

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 - 06:17 AM EDT

PDB ID	:	7SO8
Title	:	Crystal structure of Glutathione S-Transferase from Shrimp Litopenaeus van-
		namei in complex with silver ions and a molecules of Glutathione binding in
		G-site and H-site
Authors	:	Escudero-Garcia, A.; Rudino-Pinera, E.; Miranda-Blancas, R.
Deposited on		
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 (i) 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 (i)) were used in the production of this report:

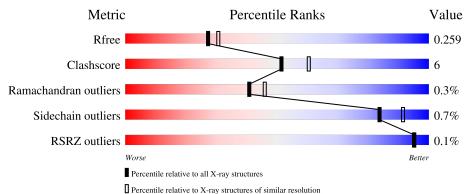
MolProbity		4 021 467
MOIFIODILY	•	4.020-407
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	219	89%	11%
1	В	219	87%	13%
1	С	219	90%	9%
1	D	219	87%	12% •



Mol	Chain	Length	Quality of chain	
1	Е	219	83%	16% ·
1	F	219	87%	13%
1	G	219	86%	13%
1	Н	219	82%	18%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15875 atoms, of which 0 are hydrogens and 0 are deuteriums.

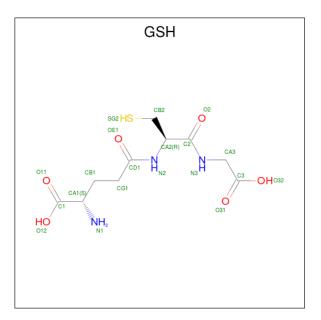
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	219	Total	С	Ν	0	S	0	1	0
	A	219	1809	1178	292	328	11	0	1	0
1	С	219	Total	С	Ν	0	S	0	2	0
		219	1818	1183	293	331	11	0	2	0
1	Е	219	Total	С	Ν	0	S	0	2	0
	Ľ	219	1820	1184	296	329	11	0	2	0
1	G	219	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	G	219	1809	1178	292	328	11	0	T	0
1	Н	219	Total	С	Ν	Ο	\mathbf{S}	9	1	0
	11	213	1809	1178	292	328	11	3		U
1	F	219	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	I.	219	1809	1178	292	328	11	0	T	0
1	В	219	Total	С	Ν	0	S	9	1	0
	D	219	1809	1178	292	328	11	9	L	0
1	D	219	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	D	219	1811	1178	294	328	11	0		0

• Molecule 1 is a protein called Glutathione transferase.

• Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$) (labeled as "Ligand of Interest" by depositor).

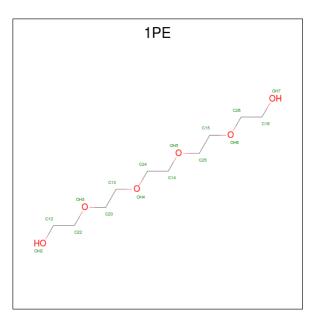




Mol	Chain	Residues		Atc	ms			ZeroOcc	AltConf
2	А	1	Total	С	Ν	0	S	0	0
	A	1	20	10	3	6	1	0	0
2	С	1	Total	С	Ν	0	\mathbf{S}	0	0
	U	1	20	10	3	6	1	0	0
2	Е	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	Ľ	1	20	10	3	6	1	0	0
2	G	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	u	1	20	10	3	6	1	0	0
2	Н	1	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
	11	1	20	10	3	6	1	0	0
2	F	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	-	Ĩ	20	10	3	6	1	Ŭ	0
2	F	1	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
	-	I.	20	10	3	6	1	Ŭ	0
2	В	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	D	1	20	10	3	6	1	Ŭ	0
2	В	1	Total	\mathbf{C}	Ν	0	\mathbf{S}	0	0
		*	20	10	3	6	1	Ŭ	, v
2	D	1	Total	С	Ν	0	\mathbf{S}	0	0
			20	10	3	6	1		0

• Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).





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

• Molecule 4 is SILVER ION (three-letter code: AG) (formula: Ag) (labeled as "Ligand of Interest" by depositor).

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

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	128	Total O 128 128	0	0
5	С	178	Total O 178 178	0	0
5	Е	152	Total O 152 152	0	0
5	G	145	Total O 145 145	0	0
5	Н	154	Total O 154 154	0	0



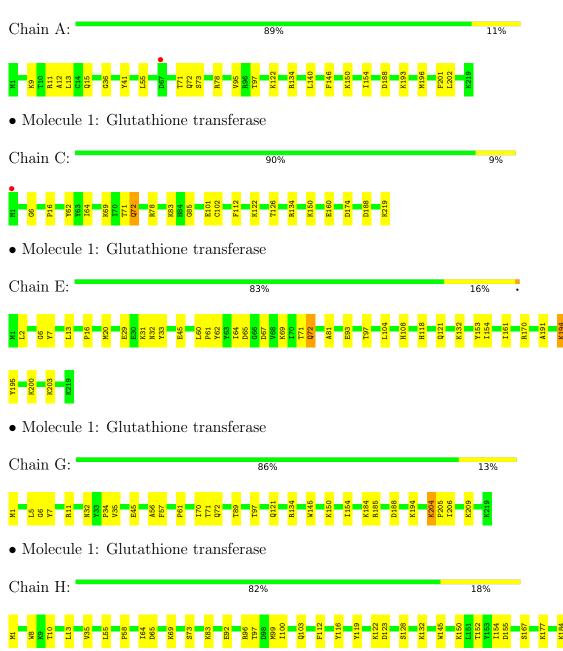
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	147	Total O 147 147	0	0
5	В	127	Total O 127 127	0	0
5	D	131	Total O 131 131	0	0



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.

