Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:30 PM UTC

PDB ID	:	3VWX / pdb_00003vwx
Title	:	Structural analysis of an epsilon-class glutathione S-transferase from housefly, Musca domestica
Authors	:	Nakamura, C.; Sue, M.; Miyamoto, T.; Yajima, S.
Deposited on	:	2012-09-05
Resolution	:	1.80 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*
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:

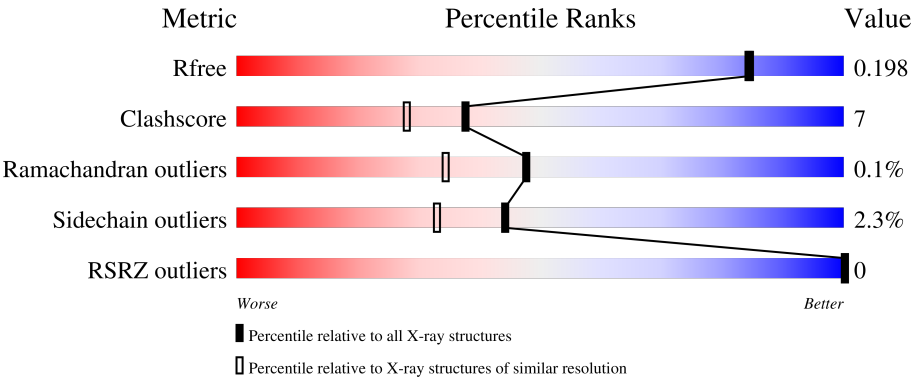
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	A	222	78% 18%
1	B	222	81% 17%
1	C	222	88% 10%
1	D	222	87% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8000 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.

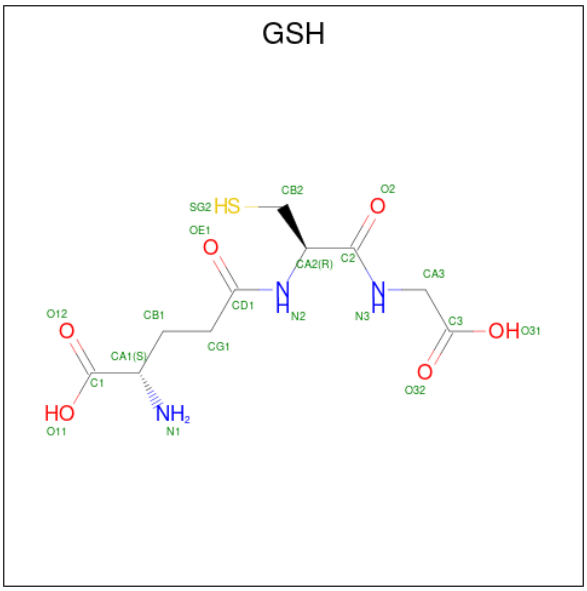
- Molecule 1 is a protein called Glutathione s-transferase 6B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1739	1132	284	318	5			
1	B	218	Total	C	N	O	S	0	0	0
			1739	1132	284	318	5			
1	C	220	Total	C	N	O	S	0	0	0
			1754	1142	286	321	5			
1	D	220	Total	C	N	O	S	0	0	0
			1754	1142	286	321	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	ALA	PRO	engineered mutation	UNP Q9U795
B	70	ALA	PRO	engineered mutation	UNP Q9U795
C	70	ALA	PRO	engineered mutation	UNP Q9U795
D	70	ALA	PRO	engineered mutation	UNP Q9U795

- Molecule 2 is GLUTATHIONE (CCD ID: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



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	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is water.

