0
2	C	301	GSH	2	0
2	D	302	GSH	1	0
3	A	302	TAM	14	0
6	G	303	1PE	8	0
2	F	301	GSH	4	0
2	B	301	GSH	2	0
5	D	304	GOL	6	0
2	A	301	GSH	15	0

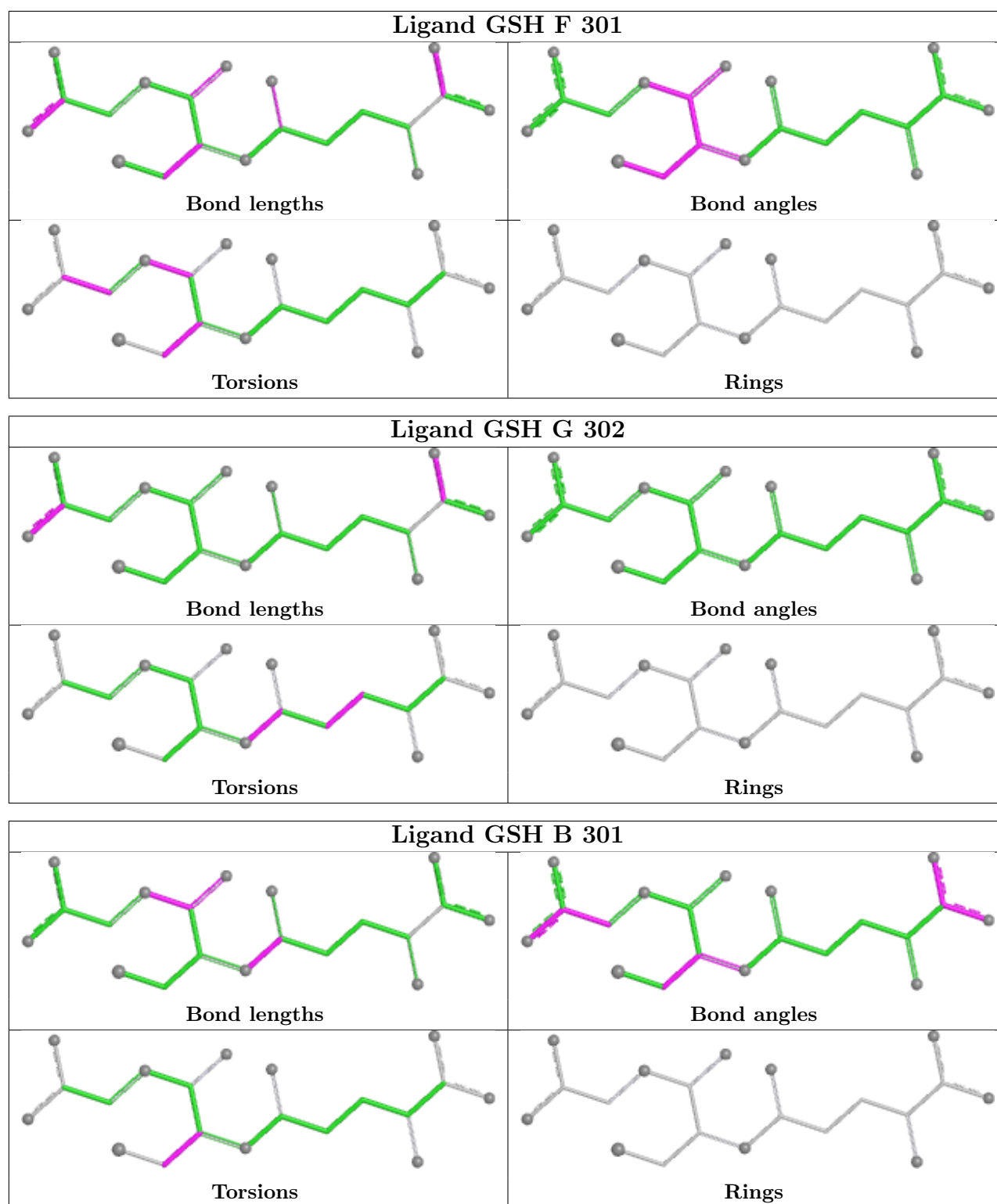
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