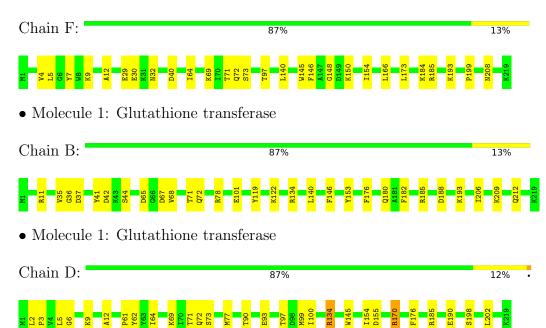


• Molecule 1: Glutathione transferase



R185 L202 P205 1206 C207 N208 K209 K209 K209

• Molecule 1: Glutathione transferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	57.39Å 93.02 Å 169.11 Å	Depositor
a, b, c, α , β , γ	90.00° 90.75° 90.00°	Depositor
Resolution (Å)	56.37 - 2.20	Depositor
Resolution (A)	56.37 - 2.20	EDS
% Data completeness	98.2 (56.37-2.20)	Depositor
(in resolution range)	98.2(56.37 - 2.20)	EDS
R _{merge}	0.62	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.68 (at 2.20 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D.	0.191 , 0.260	Depositor
R, R_{free}	0.191 , 0.259	DCC
R_{free} test set	4472 reflections (5.04%)	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 , 44.6	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15875	wwPDB-VP
Average B, all atoms $(Å^2)$	16.0	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.

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.



¹Intensities estimated from amplitudes.

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: 1PE, AG, 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		
WIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.44	0/1858	0.62	0/2507	
1	В	0.41	0/1858	0.57	0/2507	
1	С	0.46	0/1867	0.58	0/2519	
1	D	0.43	0/1860	0.61	0/2510	
1	Е	0.46	0/1869	0.61	0/2521	
1	F	0.43	0/1858	0.62	0/2507	
1	G	0.45	0/1858	0.59	0/2507	
1	Н	0.44	0/1858	0.62	0/2507	
All	All	0.44	0/14886	0.60	0/20085	

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	А	1809	0	1794	15	0
1	В	1809	0	1794	17	0
1	С	1818	0	1799	17	0
1	D	1811	0	1794	20	0
1	Е	1820	0	1806	23	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
1	F	1809	0	1794	21	0		
1	G	1809	0	1794	21	0		
1	Н	1809	0	1794	31	0		
2	А	20	0	15	2	0		
2	В	40	0	30	1	0		
2	С	20	0	15	1	0		
2	D	20	0	14	0	0		
2	Е	20	0	15	2	0		
2	F	40	0	30	3	0		
2	G	20	0	15	0	0		
2	Н	20	0	15	2	0		
3	С	16	0	22	4	0		
4	D	1	0	0	0	0		
4	Е	1	0	0	0	0		
4	G	1	0	0	0	0		
5	А	128	0	0	5	0		
5	В	127	0	0	2	0		
5	С	178	0	0	8	0		
5	D	131	0	0	4	0		
5	Е	152	0	0	4	0		
5	F	147	0	0	5	0		
5	G	145	0	0	4	0		
5	Н	154	0	0	9	0		
All	All	15875	0	14540	164	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 6.

The worst 5 of 164 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:G:5:LEU:HD12	5:G:416:HOH:O	1.48	1.12
1:E:132:LYS:HG2	5:E:546:HOH:O	1.78	0.84
1:G:121:GLN:HG2	5:G:528:HOH:O	1.79	0.83
1:G:70:ILE:HG23	1:H:99:MET:HE2	1.61	0.82
1:C:174:ASP:HB3	3:C:302:1PE:H261	1.64	0.78

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	Perce	entiles
1	А	218/219~(100%)	214~(98%)	3~(1%)	1 (0%)	29	31
1	В	218/219~(100%)	213~(98%)	5(2%)	0	100	100
1	С	219/219~(100%)	211 (96%)	7 (3%)	1 (0%)	29	31
1	D	218/219~(100%)	211~(97%)	5(2%)	2(1%)	17	16
1	Е	219/219~(100%)	212~(97%)	6 (3%)	1 (0%)	29	31
1	F	218/219~(100%)	212~(97%)	5(2%)	1 (0%)	29	31
1	G	218/219~(100%)	212~(97%)	6 (3%)	0	100	100
1	Н	218/219~(100%)	210 (96%)	8 (4%)	0	100	100
All	All	1746/1752~(100%)	1695 (97%)	45 (3%)	6 (0%)	41	46

