



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 06:46 PM EDT

PDB ID : 1OYJ  
Title : Crystal structure solution of Rice GST1 (OsGSTU1) in complex with glutathione.  
Authors : Dixon, D.P.; McEwen, A.G.; Laphorn, A.J.; Edwards, R.  
Deposited on : 2003-04-04  
Resolution : 1.95 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 types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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

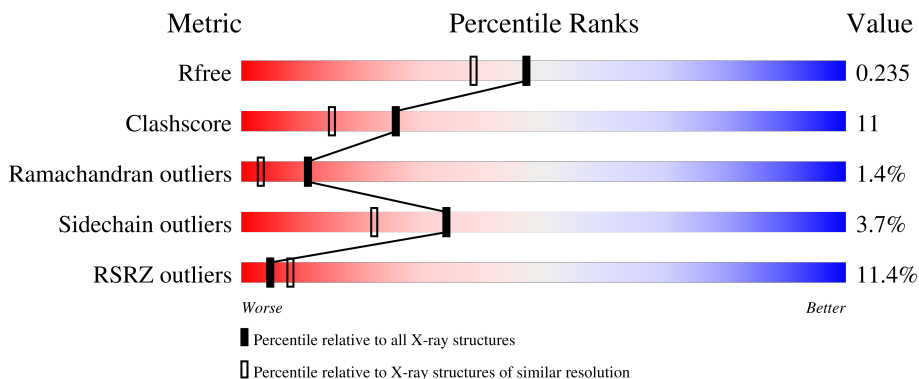
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	231	 6% 82% 14%
1	B	231	 12% 77% 15%
1	C	231	 9% 85% 10%
1	D	231	 17% 74% 19%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	831	-	-	X	-
4	GSH	A	800	X	-	-	-
4	GSH	B	801	X	-	-	-
4	GSH	C	802	X	-	-	-
4	GSH	C	803	X	-	-	-
4	GSH	C	804	X	X	-	-
4	GSH	D	805	X	-	-	-
5	GOL	A	814	-	-	X	-
5	GOL	C	812	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7954 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called glutathione s-transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	228	Total 1807	C 1156	N 319	O 326	S 6	0	3	0
1	B	224	Total 1778	C 1140	N 314	O 318	S 6	2	4	0
1	C	227	Total 1784	C 1143	N 317	O 318	S 6	2	0	0
1	D	223	Total 1757	C 1127	N 309	O 315	S 6	0	3	0

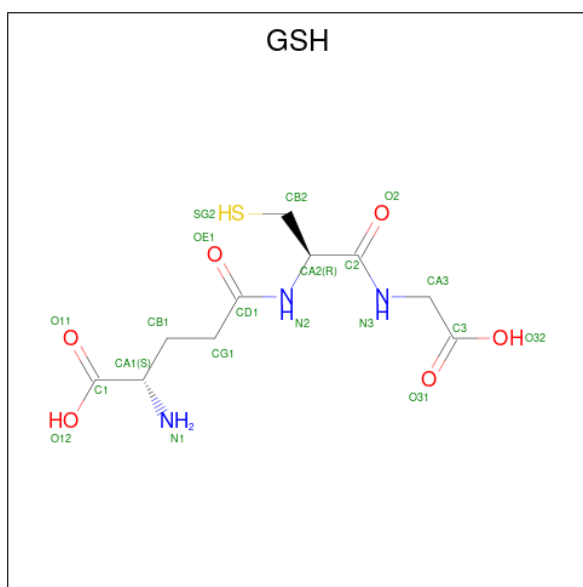
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mg 2	0	0
2	C	1	Total 1	Mg 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total 7	Cl 7	0	0
3	B	3	Total 3	Cl 3	0	0
3	C	6	Total 6	Cl 6	0	0
3	D	4	Total 4	Cl 4	0	0

- Molecule 4 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
			Total	C	N	O	S		
4	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 5 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
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	140	Total O 140 140	0	0
6	B	109	Total O 109 109	0	0
6	C	224	Total O 224 224	0	0

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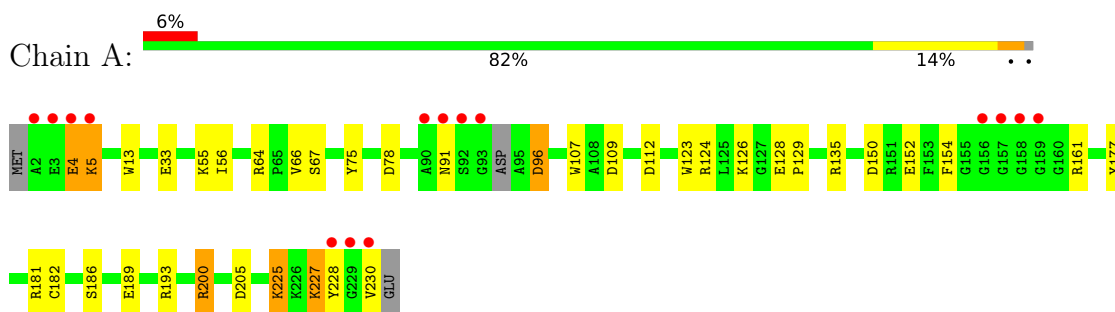
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	D	138	Total 138	O 138	0	0

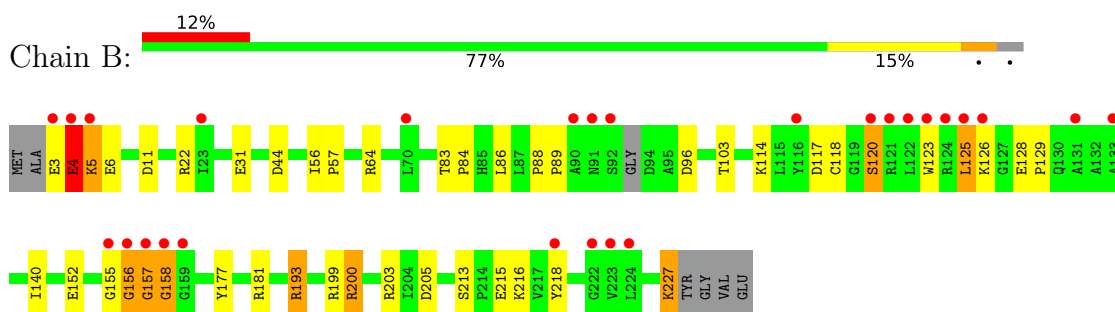
### 3 Residue-property plots [i](#)

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.