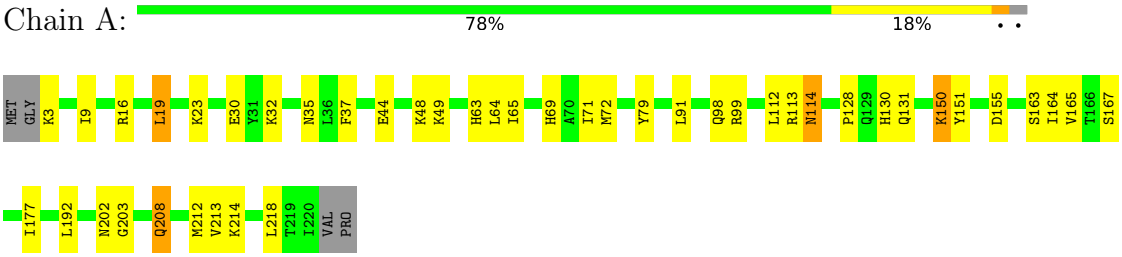
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	231	Total	O	0	0
			231	231		
3	B	235	Total	O	0	0
			235	235		
3	C	246	Total	O	0	0
			246	246		
3	D	222	Total	O	0	0
			222	222		

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.

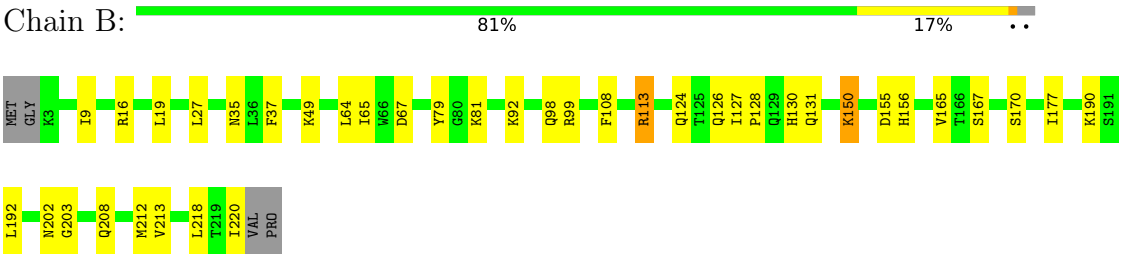
• Molecule 1: Glutathione s-transferase 6B

Chain A:



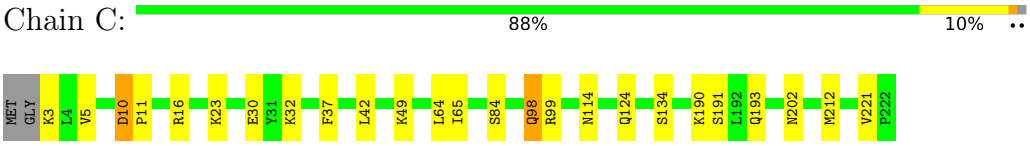
• Molecule 1: Glutathione s-transferase 6B

Chain B:



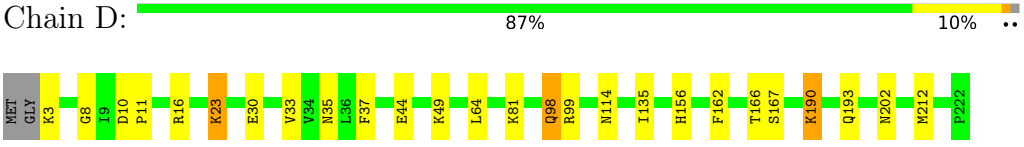
• Molecule 1: Glutathione s-transferase 6B

Chain C:



• Molecule 1: Glutathione s-transferase 6B

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	87.55Å 87.55Å 131.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.82 – 1.80 65.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (65.82-1.80) 98.3 (65.82-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.164 , 0.191 0.170 , 0.198	Depositor DCC
R_{free} test set	5131 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l 0.068 for h,-h-k,-l 0.068 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8000	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GSH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.48	7/1781 (0.4%)	1.09	1/2414 (0.0%)
1	B	1.47	7/1781 (0.4%)	1.09	0/2414
1	C	1.37	4/1797 (0.2%)	1.05	3/2436 (0.1%)
1	D	1.35	3/1797 (0.2%)	1.06	0/2436
All	All	1.42	21/7156 (0.3%)	1.07	4/9700 (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	A	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	LEU	N-CA	6.50	1.54	1.46
1	B	19	LEU	N-CA	6.31	1.53	1.46
1	D	135	ILE	N-CA	6.25	1.53	1.46
1	B	108	PHE	CA-C	-5.76	1.45	1.52
1	B	177	ILE	N-CA	-5.71	1.39	1.46
1	D	98	GLN	CD-NE2	-5.65	1.21	1.33
1	B	27	LEU	CA-CB	5.61	1.61	1.53
1	C	134	SER	C-O	-5.59	1.17	1.24
1	A	71	ILE	N-CA	5.56	1.53	1.46
1	C	98	GLN	CD-NE2	-5.49	1.21	1.33
1	A	203	GLY	N-CA	5.46	1.52	1.45
1	D	114	ASN	CA-CB	-5.45	1.44	1.53
1	A	69	HIS	N-CA	-5.42	1.39	1.46
1	B	170	SER	N-CA	-5.38	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	TYR	N-CA	5.29	1.52	1.45
1	A	208	GLN	N-CA	-5.26	1.40	1.46
1	A	79	TYR	N-CA	5.26	1.52	1.45
1	A	177	ILE	N-CA	-5.26	1.40	1.46
1	C	84	SER	CA-C	5.26	1.59	1.52
1	C	65	ILE	CB-CG1	-5.13	1.43	1.53
1	B	203	GLY	N-CA	5.08	1.52	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ASN	N-CA-C	5.63	118.95	111.75
1	C	10	ASP	CA-C-N	-5.32	114.19	119.56
1	C	10	ASP	C-N-CA	-5.32	114.19	119.56
1	C	221	VAL	CA-C-O	5.03	122.46	119.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	LYS	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	1739	0	1759	33	0
1	B	1739	0	1759	28	0
1	C	1754	0	1775	16	0
1	D	1754	0	1775	22	0
2	A	20	0	15	0	0
2	B	20	0	15	0	0
2	C	20	0	15	0	0
2	D	20	0	15	0	0
3	A	231	0	0	5	0
3	B	235	0	0	5	0
3	C	246	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	222	0	0	6	0
All	All	8000	0	7128	99	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 7.