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	170	ARG
1	А	12	ALA
1	Е	72	GLN
1	F	12	ALA
1	D	12	ALA

5.3.2 Protein sidechains (i)

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	А	192/191~(100%)	192 (100%)	0	100 100	



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	В	192/191~(100%)	191 (100%)	1 (0%)	88	94
1	\mathbf{C}	193/191~(101%)	193~(100%)	0	100	100
1	D	192/191~(100%)	188~(98%)	4 (2%)	53	67
1	Ε	193/191~(101%)	190~(98%)	3~(2%)	62	76
1	F	192/191~(100%)	192~(100%)	0	100	100
1	G	192/191~(100%)	191 (100%)	1 (0%)	88	94
1	Н	192/191~(100%)	189~(98%)	3~(2%)	62	76
All	All	1538/1528~(101%)	1526~(99%)	12 (1%)	84	90

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	122	LYS
1	D	134[A]	ARG
1	D	198	SER
1	D	134[B]	ARG
1	G	204	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	Е	121	GLN
1	G	59	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)

Of 14 ligands modelled in this entry, 3 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	Bo	ond leng	ths	B	ond ang	gles
10101		Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	GSH	F	302	-	18,19,19	0.71	1 (5%)	23,24,24	0.99	1 (4%)
2	GSH	В	302	-	18,19,19	2.33	3 (16%)	23,24,24	2.87	10 (43%)
3	1PE	С	302	-	$15,\!15,\!15$	1.07	1 (6%)	14,14,14	0.92	0
2	GSH	Н	301	-	18,19,19	0.74	0	23,24,24	0.72	0
2	GSH	D	302	-	18,19,19	0.79	1 (5%)	23,24,24	0.83	0
2	GSH	F	301	-	18,19,19	2.19	4 (22%)	23,24,24	2.26	7 (30%)
2	GSH	С	301	-	18,19,19	0.69	0	23,24,24	1.18	1 (4%)
2	GSH	G	302	-	18,19,19	0.76	1 (5%)	23,24,24	0.78	0
2	GSH	А	301	-	18,19,19	0.71	0	23,24,24	0.82	0
2	GSH	Е	302	-	18,19,19	0.78	0	23,24,24	0.74	0
2	GSH	В	301	-	18,19,19	0.84	1 (5%)	23,24,24	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	F	302	-	-	6/24/24/24	-
2	GSH	В	302	-	-	10/24/24/24	-
3	1PE	С	302	-	-	8/13/13/13	-
2	GSH	Н	301	-	-	8/24/24/24	-
2	GSH	D	302	-	-	14/24/24/24	-
2	GSH	F	301	-	-	6/24/24/24	-
2	GSH	С	301	-	-	13/24/24/24	-
2	GSH	G	302	-	-	15/24/24/24	-
2	GSH	А	301	-	-	14/24/24/24	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	Е	302	-	-	12/24/24/24	-
2	GSH	В	301	-	-	3/24/24/24	-

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

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	В	302	GSH	C2-N3	6.30	1.47	1.33
2	В	302	GSH	CD1-N2	6.05	1.47	1.34
2	F	301	GSH	CD1-N2	5.99	1.46	1.34
2	F	301	GSH	C2-N3	5.33	1.45	1.33
2	В	301	GSH	O12-C1	-2.68	1.21	1.30

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	В	302	GSH	CB2-CA2-N2	-8.14	99.67	111.28
2	F	301	GSH	CA2-CB2-SG2	-6.45	106.94	114.19
2	В	302	GSH	CA2-CB2-SG2	-6.02	107.43	114.19
2	В	302	GSH	CA2-N2-CD1	5.30	135.27	121.65
2	В	302	GSH	CA2-C2-N3	3.34	123.28	116.54

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	301	GSH	O11-C1-CA1-N1
2	А	301	GSH	CG1-CD1-N2-CA2
2	А	301	GSH	OE1-CD1-N2-CA2
2	А	301	GSH	C2-CA2-CB2-SG2
2	С	301	GSH	CG1-CD1-N2-CA2

There are no ring outliers.