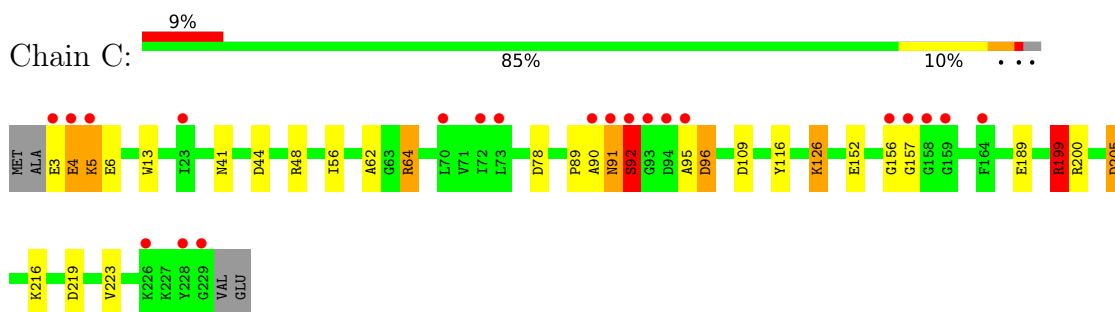
- Molecule 1: glutathione s-transferase



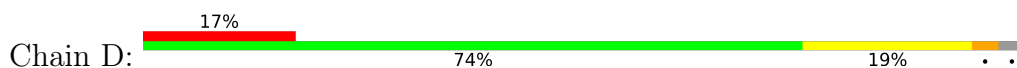
- Molecule 1: glutathione s-transferase



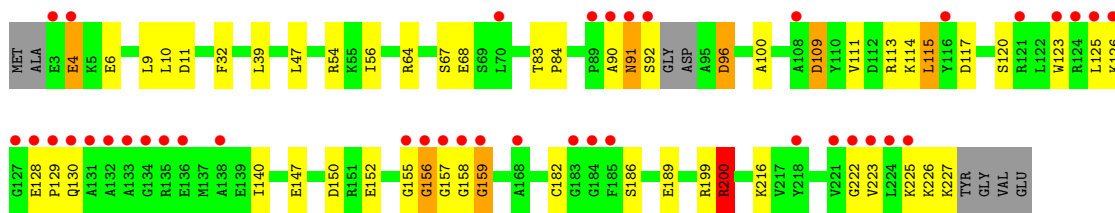
- Molecule 1: glutathione s-transferase



- Molecule 1: glutathione s-transferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.83Å 91.13Å 165.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 35.40 – 1.95	Depositor EDS
% Data completeness (in resolution range)	84.5 (40.00-1.95) 84.5 (35.40-1.95)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.178 , 0.227 0.190 , 0.235	Depositor DCC
$R_{free}$ test set	3635 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7954	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.87 % 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 6.3776e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	1.21	4/1868 (0.2%)	1.07	9/2528 (0.4%)
1	B	1.15	1/1843 (0.1%)	1.13	12/2494 (0.5%)
1	C	1.15	3/1830 (0.2%)	1.22	11/2476 (0.4%)
1	D	1.00	1/1819 (0.1%)	1.05	7/2463 (0.3%)
All	All	1.13	9/7360 (0.1%)	1.12	39/9961 (0.4%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	LYS	CD-CE	16.32	1.92	1.51
1	A	123	TRP	CB-CG	-5.83	1.39	1.50
1	D	200	ARG	CG-CD	5.65	1.66	1.51
1	A	13	TRP	CG-CD1	-5.54	1.28	1.36
1	C	200	ARG	CG-CD	5.40	1.65	1.51
1	C	5	LYS	CE-NZ	5.33	1.62	1.49
1	C	199	ARG	CG-CD	5.22	1.65	1.51
1	A	154	PHE	CE2-CZ	5.20	1.47	1.37
1	A	107	TRP	CB-CG	5.16	1.59	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ARG	NE-CZ-NH1	-23.81	108.39	120.30
1	C	199	ARG	NE-CZ-NH2	15.74	128.17	120.30
1	A	205	ASP	CB-CG-OD2	10.40	127.66	118.30
1	B	200	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	B	199	ARG	NE-CZ-NH2	8.93	124.76	120.30
1	B	199	ARG	NE-CZ-NH1	-8.81	115.90	120.30
1	C	199	ARG	CD-NE-CZ	8.56	135.59	123.60
1	A	200	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	117	ASP	CB-CG-OD2	8.04	125.54	118.30
1	D	199	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	D	199	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	B	44	ASP	CB-CG-OD2	7.17	124.76	118.30
1	B	200	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	96	ASP	CB-CG-OD2	6.75	124.38	118.30
1	C	205	ASP	CB-CG-OD2	6.69	124.32	118.30
1	C	78	ASP	CB-CG-OD2	6.44	124.10	118.30
1	B	11	ASP	CB-CG-OD1	6.26	123.94	118.30
1	D	150	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	205	ASP	CB-CG-OD2	6.18	123.86	118.30
1	D	109	ASP	CB-CG-OD2	6.05	123.74	118.30
1	C	199	ARG	CG-CD-NE	-6.01	99.18	111.80
1	D	96	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	78	ASP	CB-CG-OD2	5.95	123.65	118.30
1	C	200	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	203	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	A	109	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	135	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	200	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	193	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	D	200	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	64	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	D	200	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	22	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	A	96	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	22	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	C	109	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	157	GLY	N-CA-C	-5.16	100.21	113.10
1	A	112	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	219	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	199	ARG	Sidechain

## 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	1807	0	1765	28	0
1	B	1778	0	1743	41	0
1	C	1784	0	1753	39	0
1	D	1757	0	1709	50	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
3	A	7	0	0	2	0
3	B	3	0	0	3	0
3	C	6	0	0	0	0
3	D	4	0	0	1	0
4	A	40	0	29	2	0
4	B	20	0	15	0	0
4	C	60	0	41	3	0
4	D	20	0	15	2	0
5	A	12	0	16	5	0
5	B	6	0	8	1	0
5	C	24	0	32	5	0
5	D	12	0	16	1	0
6	A	140	0	0	7	0
6	B	109	0	0	5	1
6	C	224	0	0	11	1
6	D	138	0	0	7	0
All	All	7954	0	7142	154	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (154) 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:157:GLY:HA2	3:B:831:CL:CL	1.85	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HA	5:A:814:GOL:H31	1.16	1.12
1:B:157:GLY:CA	3:B:831:CL:CL	2.40	1.06
1:A:182:CYS:SG	6:A:975:HOH:O	2.13	1.05
1:C:6:GLU:OE1	1:C:6:GLU:HA	1.56	1.02
1:B:193:ARG:HH11	1:B:193:ARG:HG3	1.23	1.01
1:A:66:VAL:HA	5:A:814:GOL:C3	1.97	0.95
1:B:118:CYS:SG	6:B:940:HOH:O	2.27	0.91
1:B:5[B]:LYS:HG3	6:B:885:HOH:O	1.71	0.89
1:D:182:CYS:SG	6:D:931:HOH:O	2.31	0.88
1:C:116:TYR:OH	6:C:1014:HOH:O	1.93	0.86
1:C:5:LYS:HG2	1:C:6:GLU:H	1.41	0.84
1:C:91:ASN:O	1:C:92:SER:HB2	1.76	0.83
1:B:157:GLY:HA3	3:B:831:CL:CL	2.15	0.82
1:A:225:LYS:O	6:A:948:HOH:O	1.96	0.82
4:C:802:GSH:SG2	6:C:965:HOH:O	2.23	0.81
1:D:125:LEU:O	1:D:130:GLN:HB2	1.82	0.80
1:C:205:ASP:OD2	6:C:896:HOH:O	2.00	0.79
1:A:33:GLU:OE1	6:A:886:HOH:O	2.01	0.78
1:B:218:TYR:OH	1:C:152:GLU:OE2	2.02	0.78
1:D:147:GLU:OE1	6:D:855:HOH:O	2.01	0.77
1:C:6:GLU:OE1	1:C:6:GLU:CA	2.30	0.77
1:C:189:GLU:HG2	6:C:948:HOH:O	1.86	0.73
1:B:157:GLY:O	1:B:158:GLY:O	2.07	0.73
1:D:222:GLY:O	1:D:225:LYS:N	2.21	0.72
1:D:9:LEU:CD1	1:D:11:ASP:HB2	2.20	0.71
1:B:181:ARG:HH11	1:C:152:GLU:CD	1.94	0.70
1:B:177:TYR:OH	1:B:181:ARG:NH2	2.24	0.70
1:C:216:LYS:NZ	5:C:812:GOL:H32	2.08	0.69
1:D:157:GLY:O	1:D:159:GLY:N	2.26	0.69
1:D:147:GLU:O	6:D:929:HOH:O	2.09	0.69
1:D:152:GLU:HG2	1:D:200:ARG:HD3	1.74	0.69
1:D:128:GLU:N	1:D:129:PRO:CD	2.56	0.69
4:C:803:GSH:O12	6:C:901:HOH:O	2.11	0.68
1:C:44:ASP:O	1:C:48:ARG:HG3	1.95	0.67
1:D:155:GLY:O	1:D:156:GLY:C	2.32	0.67
1:C:189:GLU:HB3	6:C:948:HOH:O	1.95	0.66
1:A:4:GLU:O	1:A:5:LYS:CB	2.44	0.66
1:A:66:VAL:HG13	5:A:814:GOL:H32	1.78	0.65
1:B:120:SER:HA	1:B:123:TRP:CZ2	2.32	0.65
1:D:155:GLY:O	1:D:157:GLY:N	2.31	0.64
1:B:193:ARG:HH11	1:B:193:ARG:CG	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LYS:NZ	6:C:923:HOH:O	2.30	0.64
1:B:5[A]:LYS:NZ	6:B:872:HOH:O	2.30	0.63
1:C:6:GLU:CG	1:C:62:ALA:HA	2.29	0.62
1:D:186:SER:HB3	1:D:189:GLU:HG2	1.82	0.62
1:C:64:ARG:NH2	1:D:96:ASP:OD1	2.25	0.61
1:D:186:SER:HB3	1:D:189:GLU:CG	2.30	0.61
1:D:9:LEU:C	1:D:9:LEU:HD13	2.22	0.60
1:B:193:ARG:HG3	1:B:193:ARG:NH1	2.02	0.60
1:B:125:LEU:N	1:B:125:LEU:HD13	2.17	0.59
1:C:96:ASP:OD1	1:D:64:ARG:NH1	2.26	0.59
1:D:126:LYS:O	1:D:129:PRO:HD2	2.03	0.59
1:A:56:ILE:C	1:A:56:ILE:HD12	2.22	0.59
1:D:128:GLU:N	1:D:129:PRO:HD2	2.17	0.59
1:B:125:LEU:N	1:B:125:LEU:CD1	2.66	0.59
1:D:39:LEU:HD13	4:D:805:GSH:HA32	1.84	0.59
1:D:9:LEU:HD12	1:D:11:ASP:HB2	1.83	0.59
1:A:64:ARG:NH2	1:B:96:ASP:OD1	2.22	0.58
1:A:96:ASP:OD1	1:B:64[A]:ARG:NH2	2.30	0.58
1:B:114:LYS:HB3	1:B:140:ILE:HD13	1.86	0.58
1:A:75:TYR:HA	6:A:865:HOH:O	2.04	0.57
1:D:156:GLY:CA	6:D:861:HOH:O	2.50	0.57
5:C:810:GOL:H32	6:C:912:HOH:O	2.03	0.57
1:D:120:SER:HA	1:D:123:TRP:CZ2	2.39	0.57
1:C:189:GLU:CG	6:C:948:HOH:O	2.46	0.57
1:D:156:GLY:N	6:D:861:HOH:O	2.30	0.57
1:A:126:LYS:O	1:A:129:PRO:HD2	2.04	0.56
1:C:6:GLU:HG3	1:C:62:ALA:HA	1.87	0.56
1:A:227:LYS:C	1:A:228:TYR:HD1	2.09	0.56
1:B:152:GLU:CG	1:B:200:ARG:HD3	2.35	0.56
1:D:222:GLY:O	1:D:225:LYS:HB2	2.05	0.56
5:A:814:GOL:H2	1:B:103:THR:HA	1.88	0.55
1:D:32:PHE:O	5:D:807:GOL:H31	2.06	0.55
1:B:152:GLU:HG3	1:B:200:ARG:HD3	1.90	0.54
1:A:152:GLU:CG	1:A:200:ARG:HD3	2.37	0.54
1:D:111:VAL:HG13	1:D:115:LEU:HD13	1.90	0.54
1:D:90:ALA:C	1:D:92:SER:N	2.60	0.53
1:A:152:GLU:HG2	1:A:200:ARG:HD3	1.91	0.53
1:D:47:LEU:HD22	1:D:54:ARG:HD2	1.90	0.53
1:B:155:GLY:O	1:B:156:GLY:C	2.47	0.53
1:C:91:ASN:OD1	1:C:91:ASN:N	2.29	0.53
1:B:120:SER:HA	1:B:123:TRP:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:HG2	3:A:826:CL:CL	2.47	0.51
1:C:13:TRP:CE2	5:C:812:GOL:H2	2.46	0.51
1:C:189:GLU:CB	6:C:948:HOH:O	2.57	0.51
1:C:56:ILE:C	1:C:56:ILE:HD12	2.31	0.51
1:B:4:GLU:CD	1:B:4:GLU:C	2.70	0.50
1:B:181:ARG:NE	1:C:152:GLU:OE1	2.43	0.49
1:C:6:GLU:HG2	1:C:62:ALA:HA	1.94	0.49
1:D:114:LYS:HB3	1:D:140:ILE:HD13	1.93	0.49
1:B:213:SER:HB2	1:B:215:GLU:OE2	2.13	0.49
1:A:67:SER:N	5:A:814:GOL:O3	2.33	0.49
1:C:216:LYS:HZ3	5:C:812:GOL:H32	1.78	0.49
1:B:215:GLU:H	1:B:215:GLU:CD	2.16	0.48
1:D:157:GLY:HA2	3:D:832:CL:CL	2.50	0.48
1:D:152:GLU:CG	1:D:200:ARG:HD3	2.42	0.48
1:A:161:ARG:HB2	6:A:895:HOH:O	2.14	0.48
1:C:199:ARG:HD2	6:C:1004:HOH:O	2.13	0.48
1:B:128:GLU:N	1:B:129:PRO:CD	2.77	0.47
1:C:3:GLU:O	1:C:4:GLU:O	2.32	0.47
1:D:186:SER:HB3	1:D:189:GLU:HG3	1.97	0.47
1:D:9:LEU:HD13	1:D:10:LEU:N	2.29	0.47
1:C:56:ILE:HD11	4:C:802:GSH:HB23	1.97	0.47
1:C:91:ASN:O	1:C:92:SER:CB	2.53	0.46
1:C:216:LYS:HZ1	5:C:812:GOL:H32	1.78	0.46
1:D:56:ILE:C	1:D:56:ILE:HD12	2.36	0.46
1:D:223:VAL:C	1:D:225:LYS:H	2.18	0.46
1:D:109:ASP:OD2	1:D:113:ARG:HD2	2.15	0.46
1:B:3:GLU:HA	6:B:939:HOH:O	2.15	0.46
1:A:177:TYR:CZ	1:A:181:ARG:HD2	2.51	0.46
1:A:124:ARG:NH1	6:A:924:HOH:O	2.48	0.46
1:C:156:GLY:O	1:C:157:GLY:C	2.55	0.45
1:A:124:ARG:NE	1:A:228:TYR:HE2	2.14	0.45
1:A:56:ILE:HD12	1:A:56:ILE:O	2.17	0.45
1:B:4:GLU:HA	1:B:4:GLU:OE1	2.15	0.45
1:D:9:LEU:CD1	1:D:9:LEU:C	2.85	0.45
1:C:6:GLU:HG3	1:C:6:GLU:O	2.17	0.45
1:D:125:LEU:O	1:D:130:GLN:CB	2.60	0.45
1:A:189:GLU:HG2	3:A:836:CL:CL	2.54	0.45
1:D:100:ALA:O	6:D:844:HOH:O	2.21	0.45
1:A:55:LYS:HG2	4:A:799:GSH:N3	2.31	0.45
1:C:5:LYS:HG2	1:C:6:GLU:N	2.20	0.45
1:D:226:LYS:O	1:D:227:LYS:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5[B]:LYS:CD	1:B:6:GLU:H	2.30	0.44
1:C:90:ALA:C	1:C:92:SER:H	2.20	0.44
1:A:128:GLU:HB3	1:A:129:PRO:HD3	1.98	0.44
1:B:86:LEU:HD21	6:B:846:HOH:O	2.18	0.44
1:D:68:GLU:OE1	4:D:805:GSH:N1	2.46	0.44
1:B:4:GLU:OE1	1:B:4:GLU:CA	2.65	0.44
1:C:56:ILE:HD12	1:C:56:ILE:O	2.18	0.44
1:B:227:LYS:HD2	1:B:227:LYS:HA	1.65	0.44
1:D:91:ASN:C	1:D:91:ASN:OD1	2.57	0.43
1:B:5[B]:LYS:HG3	1:B:6:GLU:N	2.34	0.43
6:A:949:HOH:O	5:B:806:GOL:H12	2.19	0.43
1:B:83:THR:HB	1:B:84:PRO:HD2	2.01	0.43
1:C:89:PRO:CB	1:C:91:ASN:OD1	2.67	0.42
1:D:91:ASN:OD1	1:D:91:ASN:O	2.37	0.42
1:D:222:GLY:O	1:D:223:VAL:C	2.56	0.42
1:D:223:VAL:C	1:D:225:LYS:N	2.72	0.42
1:B:5[B]:LYS:HD2	1:B:6:GLU:H	1.85	0.42
1:D:83:THR:HB	1:D:84:PRO:HD2	2.02	0.42
1:A:124:ARG:CZ	1:A:228:TYR:HE2	2.33	0.42
1:A:152:GLU:HG2	1:A:200:ARG:CD	2.48	0.42
1:D:67:SER:O	1:D:68:GLU:HB2	2.20	0.42
1:D:64:ARG:HD2	6:D:953:HOH:O	2.20	0.41
1:D:225:LYS:O	1:D:226:LYS:HG3	2.20	0.41
1:A:56:ILE:HD11	4:A:799:GSH:HB23	2.02	0.41
1:D:123:TRP:HB2	1:D:225:LYS:HE3	2.02	0.41
1:B:181:ARG:NH1	1:C:152:GLU:OE1	2.52	0.41
1:B:88:PRO:HA	1:B:89:PRO:HD3	1.98	0.41
1:C:6:GLU:HG3	1:C:62:ALA:H	1.85	0.41
1:C:3:GLU:HB3	1:C:4:GLU:H	1.71	0.40
1:B:56:ILE:HB	1:B:57:PRO:HA	2.03	0.40