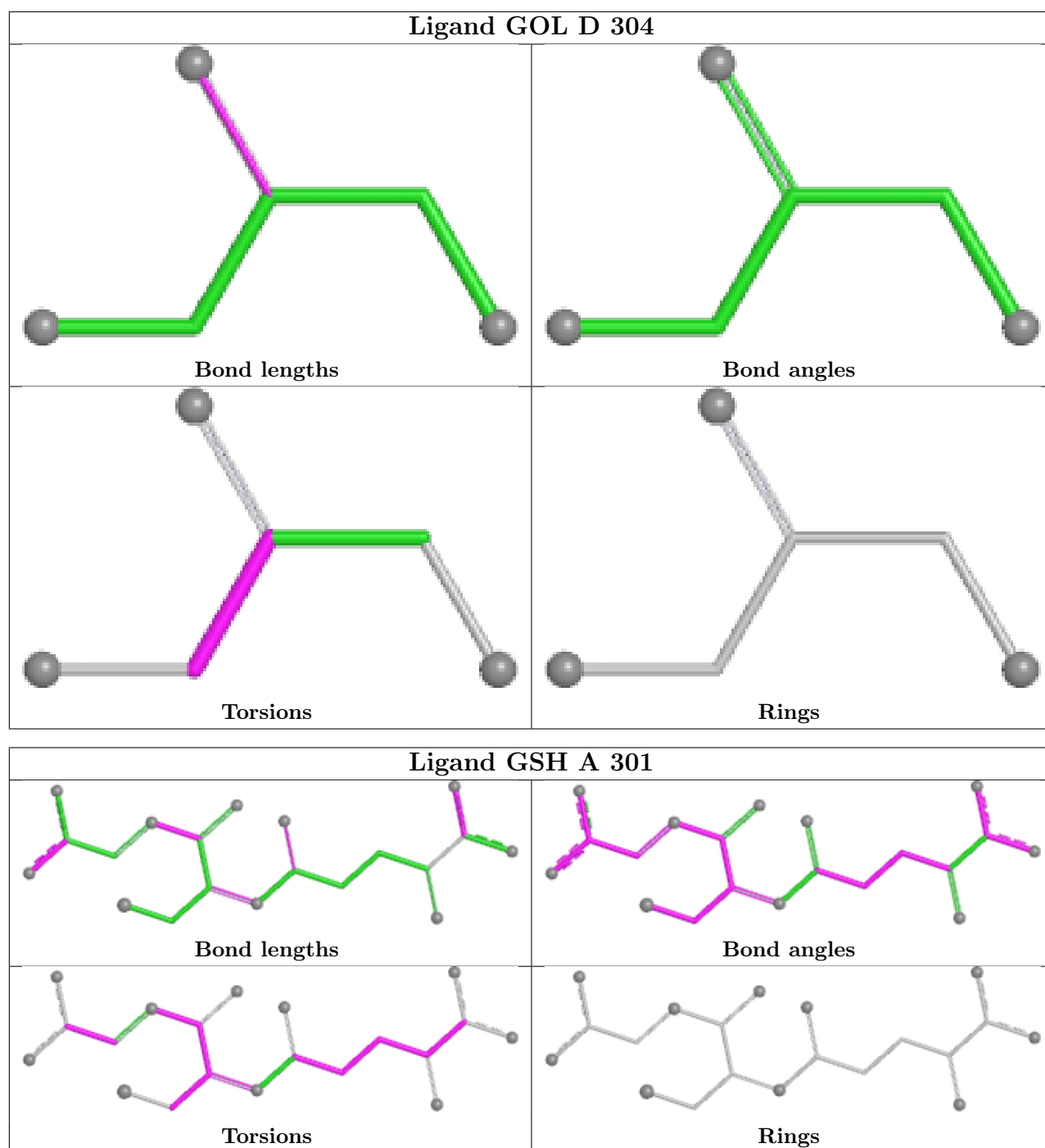












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/219 (99%)	-0.37	2 (0%) 81 79	5, 13, 32, 50	0
1	B	218/219 (99%)	-0.29	2 (0%) 81 79	5, 16, 28, 44	0
1	C	219/219 (100%)	-0.43	2 (0%) 81 79	4, 12, 27, 43	0
1	D	218/219 (99%)	-0.47	1 (0%) 87 85	4, 11, 24, 34	1 (0%)
1	E	219/219 (100%)	-0.46	0 100 100	5, 12, 27, 34	3 (1%)
1	F	218/219 (99%)	-0.46	0 100 100	4, 12, 28, 35	2 (0%)
1	G	219/219 (100%)	-0.41	0 100 100	6, 13, 27, 38	2 (0%)
1	H	218/219 (99%)	-0.44	1 (0%) 87 85	5, 12, 26, 50	1 (0%)
All	All	1746/1752 (99%)	-0.42	8 (0%) 87 85	4, 13, 28, 50	9 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	67	ASP	4.3
1	C	1	MET	3.1
1	B	66	GLY	2.9
1	C	66	GLY	2.6
1	H	78	ARG	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

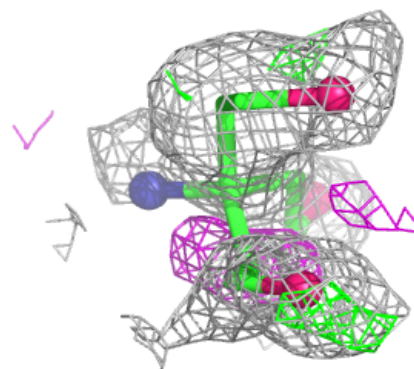
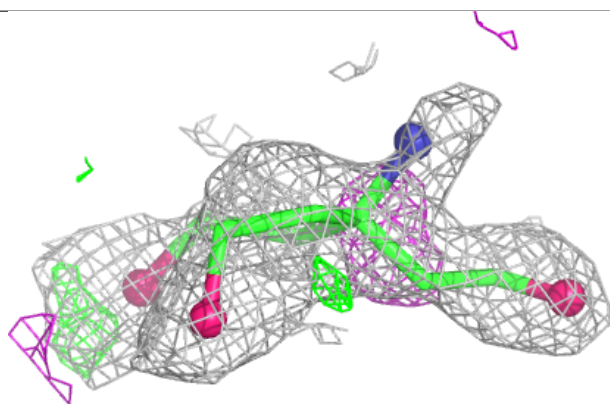
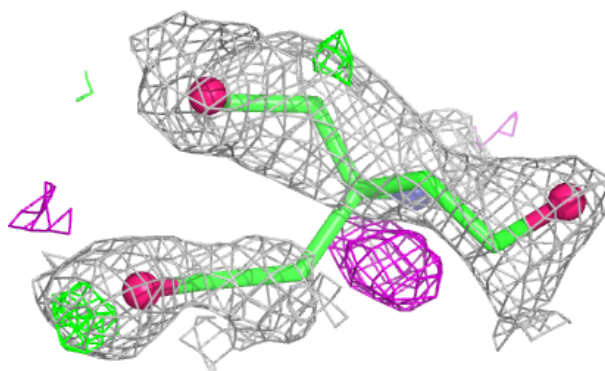
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TAM	A	302	11/11	0.69	0.18	21,27,40,41	0
2	GSH	F	302	20/20	0.71	0.18	31,46,58,62	0
2	GSH	H	301	20/20	0.72	0.19	21,50,62,70	0
2	GSH	B	302	20/20	0.76	0.15	24,46,55,57	0
2	GSH	A	301	20/20	0.79	0.14	26,36,57,60	0
5	GOL	D	303	6/6	0.80	0.27	11,31,51,58	0
5	GOL	D	304	6/6	0.85	0.16	20,30,43,52	0
2	GSH	G	302	20/20	0.88	0.11	15,29,42,51	0
2	GSH	F	301	20/20	0.90	0.08	17,26,36,39	0
6	1PE	G	303	16/16	0.90	0.09	13,23,31,33	0
2	GSH	E	302	20/20	0.91	0.09	4,17,32,38	0
2	GSH	C	301	20/20	0.93	0.07	11,20,33,40	0
2	GSH	D	302	20/20	0.94	0.07	9,22,32,34	0
2	GSH	B	301	20/20	0.94	0.07	9,23,32,45	0
4	AG	E	301	1/1	0.95	0.06	37,37,37,37	1
4	AG	D	301	1/1	0.96	0.06	68,68,68,68	1
4	AG	G	301	1/1	0.97	0.04	43,43,43,43	1