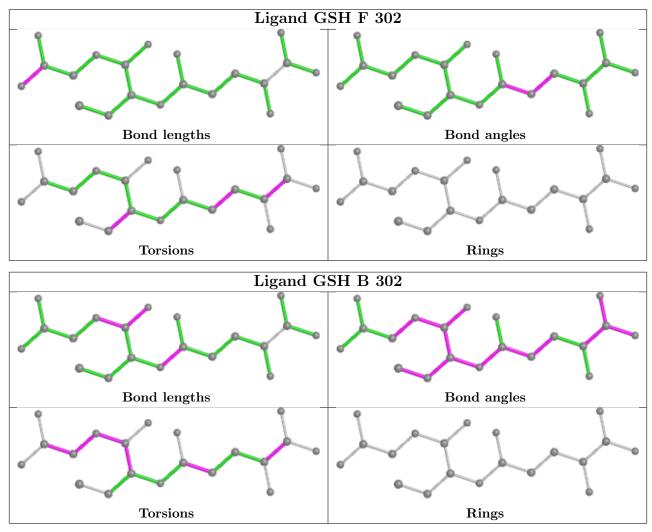
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	302	GSH	1	0
2	В	302	GSH	1	0
3	С	302	1PE	4	0
2	Н	301	GSH	2	0
2	F	301	GSH	2	0



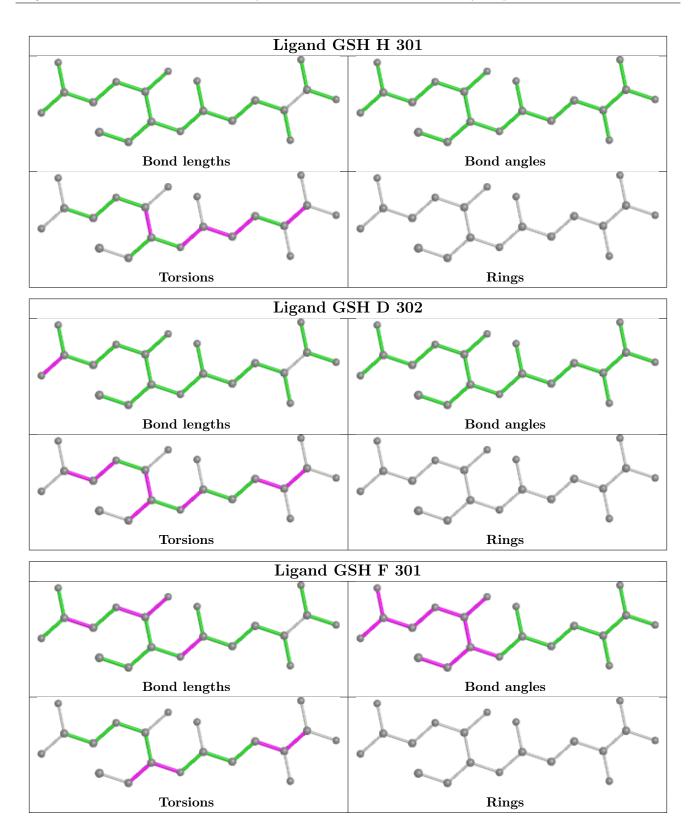
contracta from process pagem										
Mol	Chain	Res	Type	Clashes	Symm-Clashes					
2	С	301	GSH	1	0					
2	А	301	GSH	2	0					
2	Е	302	GSH	2	0					

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 then 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 sufficient must be highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