All (1) 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)
6:B:858:HOH:O	6:C:1032:HOH:O[4_456]	1.98	0.22

## 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	227/231 (98%)	220 (97%)	5 (2%)	2 (1%)	17	8
1	B	224/231 (97%)	218 (97%)	3 (1%)	3 (1%)	12	3
1	C	225/231 (97%)	215 (96%)	7 (3%)	3 (1%)	12	3
1	D	222/231 (96%)	210 (95%)	7 (3%)	5 (2%)	6	1
All	All	898/924 (97%)	863 (96%)	22 (2%)	13 (1%)	11	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	GLY
1	C	4	GLU
1	C	92	SER
1	D	156	GLY
1	D	158	GLY
1	D	159	GLY
1	B	158	GLY
1	A	5	LYS
1	A	227	LYS
1	C	95	ALA
1	D	4[A]	GLU
1	D	4[B]	GLU
1	B	4	GLU

### 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	A	183/185 (99%)	176 (96%)	7 (4%)	33	21
1	B	180/185 (97%)	170 (94%)	10 (6%)	21	9
1	C	179/185 (97%)	174 (97%)	5 (3%)	43	33
1	D	177/185 (96%)	168 (95%)	9 (5%)	24	11
All	All	719/740 (97%)	688 (96%)	31 (4%)	34	16

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	91	ASN
1	A	150[A]	ASP
1	A	150[B]	ASP
1	A	186	SER
1	A	225	LYS
1	A	230	VAL
1	B	4	GLU
1	B	5[A]	LYS
1	B	5[B]	LYS
1	B	31[A]	GLU
1	B	31[B]	GLU
1	B	120	SER
1	B	125	LEU
1	B	126	LYS
1	B	193	ARG
1	B	227	LYS
1	C	41	ASN
1	C	91	ASN
1	C	92	SER
1	C	126	LYS
1	C	223	VAL
1	D	4[A]	GLU
1	D	4[B]	GLU
1	D	6	GLU
1	D	91	ASN
1	D	115	LEU
1	D	117	ASP
1	D	200	ARG
1	D	216[A]	LYS
1	D	216[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

### 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 39 ligands modelled in this entry, 23 are monoatomic - leaving 16 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	GSH	C	802	-	18,19,19	1.11	1 (5%)	23,24,24	1.66	3 (13%)
5	GOL	A	811	-	5,5,5	0.31	0	5,5,5	0.31	0
5	GOL	D	807	-	5,5,5	0.68	0	5,5,5	1.44	1 (20%)
4	GSH	A	800	2	18,19,19	1.23	2 (11%)	23,24,24	1.61	5 (21%)
5	GOL	A	814	-	5,5,5	0.30	0	5,5,5	0.78	0
4	GSH	A	799	-	18,19,19	1.17	2 (11%)	23,24,24	2.39	13 (56%)
5	GOL	C	812	-	5,5,5	0.51	0	5,5,5	1.13	0
5	GOL	D	809	-	5,5,5	0.40	0	5,5,5	0.59	0
4	GSH	D	805	-	18,19,19	1.36	4 (22%)	23,24,24	2.56	8 (34%)
5	GOL	C	808	-	5,5,5	0.47	0	5,5,5	0.82	0
4	GSH	C	803	2	18,19,19	1.35	3 (16%)	23,24,24	1.09	2 (8%)
5	GOL	C	810	-	5,5,5	0.45	0	5,5,5	1.04	0
4	GSH	C	804	-	18,19,19	1.20	4 (22%)	23,24,24	4.72	14 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GSH	B	801	-	18,19,19	1.27	2 (11%)	23,24,24	2.20	9 (39%)
5	GOL	C	813	-	5,5,5	0.42	0	5,5,5	1.01	0
5	GOL	B	806	-	5,5,5	0.42	0	5,5,5	0.80	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
4	GSH	C	802	-	1/1/6/8	3/24/24/24	-
5	GOL	A	811	-	-	2/4/4/4	-
5	GOL	D	807	-	-	1/4/4/4	-
4	GSH	A	800	2	1/1/6/8	2/24/24/24	-
5	GOL	A	814	-	-	2/4/4/4	-
4	GSH	A	799	-	-	7/24/24/24	-
5	GOL	C	812	-	-	1/4/4/4	-
5	GOL	D	809	-	-	1/4/4/4	-
4	GSH	D	805	-	1/1/6/8	9/24/24/24	-
5	GOL	C	808	-	-	2/4/4/4	-
4	GSH	C	803	2	1/1/6/8	1/24/24/24	-
5	GOL	C	810	-	-	2/4/4/4	-
4	GSH	C	804	-	1/1/6/8	12/24/24/24	-
4	GSH	B	801	-	1/1/6/8	5/24/24/24	-
5	GOL	C	813	-	-	4/4/4/4	-
5	GOL	B	806	-	-	4/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	805	GSH	O12-C1	-3.16	1.20	1.30
4	B	801	GSH	O12-C1	-3.04	1.20	1.30
4	D	805	GSH	O2-C2	-2.78	1.17	1.23
4	A	799	GSH	O12-C1	-2.72	1.21	1.30
4	C	803	GSH	CB2-CA2	-2.66	1.50	1.53
4	A	800	GSH	O12-C1	-2.61	1.22	1.30
4	C	804	GSH	O12-C1	-2.58	1.22	1.30
4	D	805	GSH	O32-C3	-2.53	1.22	1.30
4	D	805	GSH	CG1-CD1	2.48	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	799	GSH	O32-C3	-2.42	1.22	1.30
4	C	803	GSH	O32-C3	-2.35	1.22	1.30
4	C	802	GSH	O32-C3	-2.33	1.22	1.30
4	C	804	GSH	O32-C3	-2.31	1.23	1.30
4	C	804	GSH	CA2-N2	2.23	1.50	1.45
4	A	800	GSH	CB1-CA1	2.16	1.57	1.53
4	B	801	GSH	CB2-CA2	2.13	1.55	1.53
4	C	803	GSH	CA3-C3	2.13	1.55	1.51
4	C	804	GSH	CB2-SG2	-2.11	1.77	1.81