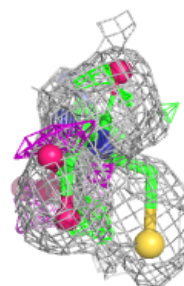
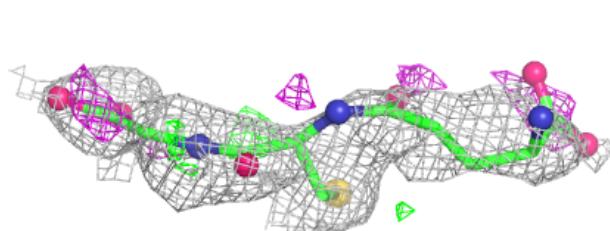
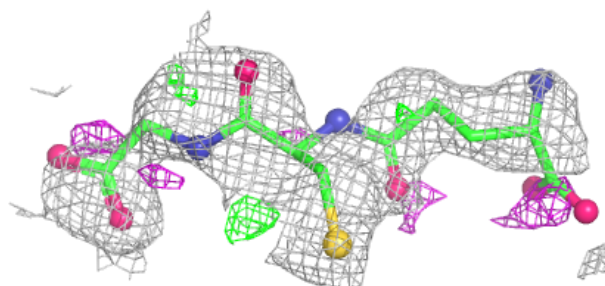
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TAM 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)

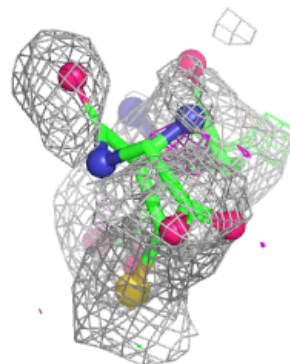
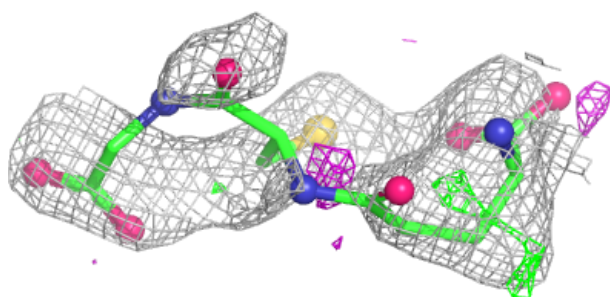
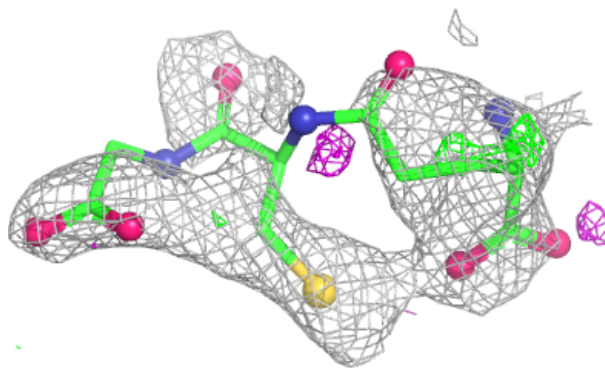
**Electron density around GSH F 302:**

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

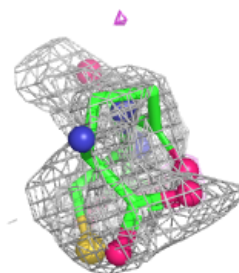
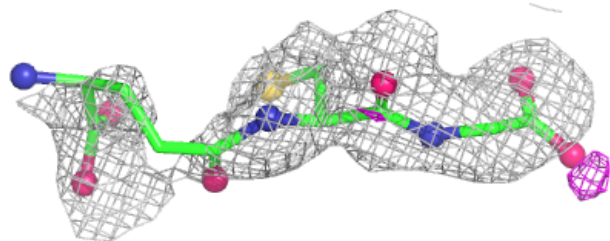
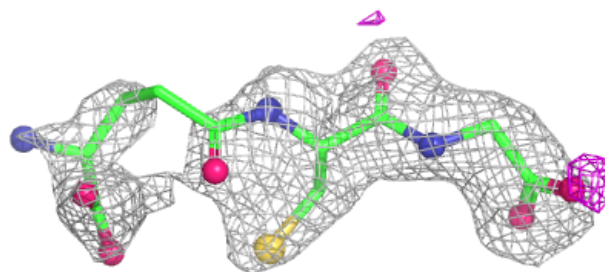


Electron density around GSH H 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