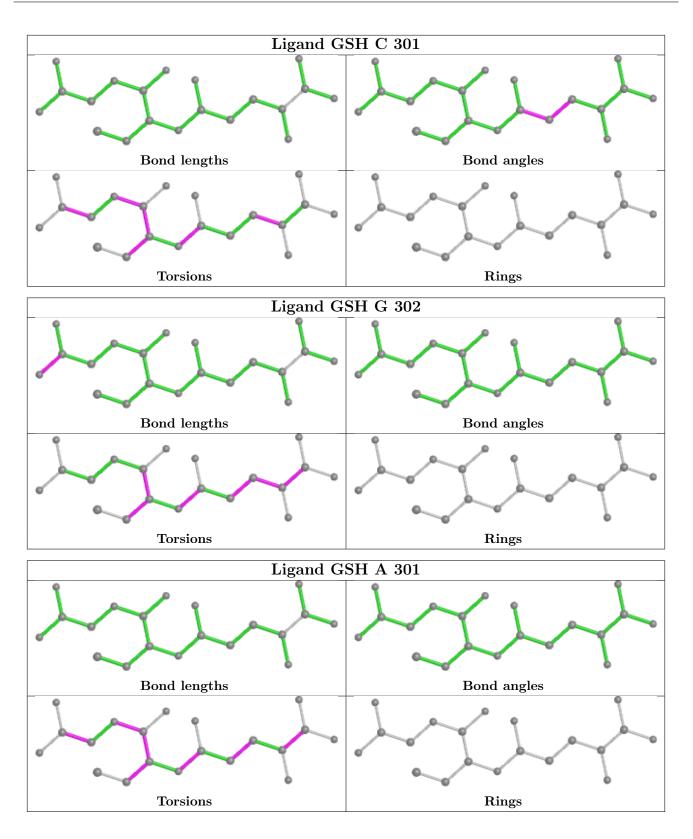






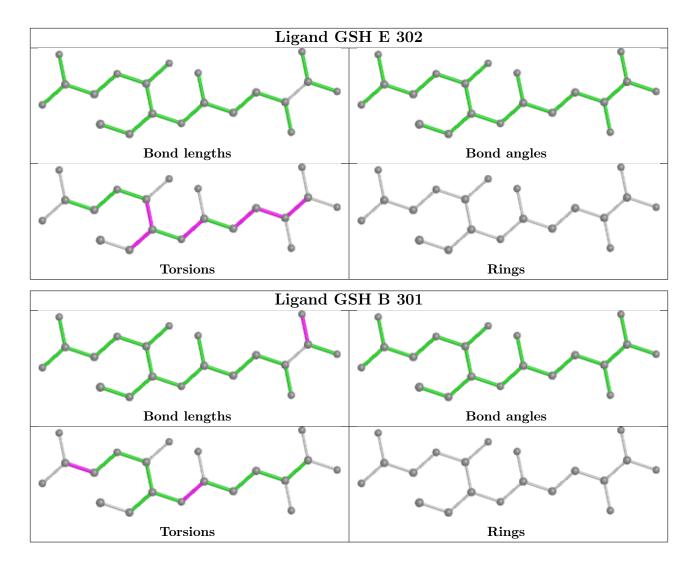












5.7 Other polymers (i)

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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	219/219~(100%)	-0.56	1 (0%) 91 90	5, 14, 37, 60	0
1	В	219/219~(100%)	-0.58	0 100 100	6, 17, 32, 60	0
1	С	219/219~(100%)	-0.69	1 (0%) 91 90	4,13,27,59	0
1	D	219/219~(100%)	-0.73	0 100 100	5, 13, 26, 51	0
1	Ε	219/219~(100%)	-0.69	0 100 100	5, 14, 29, 36	0
1	F	219/219~(100%)	-0.70	0 100 100	5, 13, 29, 46	0
1	G	219/219~(100%)	-0.66	0 100 100	7, 13, 29, 46	0
1	Н	219/219~(100%)	-0.67	0 100 100	5, 14, 30, 56	0
All	All	1752/1752~(100%)	-0.66	2 (0%) 95 95	4, 14, 30, 60	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	67	ASP	4.0
1	С	1	MET	2.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



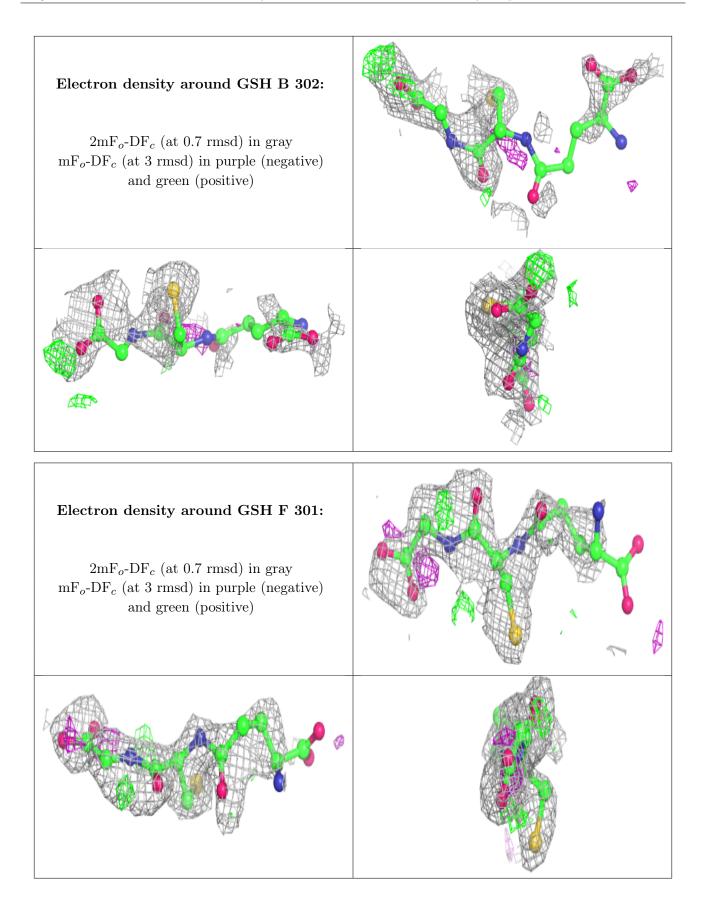
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