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	804	GSH	CB2-CA2-C2	-10.94	87.20	109.76
4	C	804	GSH	CA2-C2-N3	9.26	135.21	116.54
4	C	804	GSH	CA2-CB2-SG2	7.40	122.52	114.19
4	C	804	GSH	CB2-CA2-N2	6.68	120.82	111.28
4	D	805	GSH	CA3-N3-C2	-6.56	105.13	121.37
4	C	804	GSH	C2-CA2-N2	5.87	127.14	111.16
4	C	804	GSH	CA2-N2-CD1	-5.66	107.09	121.65
4	C	804	GSH	CA3-N3-C2	-5.36	108.09	121.37
4	C	804	GSH	CB1-CG1-CD1	-4.95	101.98	113.04
4	C	802	GSH	CB1-CA1-C1	4.87	121.89	110.30
4	A	800	GSH	CA2-CB2-SG2	-4.71	108.91	114.19
4	B	801	GSH	O12-C1-CA1	4.59	129.00	113.38
4	C	804	GSH	O2-C2-N3	-4.47	113.40	122.99
4	A	799	GSH	CA3-N3-C2	-4.46	110.31	121.37
4	C	804	GSH	O2-C2-CA2	-4.44	111.11	120.45
4	D	805	GSH	O2-C2-N3	-4.42	113.50	122.99
4	B	801	GSH	O11-C1-CA1	-4.29	107.01	122.14
4	D	805	GSH	CA2-C2-N3	4.12	124.85	116.54
4	A	799	GSH	CB1-CA1-N1	4.10	120.91	110.17
4	D	805	GSH	CA2-CB2-SG2	-4.05	109.64	114.19
4	C	804	GSH	CG1-CB1-CA1	3.75	122.58	113.84
4	B	801	GSH	CB1-CA1-C1	3.64	118.97	110.30
4	D	805	GSH	O12-C1-CA1	3.61	125.69	113.38
4	A	799	GSH	CA2-C2-N3	3.31	123.22	116.54
4	A	799	GSH	C3-CA3-N3	3.27	123.13	113.06
4	C	804	GSH	CB1-CA1-N1	3.25	118.70	110.17
4	A	799	GSH	CB1-CA1-C1	3.10	117.69	110.30
4	A	800	GSH	CB1-CG1-CD1	3.07	119.89	113.04
4	B	801	GSH	CG1-CD1-N2	3.05	121.12	115.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	805	GSH	CB1-CA1-C1	3.03	117.53	110.30
4	A	799	GSH	O12-C1-O11	-2.82	117.69	124.09
4	D	805	GSH	O11-C1-CA1	-2.80	112.27	122.14
4	B	801	GSH	C2-CA2-N2	-2.79	103.56	111.16
4	A	799	GSH	CA2-CB2-SG2	-2.77	111.08	114.19
4	B	801	GSH	CG1-CB1-CA1	2.73	120.20	113.84
4	A	799	GSH	CB2-CA2-N2	-2.63	107.54	111.28
4	A	800	GSH	O12-C1-O11	-2.59	118.21	124.09
4	C	804	GSH	O32-C3-CA3	2.55	121.59	112.74
4	B	801	GSH	CA3-N3-C2	-2.54	115.08	121.37
4	C	802	GSH	O12-C1-O11	-2.42	118.59	124.09
4	A	799	GSH	O11-C1-CA1	2.33	130.35	122.14
4	B	801	GSH	CB1-CA1-N1	2.26	116.09	110.17
4	A	799	GSH	C2-CA2-N2	-2.26	105.01	111.16
4	A	799	GSH	CG1-CD1-N2	2.23	119.70	115.83
4	A	799	GSH	OE1-CD1-CG1	-2.17	118.04	122.02
4	C	804	GSH	CB1-CA1-C1	2.15	115.42	110.30
4	A	800	GSH	O12-C1-CA1	2.14	120.69	113.38
4	D	805	GSH	O32-C3-CA3	2.13	120.16	112.74
4	C	802	GSH	CG1-CB1-CA1	2.10	118.74	113.84
4	A	800	GSH	CA2-C2-N3	-2.08	112.35	116.54
4	C	803	GSH	C2-CA2-N2	2.08	116.81	111.16
4	C	803	GSH	CA2-CB2-SG2	-2.06	111.88	114.19
4	A	799	GSH	O2-C2-CA2	-2.05	116.14	120.45
4	B	801	GSH	CA2-CB2-SG2	2.03	116.48	114.19
5	D	807	GOL	O1-C1-C2	2.03	119.92	110.20

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	800	GSH	CA1
4	B	801	GSH	CA1
4	C	802	GSH	CA1
4	C	803	GSH	CA1
4	C	804	GSH	CA1
4	D	805	GSH	CA1

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	799	GSH	C1-CA1-CB1-CG1
4	A	800	GSH	O11-C1-CA1-N1

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Mol	Chain	Res	Type	Atoms
4	B	801	GSH	O11-C1-CA1-N1
4	B	801	GSH	N1-CA1-CB1-CG1
4	B	801	GSH	C1-CA1-CB1-CG1
4	C	802	GSH	C1-CA1-CB1-CG1
4	C	804	GSH	O11-C1-CA1-N1
4	C	804	GSH	CG1-CD1-N2-CA2
4	C	804	GSH	OE1-CD1-N2-CA2
4	C	804	GSH	N2-CA2-CB2-SG2
4	D	805	GSH	O31-C3-CA3-N3
4	D	805	GSH	O32-C3-CA3-N3
5	A	811	GOL	C1-C2-C3-O3
5	B	806	GOL	O1-C1-C2-C3
5	B	806	GOL	C1-C2-C3-O3
5	B	806	GOL	O2-C2-C3-O3
5	C	808	GOL	O1-C1-C2-C3
5	C	810	GOL	C1-C2-C3-O3
5	C	813	GOL	O1-C1-C2-C3
4	A	799	GSH	O2-C2-N3-CA3
4	C	804	GSH	O2-C2-N3-CA3
4	D	805	GSH	O2-C2-N3-CA3
4	C	804	GSH	CA2-C2-N3-CA3
4	D	805	GSH	CA2-C2-N3-CA3
4	B	801	GSH	O12-C1-CA1-N1
4	D	805	GSH	O12-C1-CA1-N1
4	A	799	GSH	CA2-C2-N3-CA3
4	D	805	GSH	CA1-CB1-CG1-CD1
4	C	804	GSH	O12-C1-CA1-N1
5	C	813	GOL	O1-C1-C2-O2
4	A	799	GSH	O31-C3-CA3-N3
5	A	814	GOL	C1-C2-C3-O3
5	C	813	GOL	C1-C2-C3-O3
5	A	811	GOL	O2-C2-C3-O3
4	A	799	GSH	O32-C3-CA3-N3
4	A	800	GSH	O12-C1-CA1-N1
5	B	806	GOL	O1-C1-C2-O2
5	C	808	GOL	O1-C1-C2-O2
4	D	805	GSH	O11-C1-CA1-CB1
5	D	809	GOL	O1-C1-C2-O2
4	C	802	GSH	O11-C1-CA1-N1
4	D	805	GSH	O11-C1-CA1-N1
4	D	805	GSH	O12-C1-CA1-CB1
4	C	804	GSH	C1-CA1-CB1-CG1