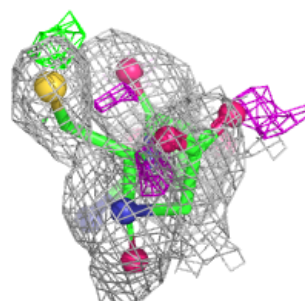
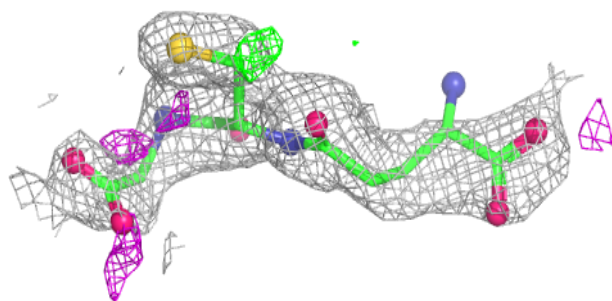
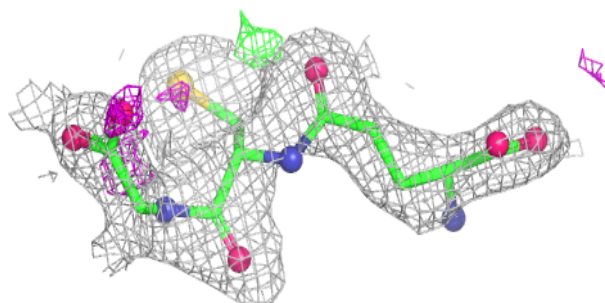
**Electron density around GSH B 302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

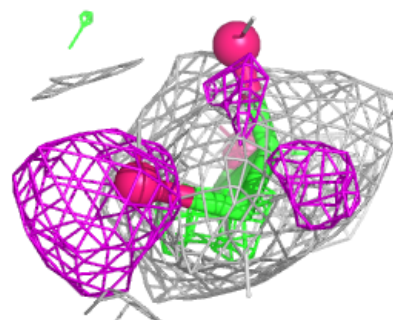
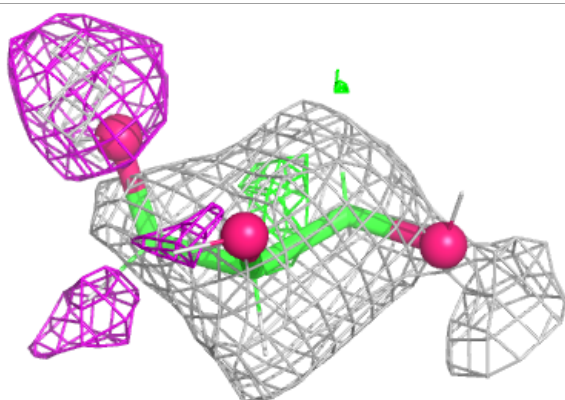
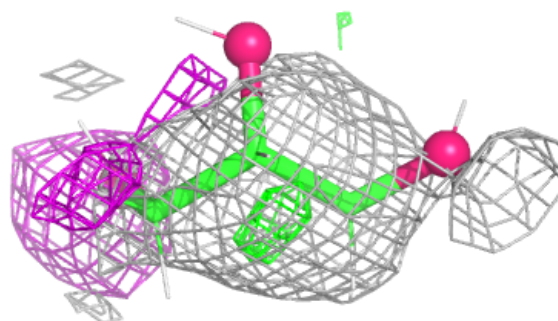


Electron density around GSH A 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

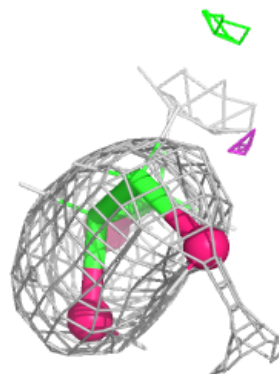
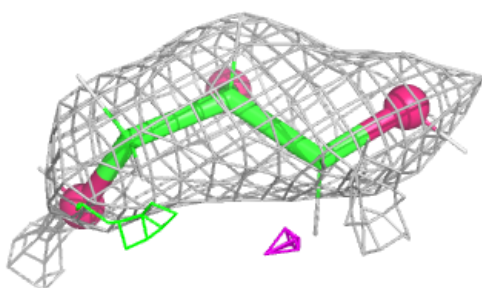
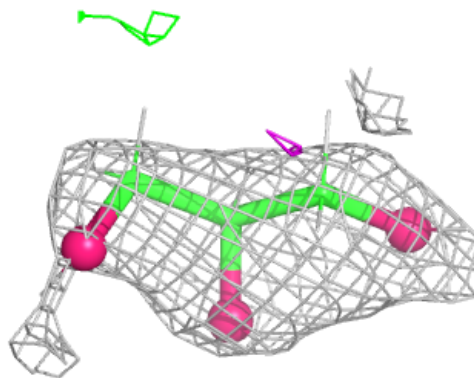
**Electron density around GOL D 303:**

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and green (positive)

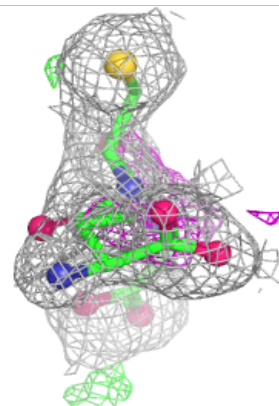
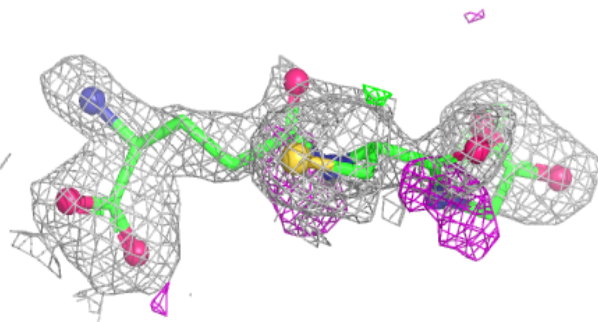
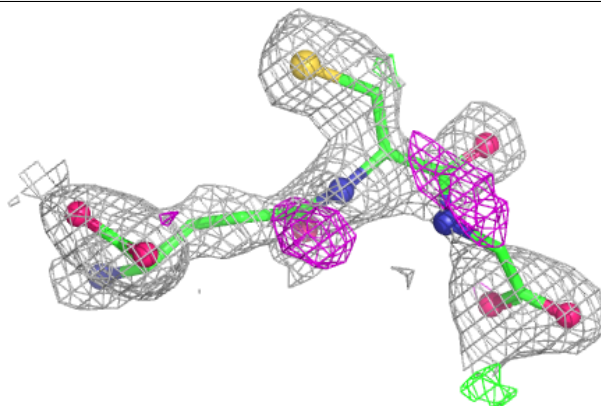