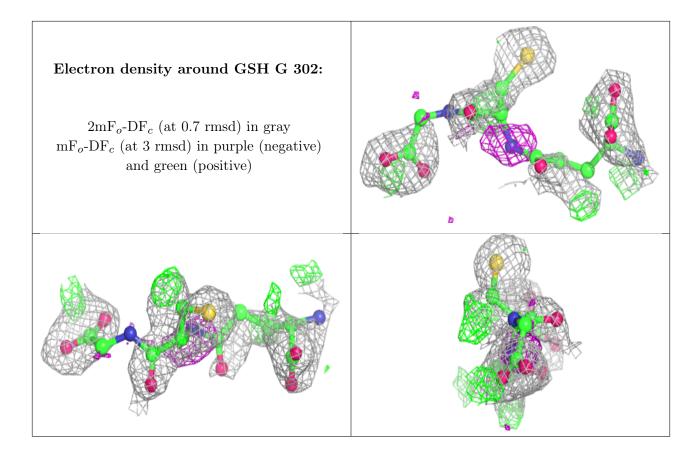
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	$\mathbf{Q}{<}0.9$
2	GSH	В	302	20/20	0.64	0.38	$35,\!62,\!80,\!87$	0
2	GSH	F	301	20/20	0.75	0.29	18,40,65,75	0
2	GSH	G	302	20/20	0.76	0.32	19,49,74,86	0
2	GSH	А	301	20/20	0.77	0.25	34,51,62,67	0
2	GSH	D	302	20/20	0.77	0.30	15,47,80,84	0
4	AG	Е	301	1/1	0.77	0.11	134,134,134,134	0
2	GSH	Н	301	20/20	0.81	0.23	$26,\!40,\!53,\!55$	0
4	AG	D	301	1/1	0.82	0.20	132,132,132,132	0
2	GSH	С	301	20/20	0.83	0.17	17,38,55,71	0
2	GSH	Е	302	20/20	0.86	0.20	16,27,39,53	0
3	1PE	С	302	16/16	0.89	0.13	9,19,32,32	0
2	GSH	F	302	20/20	0.92	0.17	12,28,37,39	0
4	AG	G	301	1/1	0.93	0.07	88,88,88,88	0
2	GSH	В	301	20/20	0.95	0.13	10,22,38,44	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.