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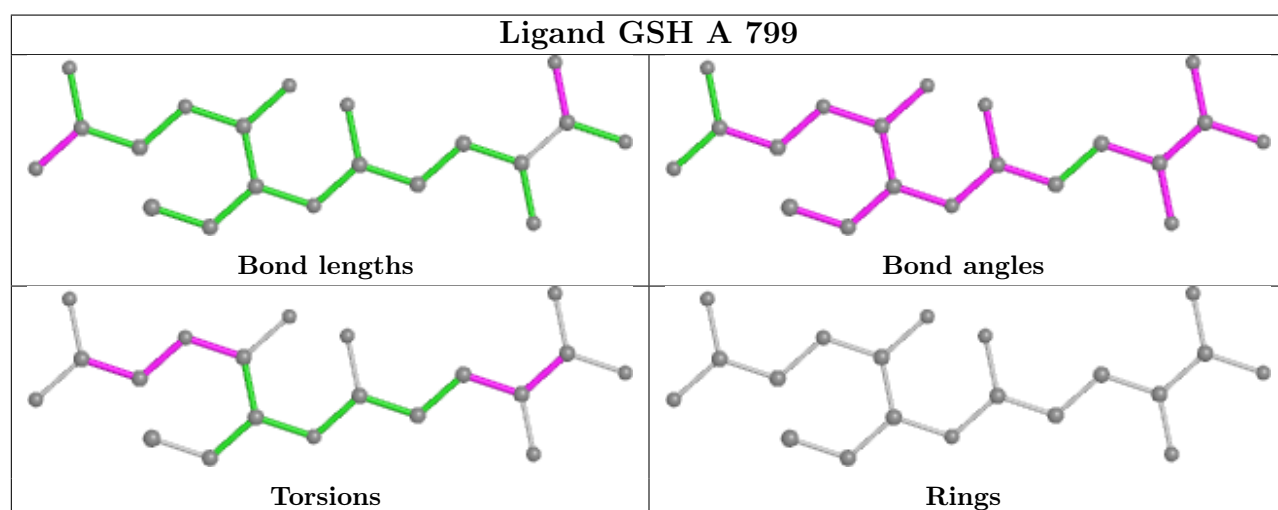
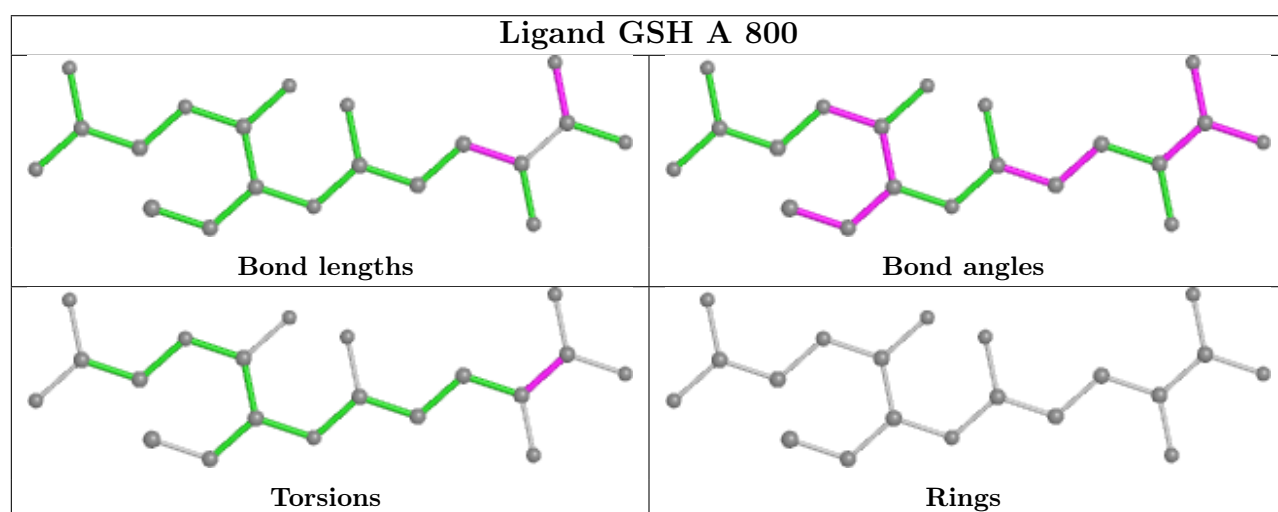
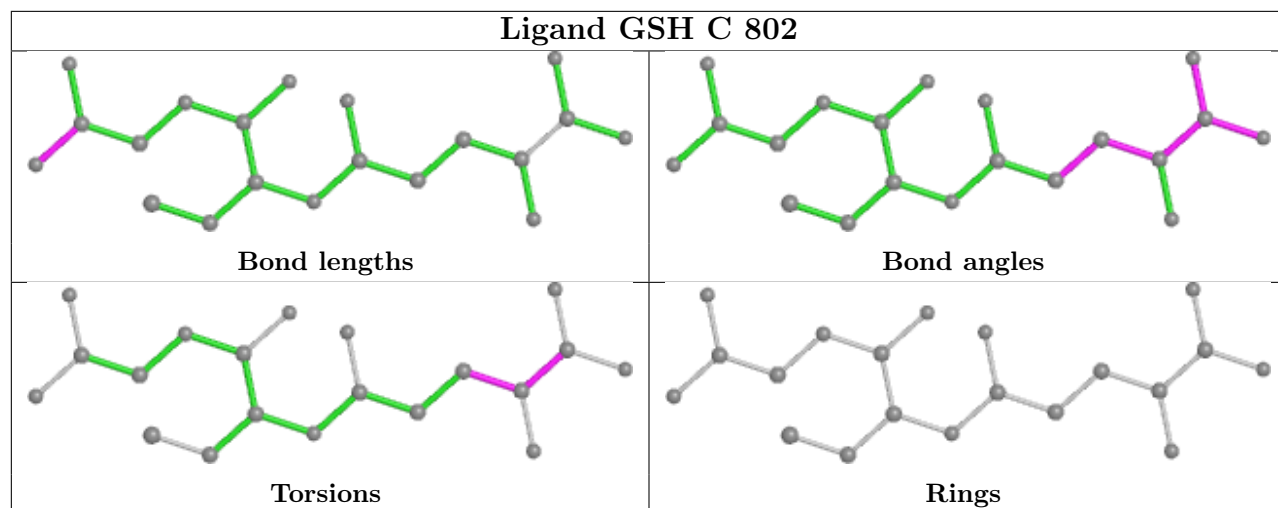
Mol	Chain	Res	Type	Atoms
4	C	804	GSH	CA1-CB1-CG1-CD1
5	C	810	GOL	O2-C2-C3-O3
4	C	804	GSH	C2-CA2-CB2-SG2
5	C	813	GOL	O2-C2-C3-O3
4	B	801	GSH	O31-C3-CA3-N3
4	C	803	GSH	CA1-CB1-CG1-CD1
4	C	802	GSH	O12-C1-CA1-N1
5	A	814	GOL	O2-C2-C3-O3
4	A	799	GSH	C3-CA3-N3-C2
4	A	799	GSH	O12-C1-CA1-N1
5	C	812	GOL	C1-C2-C3-O3
4	C	804	GSH	O32-C3-CA3-N3
5	D	807	GOL	O2-C2-C3-O3
4	C	804	GSH	O31-C3-CA3-N3

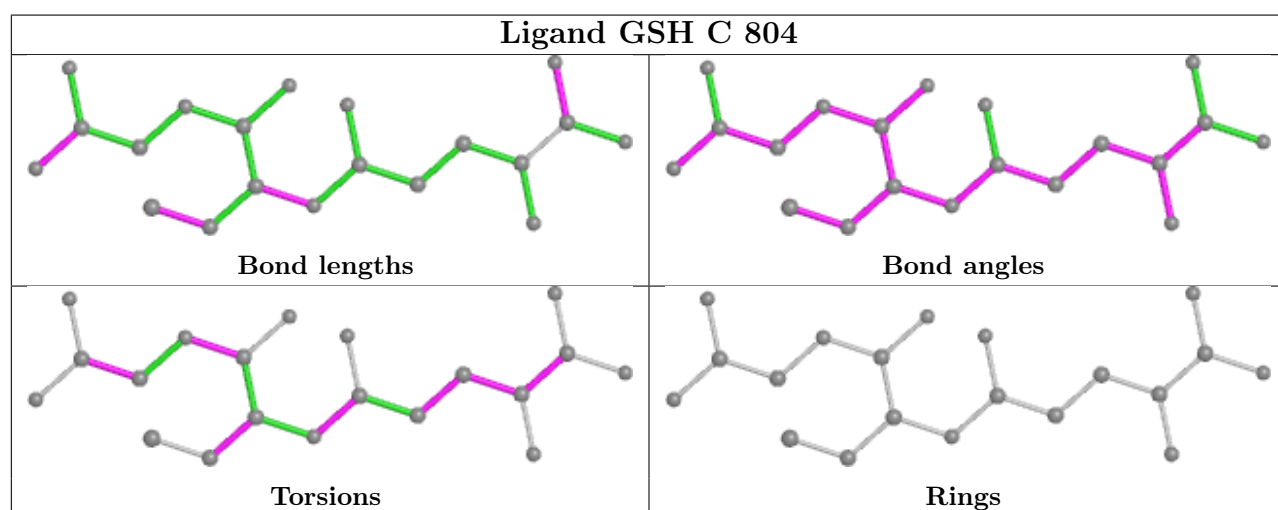
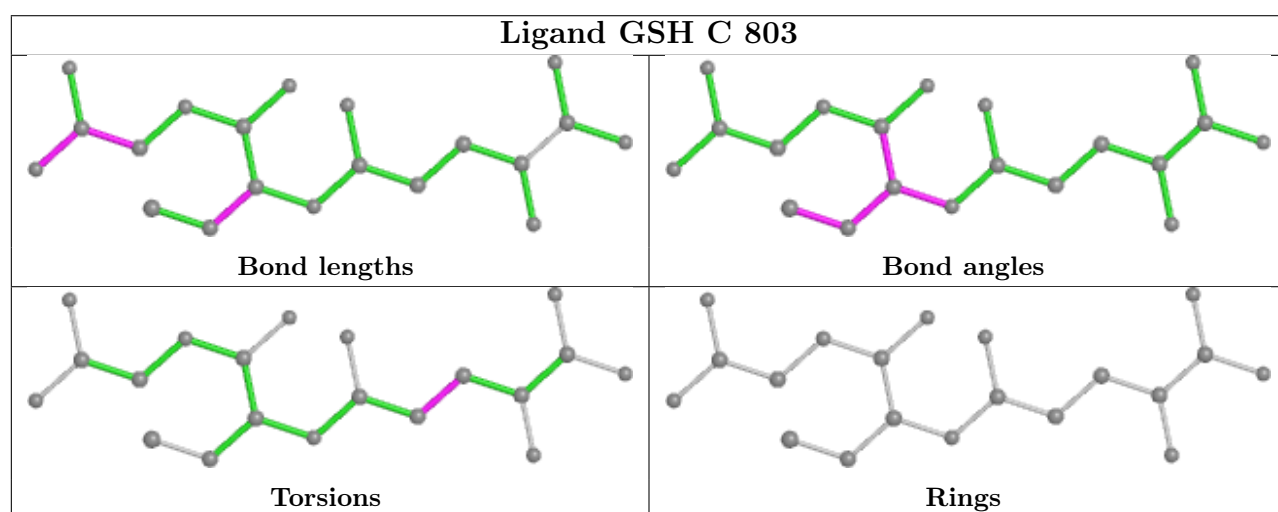
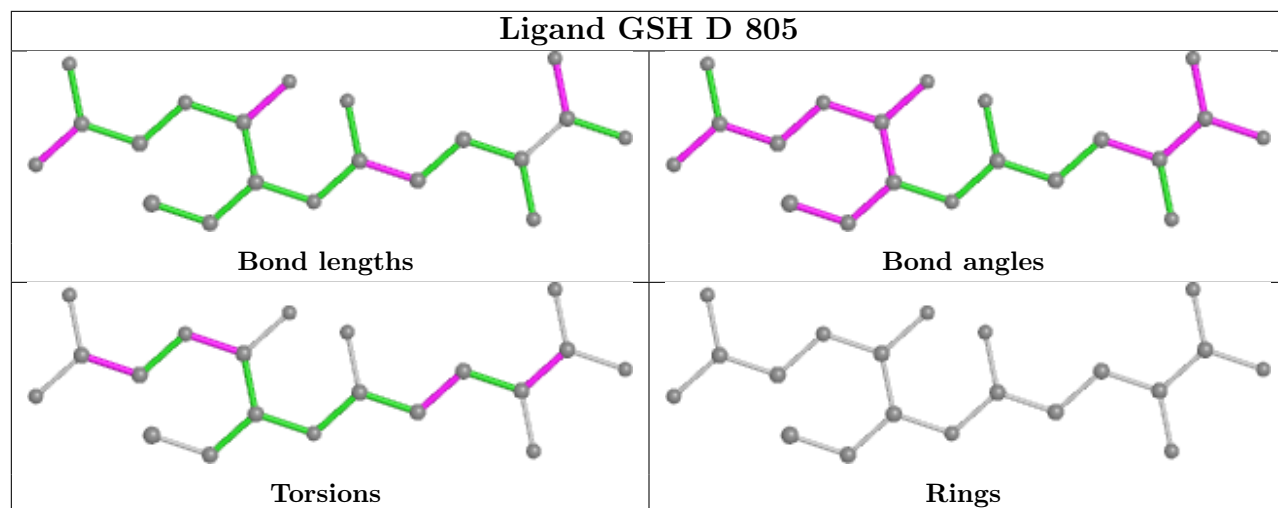
There are no ring outliers.