Electron density around GOL D 304:

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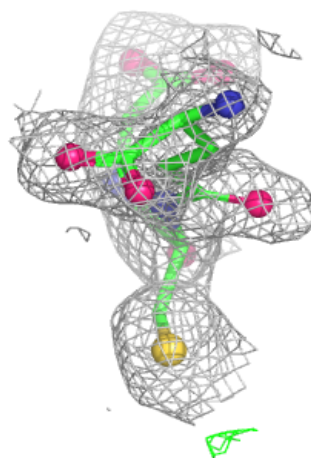
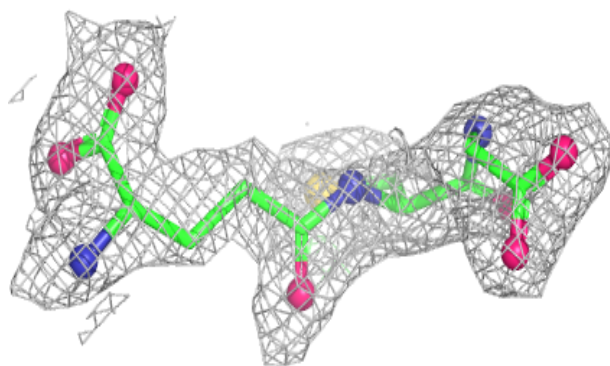
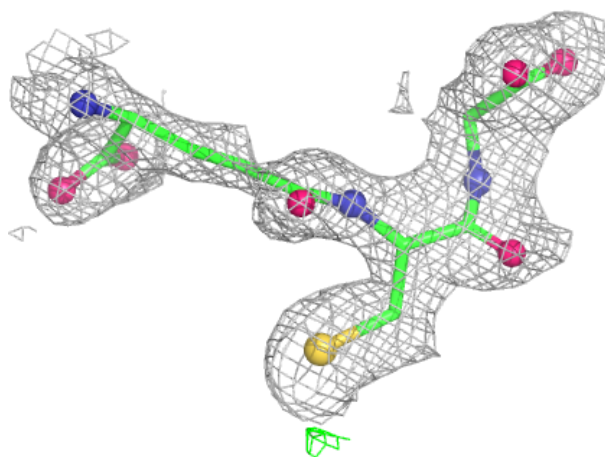
**Electron density around GSH G 302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



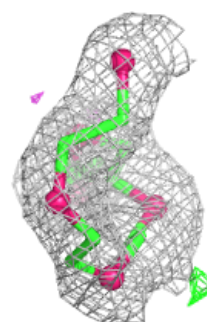
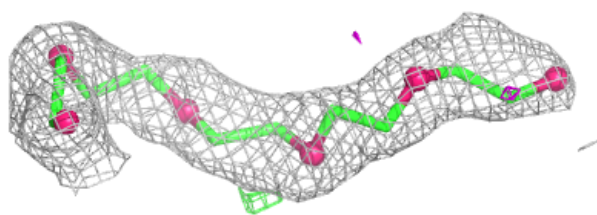
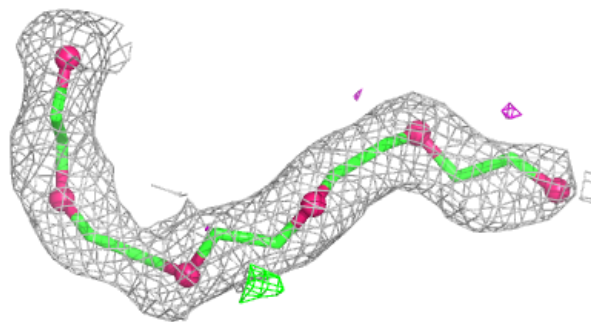
Electron density around GSH F 301:

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



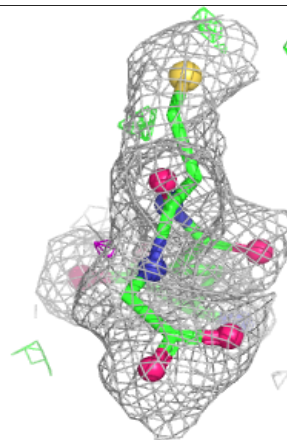
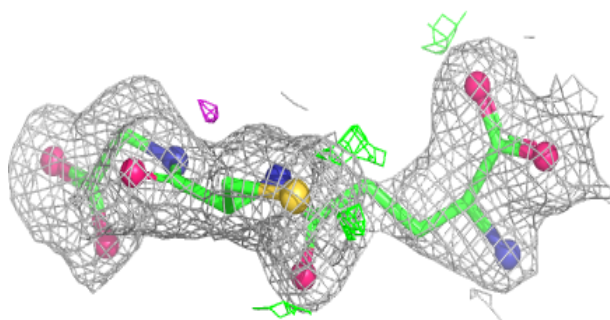
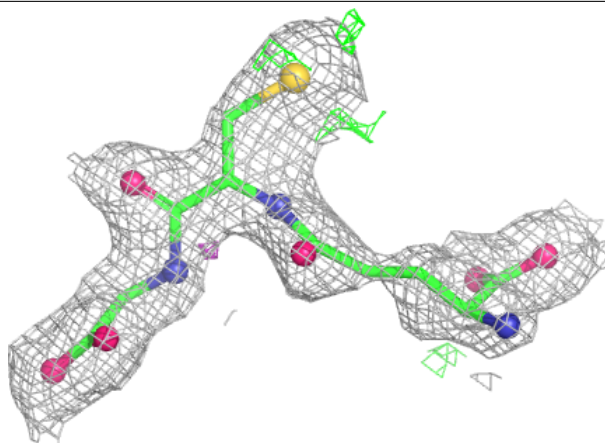
Electron density around 1PE G 303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