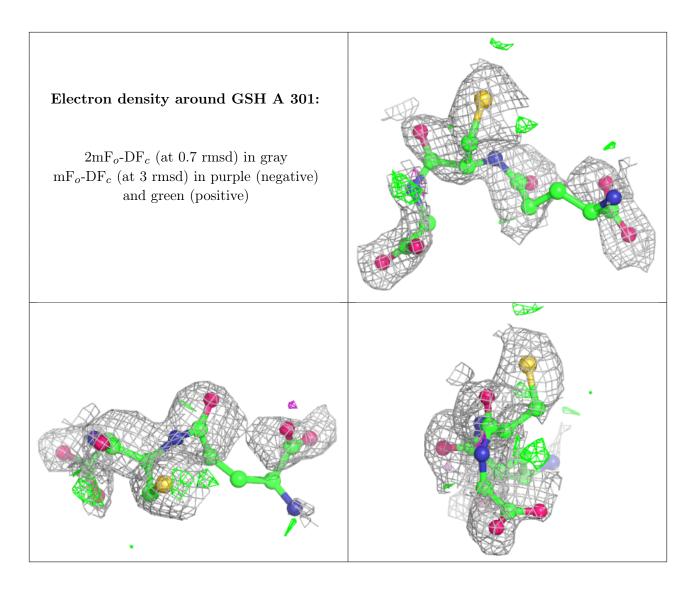






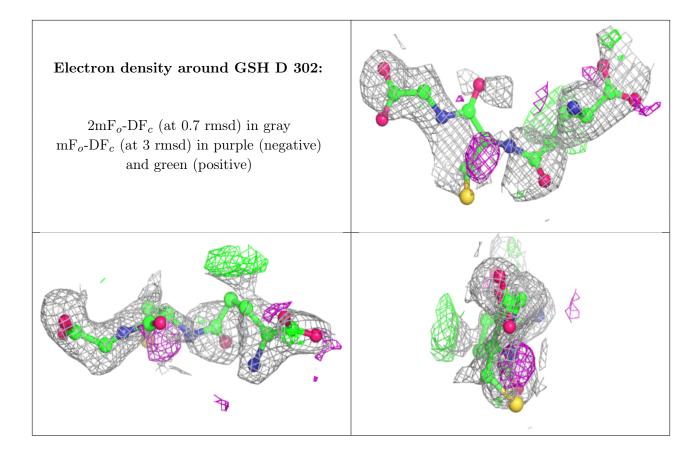




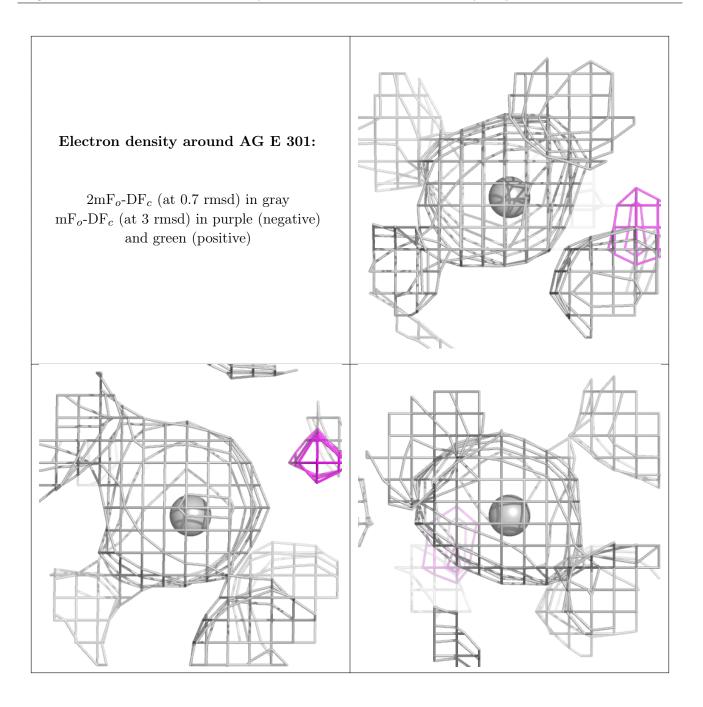




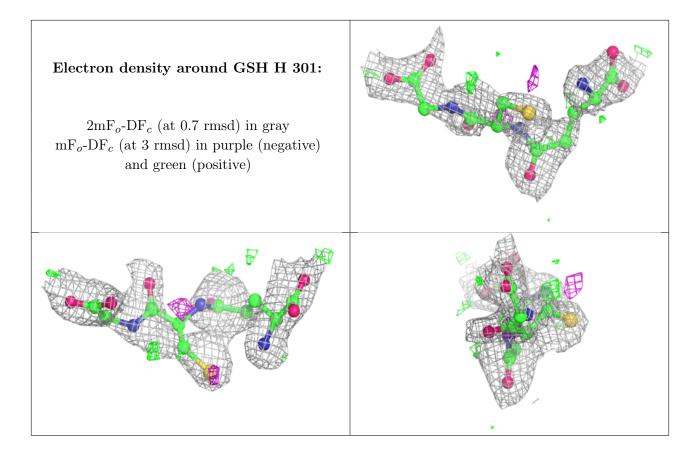




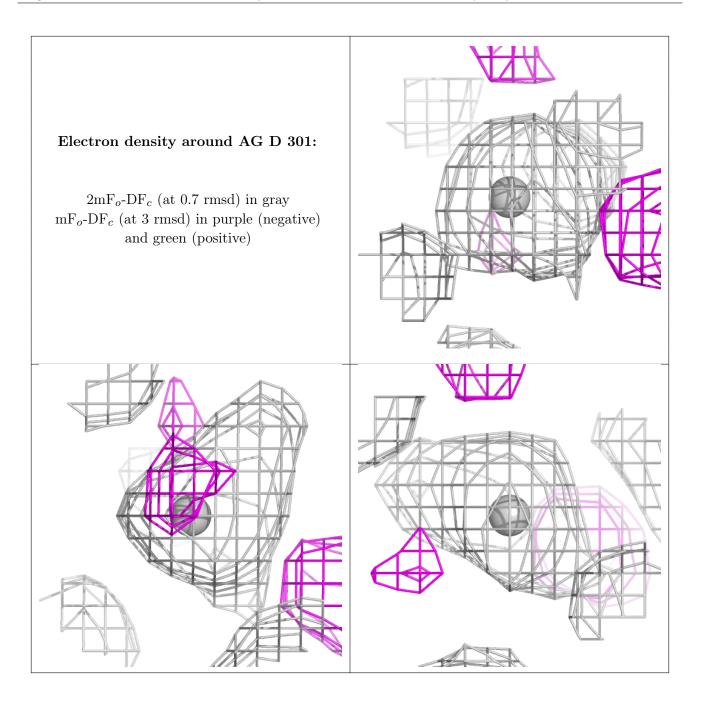