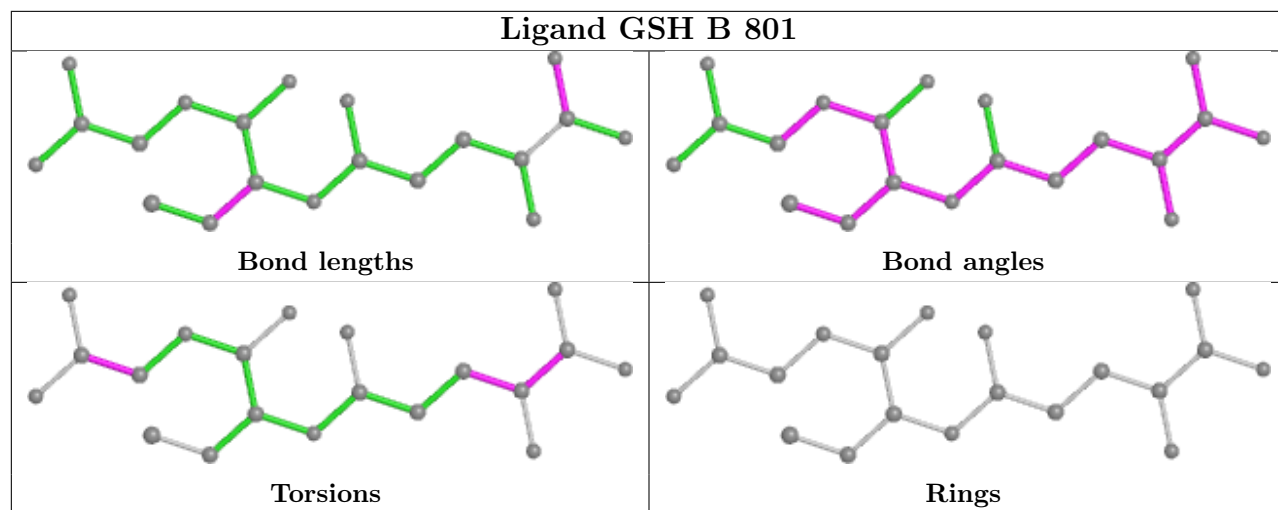
9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	802	GSH	2	0
5	D	807	GOL	1	0
5	A	814	GOL	5	0
4	A	799	GSH	2	0
5	C	812	GOL	4	0
4	D	805	GSH	2	0
4	C	803	GSH	1	0
5	C	810	GOL	1	0
5	B	806	GOL	1	0

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







## 5.7 Other polymers [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	228/231 (98%)	0.37	15 (6%) 18 26	16, 23, 55, 84	0
1	B	224/231 (96%)	0.57	27 (12%) 4 7	20, 28, 56, 66	1 (0%)
1	C	227/231 (98%)	0.40	21 (9%) 8 14	19, 25, 53, 76	1 (0%)
1	D	223/231 (96%)	0.84	40 (17%) 1 1	23, 33, 66, 75	0
All	All	902/924 (97%)	0.54	103 (11%) 5 8	16, 27, 61, 84	2 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	VAL	12.1
1	A	229	GLY	10.4
1	A	2	ALA	9.9
1	D	156	GLY	9.1
1	B	158	GLY	8.7
1	C	93	GLY	8.5
1	C	91	ASN	8.3
1	A	158	GLY	7.7
1	B	156	GLY	7.5
1	A	156	GLY	7.0
1	B	157	GLY	6.9
1	A	91	ASN	6.9
1	B	123	TRP	6.5
1	D	132	ALA	6.3
1	C	92	SER	6.2
1	D	157	GLY	6.2
1	D	92	SER	6.1
1	A	93	GLY	6.0
1	C	156	GLY	5.9
1	D	158	GLY	5.7
1	C	90	ALA	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	91	ASN	5.5
1	B	223	VAL	5.3
1	D	90	ALA	5.3
1	A	228	TYR	5.3
1	A	157	GLY	5.2
1	D	3	GLU	5.1
1	C	94	ASP	5.1
1	B	159	GLY	5.0
1	D	131	ALA	4.9
1	A	4	GLU	4.7
1	B	124	ARG	4.6
1	D	127	GLY	4.6
1	D	4[A]	GLU	4.4
1	D	159	GLY	4.4
1	B	3	GLU	4.4
1	C	3	GLU	4.4
1	B	126	LYS	4.4
1	D	123	TRP	4.1
1	D	221	VAL	4.1
1	A	5	LYS	4.0
1	D	223	VAL	3.9
1	B	91	ASN	3.9
1	A	3	GLU	3.8
1	D	128	GLU	3.8
1	A	90	ALA	3.7
1	D	224	LEU	3.7
1	C	228	TYR	3.7
1	B	92	SER	3.7
1	D	185	PHE	3.6
1	B	125	LEU	3.6
1	C	157	GLY	3.6
1	D	125	LEU	3.6
1	B	90	ALA	3.5
1	C	4	GLU	3.5
1	D	130	GLN	3.5
1	C	159	GLY	3.4
1	B	4	GLU	3.4
1	C	158	GLY	3.4
1	B	122	LEU	3.4
1	A	92	SER	3.3
1	C	229	GLY	3.3
1	B	120	SER	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	73	LEU	3.0
1	B	222	GLY	3.0
1	C	95	ALA	3.0
1	D	135	ARG	3.0
1	D	133	ALA	2.9
1	B	116	TYR	2.9
1	C	5	LYS	2.9
1	A	159	GLY	2.8
1	D	126	LYS	2.8
1	C	226	LYS	2.7
1	D	183	GLY	2.7
1	C	72	ILE	2.7
1	D	70	LEU	2.7
1	D	155	GLY	2.6
1	B	224	LEU	2.5
1	D	134	GLY	2.5
1	B	70	LEU	2.5
1	D	89	PRO	2.5
1	D	116	TYR	2.5
1	C	70	LEU	2.4
1	B	5[A]	LYS	2.4
1	D	129	PRO	2.4
1	B	121	ARG	2.3
1	B	131	ALA	2.3
1	D	225	LYS	2.3
1	D	218	TYR	2.3
1	D	124	ARG	2.3
1	D	168	ALA	2.3
1	D	222	GLY	2.2
1	D	184	GLY	2.2
1	D	121	ARG	2.2
1	B	218	TYR	2.2
1	C	23	ILE	2.2
1	B	133	ALA	2.2
1	D	108	ALA	2.1
1	B	155	GLY	2.1
1	D	136	GLU	2.1
1	D	138	ALA	2.1
1	C	164	PHE	2.1
1	B	23	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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<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	CL	A	838	1/1	0.30	0.16	93,93,93,93	0
5	GOL	C	812	6/6	0.68	0.23	63,67,69,69	0
5	GOL	A	811	6/6	0.74	0.23	73,80,80,81	0
5	GOL	C	810	6/6	0.75	0.21	48,53,56,63	0
3	CL	B	831	1/1	0.77	0.18	70,70,70,70	0
5	GOL	A	814	6/6	0.77	0.32	69,72,74,78	0
4	GSH	C	804	20/20	0.78	0.30	46,73,81,81	20
3	CL	C	828	1/1	0.83	0.17	67,67,67,67	0
3	CL	A	826	1/1	0.85	0.30	73,73,73,73	0
5	GOL	B	806	6/6	0.86	0.25	65,75,77,78	0
3	CL	A	825	1/1	0.87	0.26	65,65,65,65	0
5	GOL	D	809	6/6	0.87	0.15	52,61,62,64	0
4	GSH	C	802	20/20	0.89	0.12	32,39,51,53	0
5	GOL	C	813	6/6	0.89	0.11	48,64,67,69	0
2	MG	A	817	1/1	0.89	0.19	60,60,60,60	0
3	CL	A	827	1/1	0.90	0.09	62,62,62,62	0
4	GSH	A	799	20/20	0.91	0.12	29,33,54,56	0
3	CL	D	834	1/1	0.91	0.09	58,58,58,58	0
3	CL	B	835	1/1	0.92	0.27	68,68,68,68	0
4	GSH	D	805	20/20	0.92	0.13	35,43,57,58	0
4	GSH	C	803	20/20	0.92	0.12	32,37,68,69	0
3	CL	D	832	1/1	0.93	0.33	79,79,79,79	0
5	GOL	C	808	6/6	0.93	0.13	43,54,56,57	0
3	CL	A	836	1/1	0.94	0.18	61,61,61,61	0
4	GSH	A	800	20/20	0.94	0.13	33,39,69,73	0
5	GOL	D	807	6/6	0.94	0.18	40,55,58,59	0
4	GSH	B	801	20/20	0.94	0.11	29,39,57,58	0