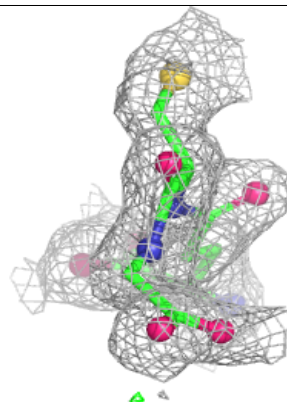
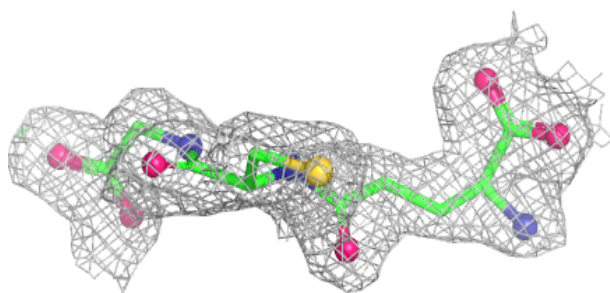
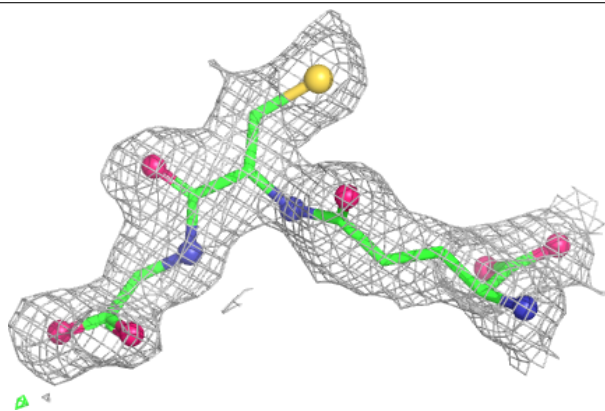


Electron density around GSH E 302:

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and green (positive)

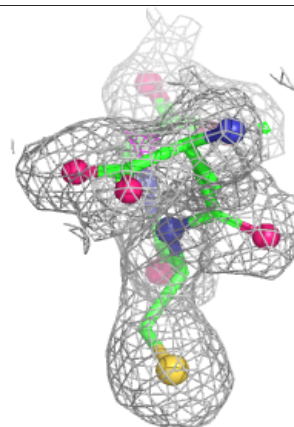
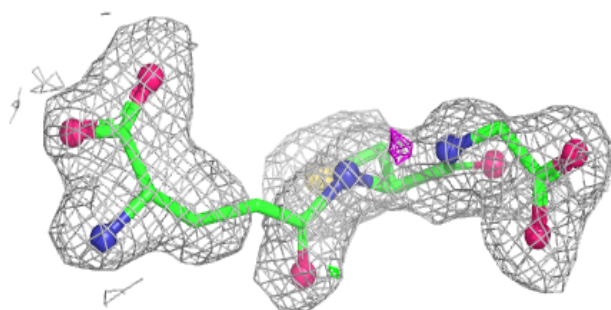
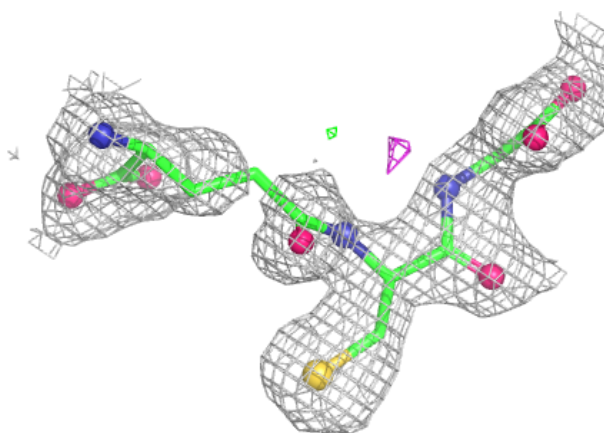
**Electron density around GSH C 301:**

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

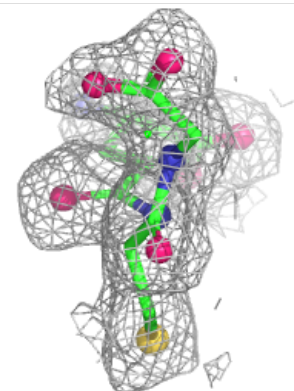
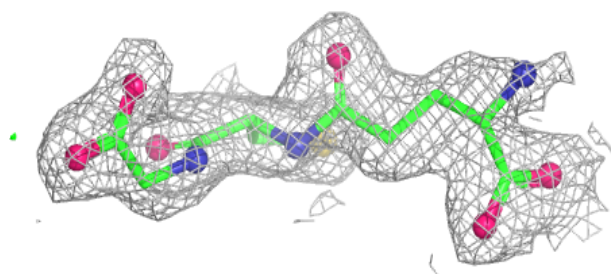
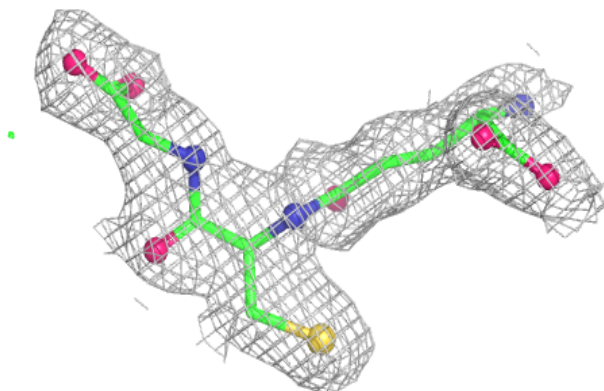