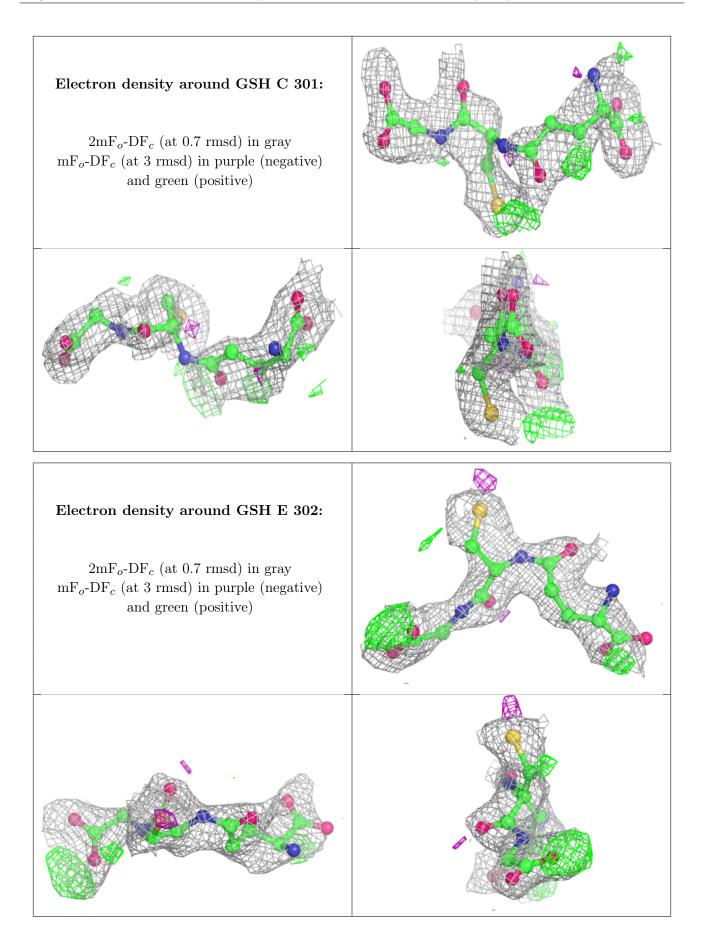




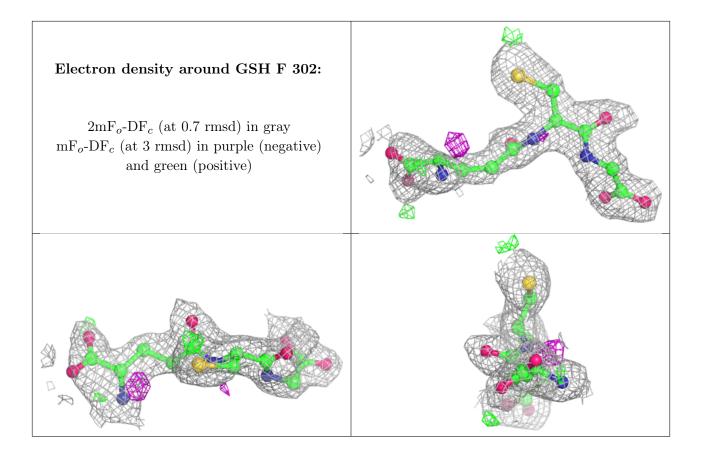




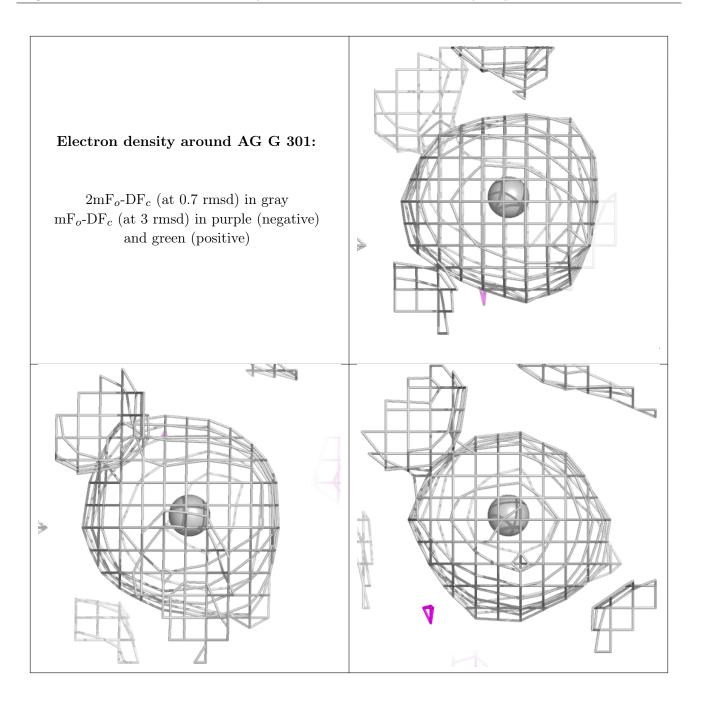




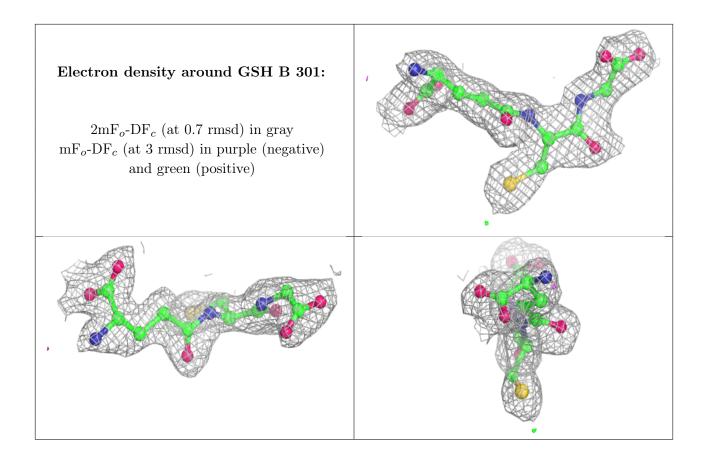












6.5 Other polymers (i)

There are no such residues in this entry.