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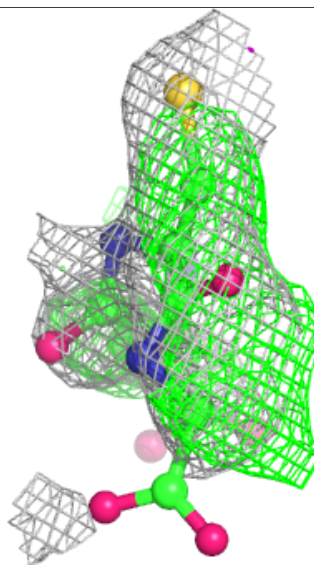
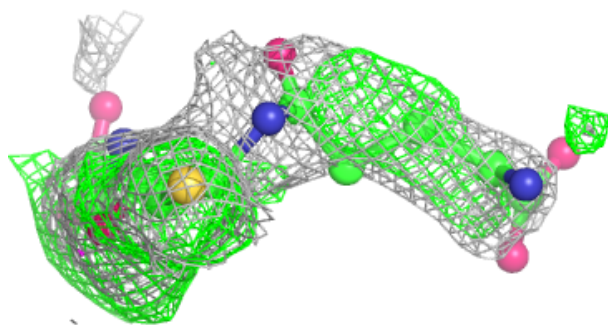
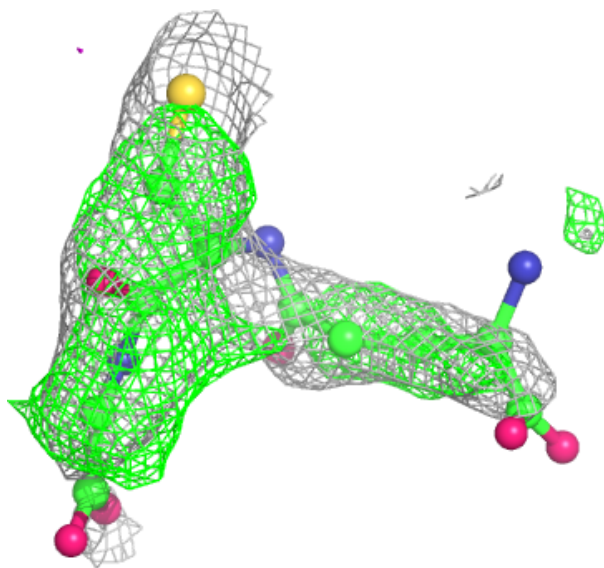
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	B	820	1/1	0.95	0.09	65,65,65,65	0
3	CL	C	829	1/1	0.95	0.11	74,74,74,74	0
3	CL	A	837	1/1	0.95	0.23	72,72,72,72	0
3	CL	A	823	1/1	0.95	0.20	58,58,58,58	0
2	MG	C	816	1/1	0.96	0.08	41,41,41,41	0
3	CL	D	819	1/1	0.96	0.16	55,55,55,55	0
3	CL	C	830	1/1	0.97	0.18	65,65,65,65	0
3	CL	C	822	1/1	0.98	0.10	52,52,52,52	0
3	CL	D	821	1/1	0.98	0.04	51,51,51,51	0
2	MG	A	815	1/1	0.98	0.04	38,38,38,38	0
3	CL	C	833	1/1	0.98	0.07	52,52,52,52	0
3	CL	C	824	1/1	0.99	0.03	54,54,54,54	0

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

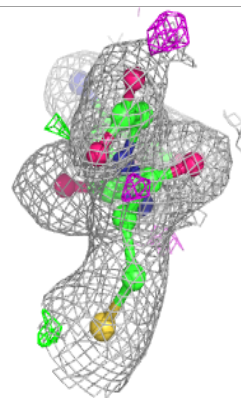
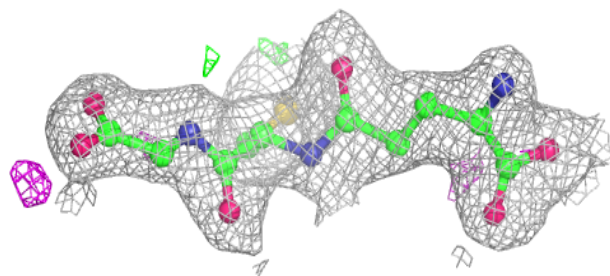
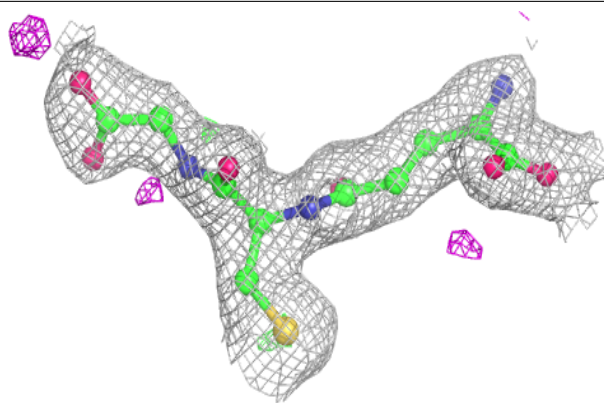
**Electron density around GSH C 804:**

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

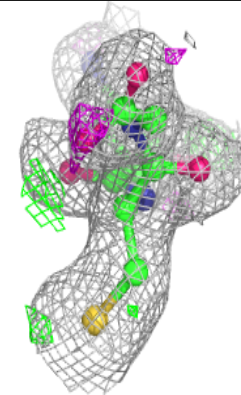
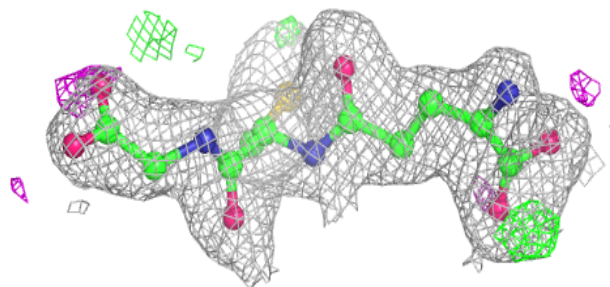
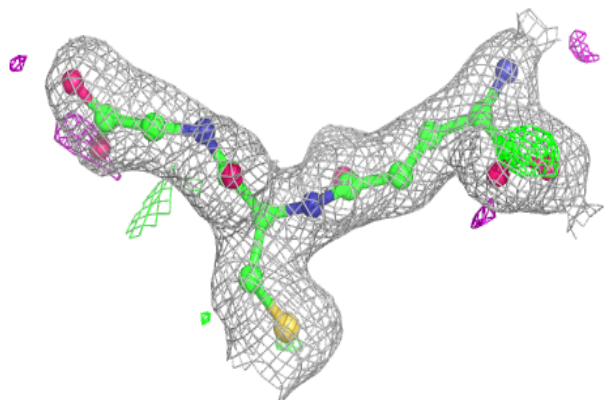