Electron density around GSH D 302:

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

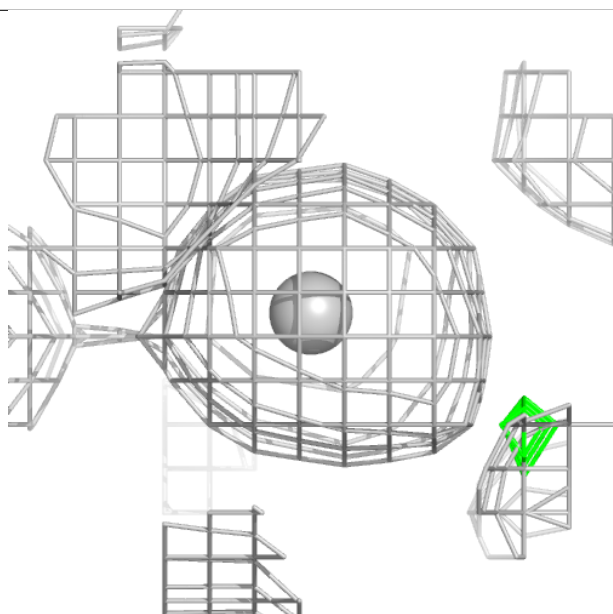
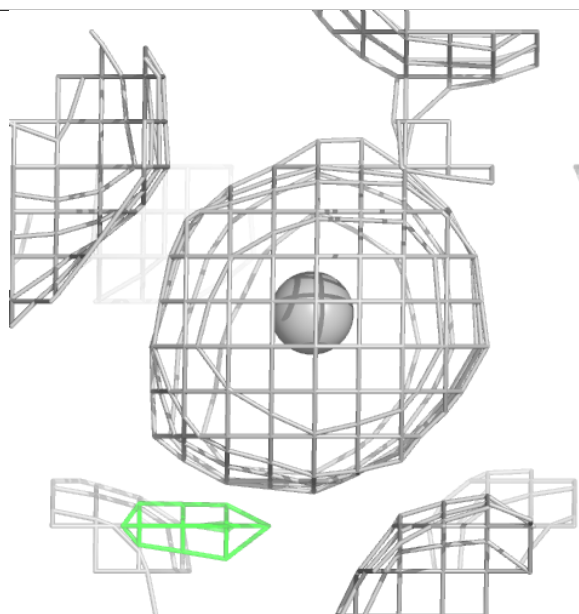
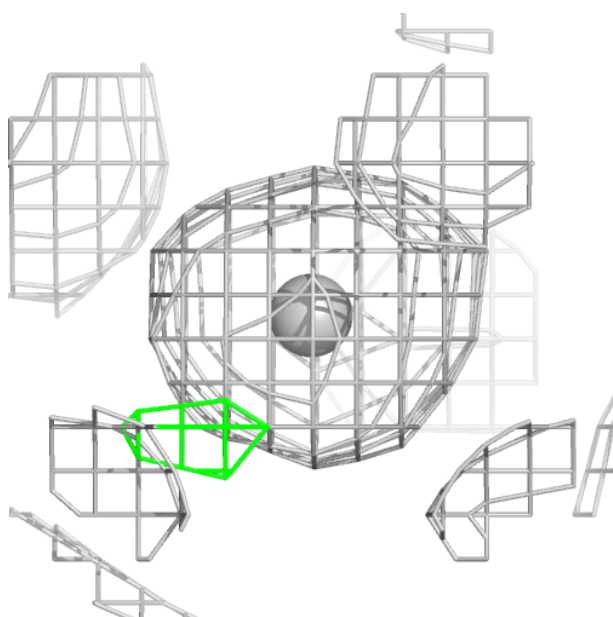
**Electron density around GSH B 301:**

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



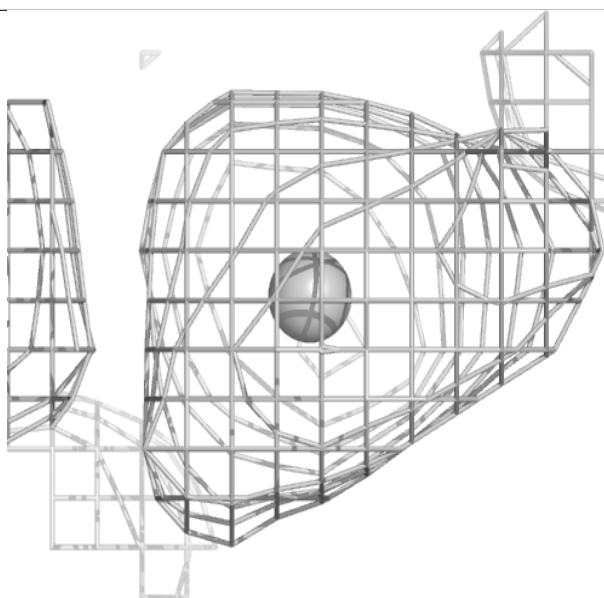
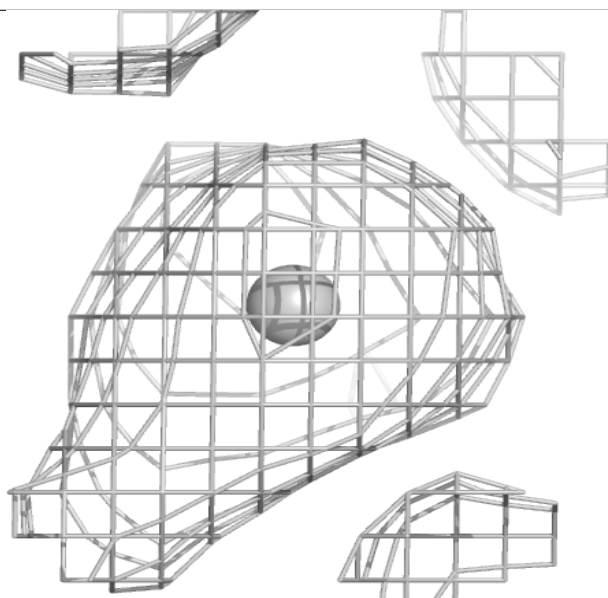
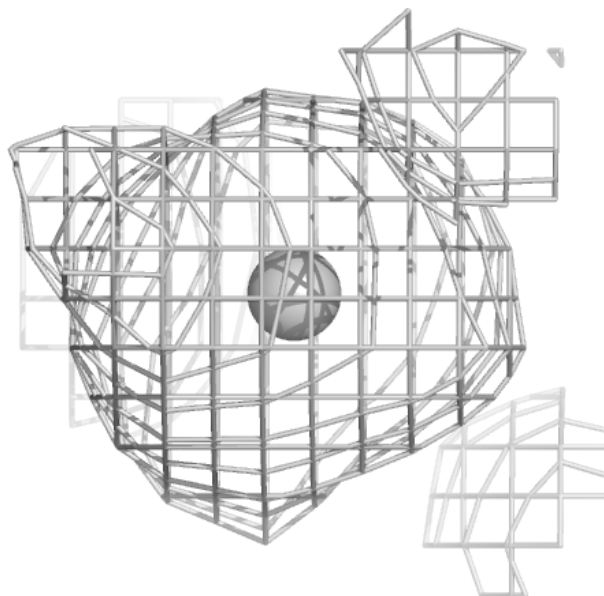
Electron density around AG E 301:

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



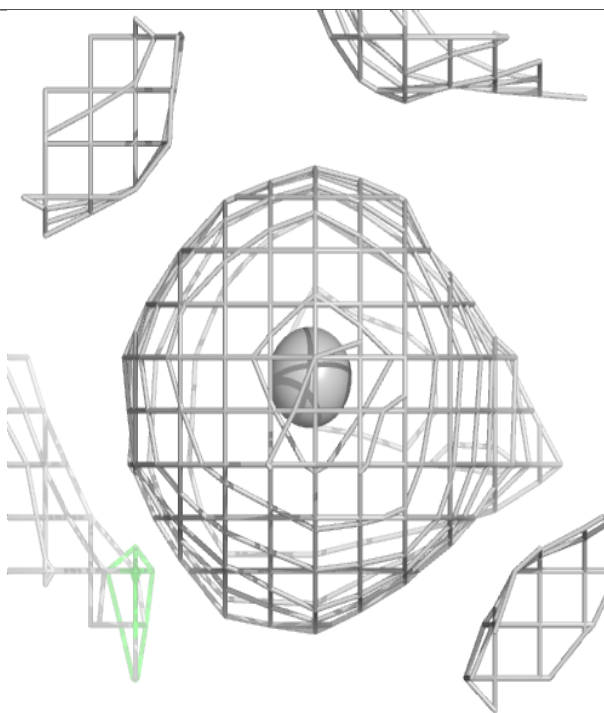
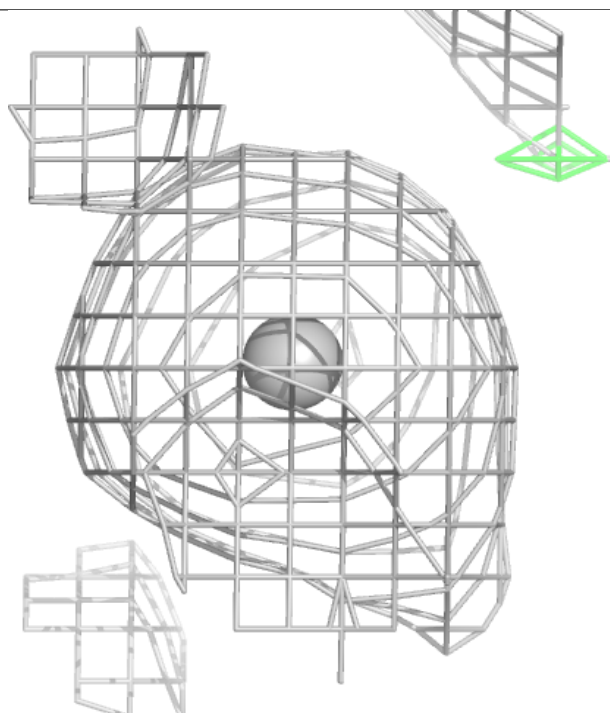
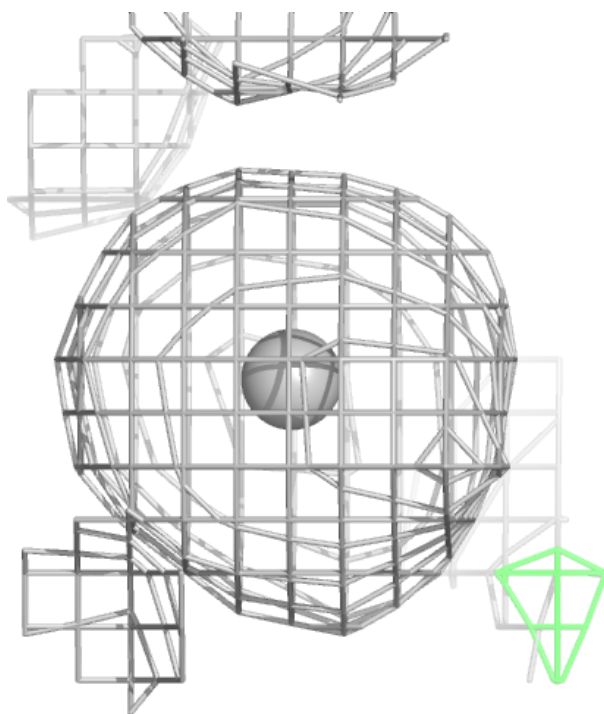
Electron density around AG D 301:

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



Electron density around AG G 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.