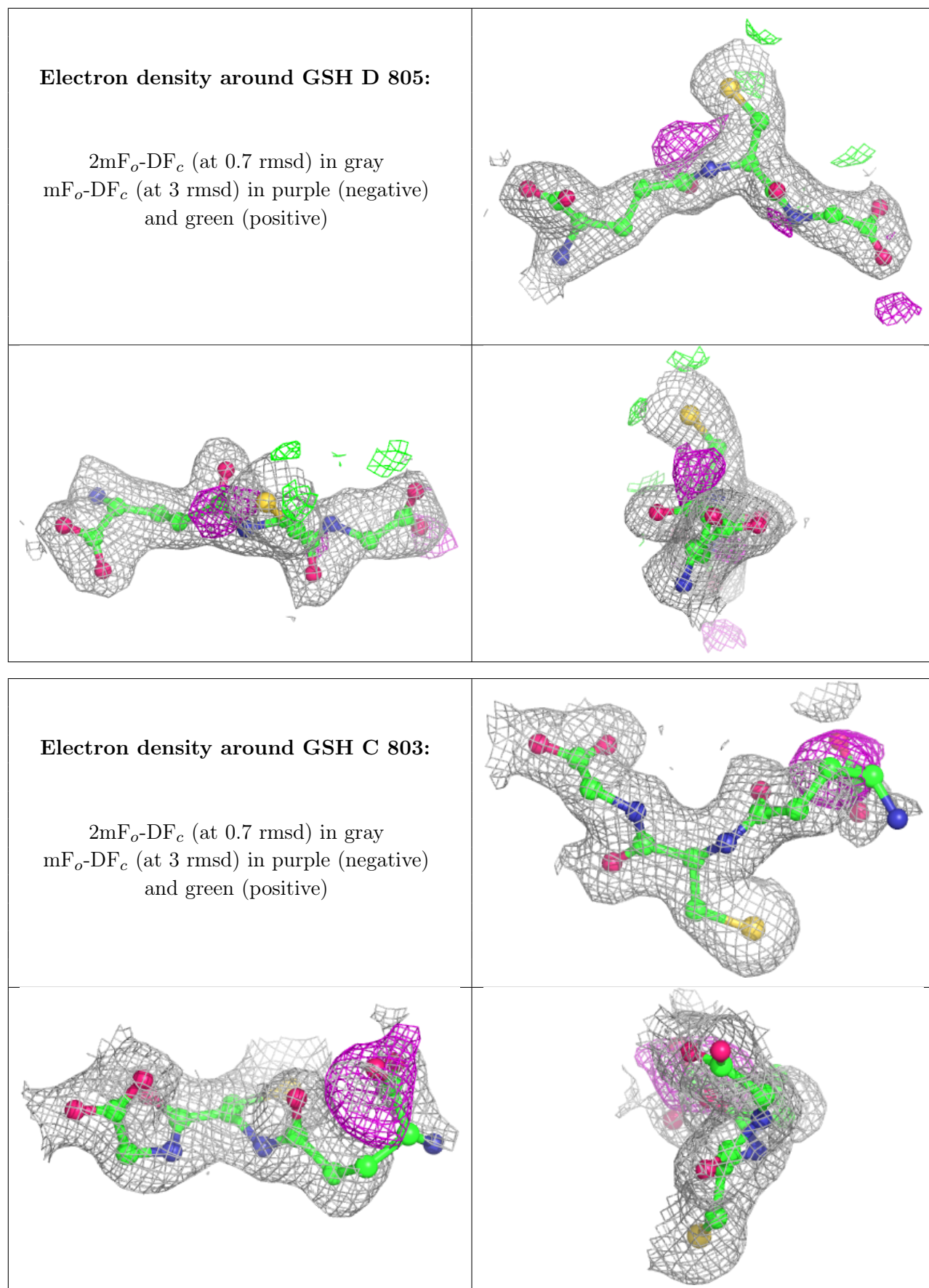
**Electron density around GSH C 802:**

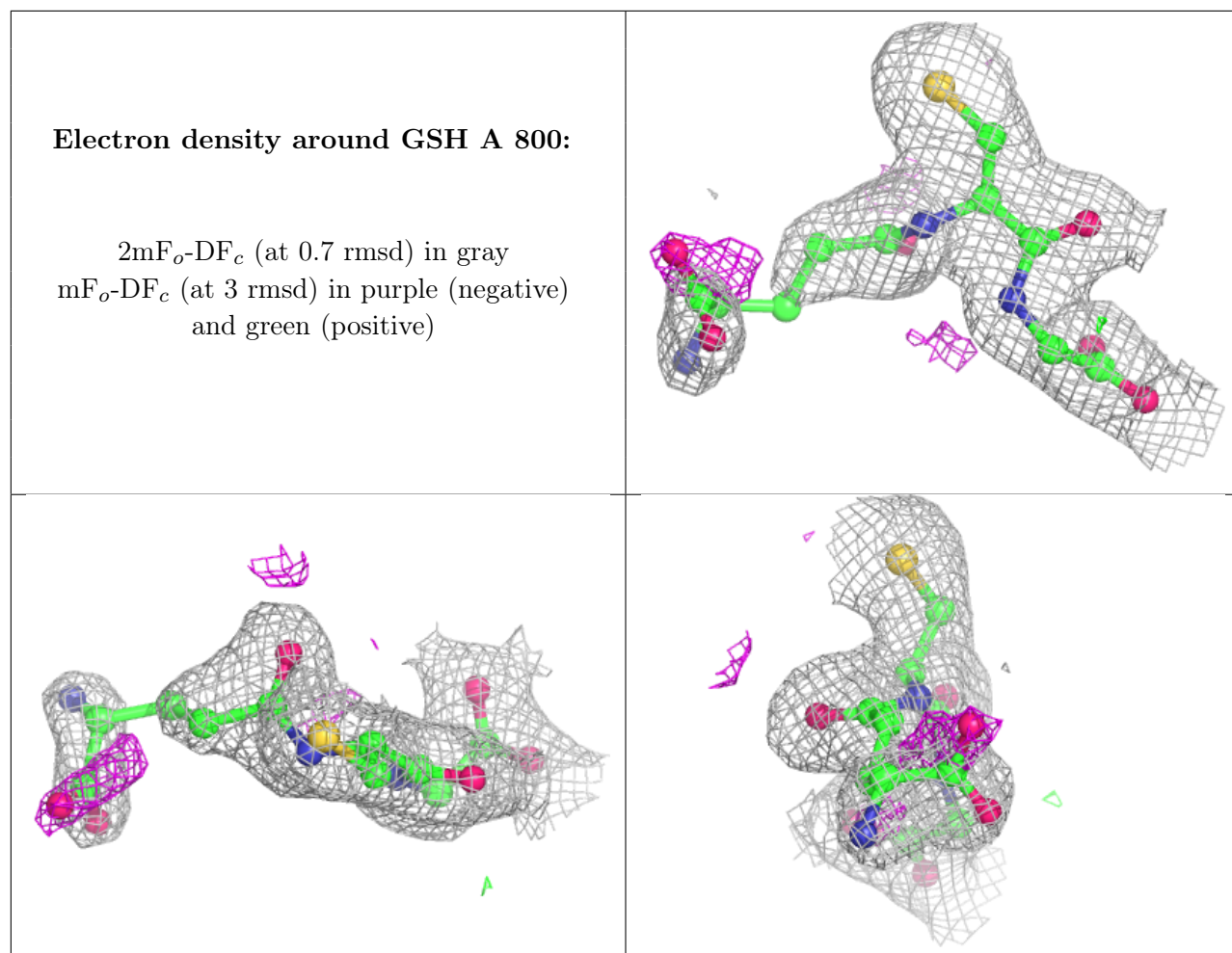
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

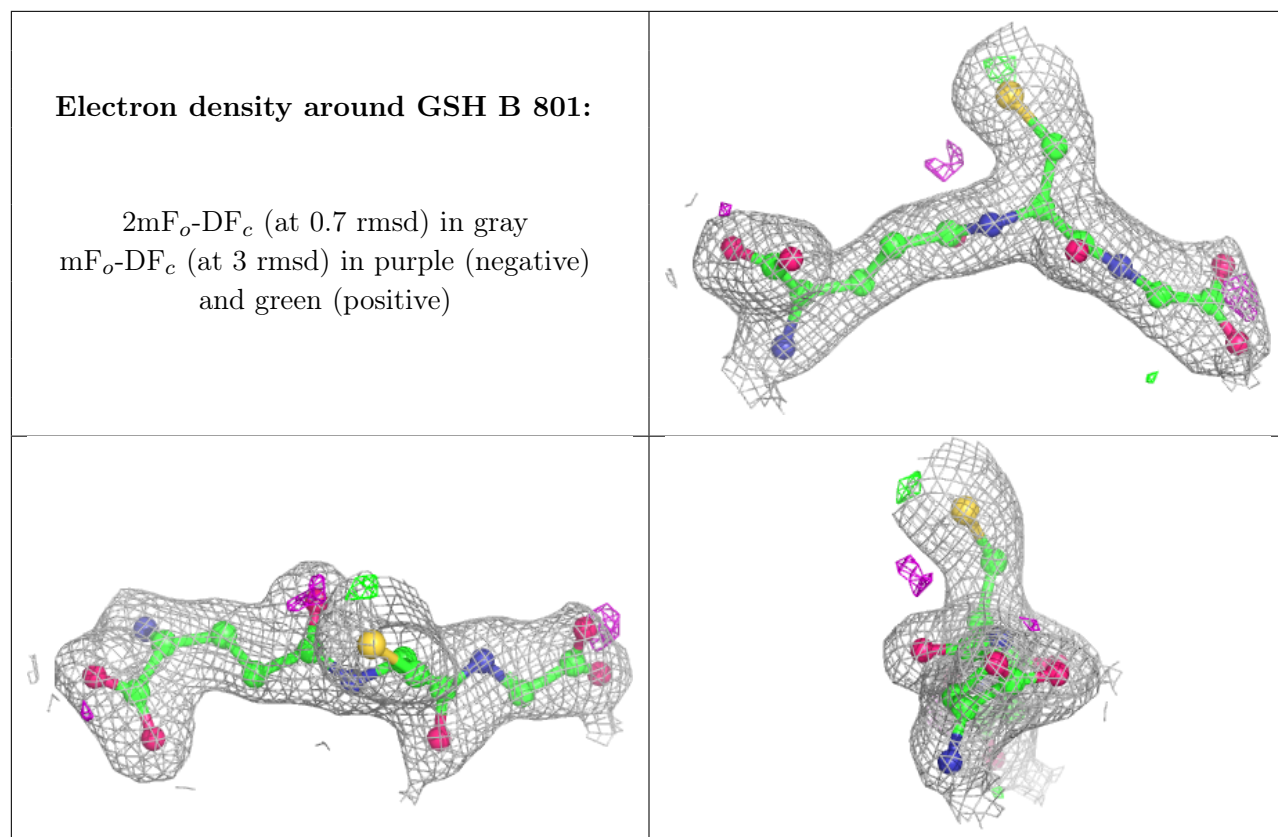
**Electron density around GSH A 799:**

$2mF_o-DF_c$  (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.