All (99) 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:114:ASN:HB3	3:C:889:HOH:O	1.49	1.12
1:B:150:LYS:HD2	1:B:150:LYS:H	1.11	1.08
1:A:150:LYS:H	1:A:150:LYS:HD2	1.28	0.96
1:D:156:HIS:HE1	3:D:1077:HOH:O	1.51	0.93
1:B:150:LYS:HD2	1:B:150:LYS:N	1.87	0.87
1:C:98:GLN:HE22	1:C:99:ARG:HH11	1.26	0.82
1:B:98:GLN:HE22	1:B:99:ARG:HH11	1.27	0.81
1:A:98:GLN:HE22	1:A:99:ARG:HH11	1.27	0.81
1:A:16:ARG:HH21	1:A:202:ASN:HD21	1.29	0.80
1:B:128:PRO:HD2	1:B:131:GLN:NE2	1.95	0.79
1:A:37:PHE:CZ	1:A:212:MET:HE1	2.17	0.79
1:B:156:HIS:HE1	3:B:910:HOH:O	1.66	0.78
1:B:37:PHE:CZ	1:B:212:MET:HE1	2.18	0.78
1:D:98:GLN:HE22	1:D:99:ARG:HH11	1.30	0.77
1:B:150:LYS:H	1:B:150:LYS:CD	1.84	0.75
1:A:150:LYS:H	1:A:150:LYS:CD	2.01	0.74
1:B:16:ARG:HH21	1:B:202:ASN:HD21	1.35	0.74
1:C:37:PHE:CD2	3:C:857:HOH:O	2.40	0.73
1:D:37:PHE:CD2	3:D:1035:HOH:O	2.40	0.73
1:B:65:ILE:HG22	3:B:908:HOH:O	1.87	0.73
1:D:3:LYS:HE3	1:D:30:GLU:HG2	1.69	0.73
1:C:124:GLN:NE2	3:C:953:HOH:O	2.22	0.72
1:A:16:ARG:HH21	1:A:202:ASN:ND2	1.89	0.71
1:A:63:HIS:ND1	3:A:819:HOH:O	2.24	0.71
1:D:98:GLN:NE2	1:D:99:ARG:HH11	1.92	0.67
1:C:98:GLN:NE2	1:C:99:ARG:HH11	1.93	0.67
1:B:16:ARG:HH21	1:B:202:ASN:ND2	1.94	0.66
1:B:208:GLN:O	1:B:212:MET:HG3	1.94	0.66
1:D:16:ARG:HH11	1:D:202:ASN:HD21	1.42	0.65
1:B:113:ARG:HD2	3:B:763:HOH:O	1.96	0.65
1:A:208:GLN:O	1:A:212:MET:HG3	1.97	0.64
1:B:165:VAL:HB	1:B:192:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:LYS:NZ	1:D:193:GLN:HE22	1.97	0.62
1:A:30:GLU:HG2	1:A:32:LYS:HE3	1.82	0.62
1:C:16:ARG:HH21	1:C:202:ASN:HD21	1.46	0.61
1:A:128:PRO:HB2	1:A:130:HIS:CE1	2.36	0.60
1:D:16:ARG:HH11	1:D:202:ASN:ND2	1.99	0.59
1:D:190:LYS:HE3	3:D:1039:HOH:O	2.02	0.59
1:A:165:VAL:HB	1:A:192:LEU:HD23	1.85	0.57
1:A:65:ILE:HG22	3:A:815:HOH:O	2.04	0.57
1:A:150:LYS:HD2	1:A:150:LYS:N	2.11	0.56
1:A:214:LYS:HE3	3:A:634:HOH:O	2.06	0.56
1:C:16:ARG:HH21	1:C:202:ASN:ND2	2.02	0.56
1:A:98:GLN:NE2	1:A:99:ARG:HH11	2.02	0.55
1:B:165:VAL:CB	1:B:192:LEU:HD23	2.35	0.55
1:B:98:GLN:NE2	1:B:99:ARG:HH11	2.01	0.55
1:B:213:VAL:HG13	1:B:218:LEU:HD11	1.86	0.55
1:A:49:LYS:HA	1:A:64:LEU:HD13	1.89	0.55
1:B:165:VAL:HB	1:B:192:LEU:CD2	2.38	0.54
1:A:128:PRO:CB	1:A:130:HIS:CE1	2.91	0.53
1:A:213:VAL:HG13	1:A:218:LEU:HD11	1.90	0.52
1:D:10:ASP:OD1	1:D:11:PRO:HD3	2.09	0.52
1:B:49:LYS:HA	1:B:64:LEU:HD13	1.91	0.52
1:A:16:ARG:HD2	1:A:202:ASN:ND2	2.26	0.51
1:D:156:HIS:CE1	3:D:1077:HOH:O	2.37	0.51
1:B:9:ILE:HD12	1:B:35:ASN:HA	1.93	0.51
1:C:30:GLU:OE2	1:C:32:LYS:NZ	2.44	0.51
1:B:150:LYS:HD3	1:B:155:ASP:OD1	2.11	0.50
1:A:114:ASN:HD22	1:A:131:GLN:CD	2.19	0.50
1:B:190:LYS:NZ	3:B:851:HOH:O	2.45	0.50
1:C:49:LYS:HA	1:C:64:LEU:HD13	1.94	0.50
1:A:150:LYS:HD3	1:A:155:ASP:HA	1.94	0.49
1:C:10:ASP:OD1	1:C:11:PRO:HD3	2.11	0.49
1:A:16:ARG:NH2	1:A:202:ASN:HD21	2.06	0.49
1:D:190:LYS:HA	1:D:193:GLN:HE21	1.77	0.49
1:C:16:ARG:HD2	1:C:202:ASN:ND2	2.28	0.48
1:A:165:VAL:CB	1:A:192:LEU:HD23	2.44	0.47
1:A:214:LYS:NZ	3:A:800:HOH:O	2.41	0.47
1:A:72:MET:HE1	1:A:163:SER:HB2	1.96	0.47
1:D:37:PHE:CZ	1:D:212:MET:HE1	2.48	0.47
1:C:114:ASN:CB	3:C:889:HOH:O	2.31	0.47
1:B:127:ILE:O	1:B:220:ILE:HA	2.15	0.47
1:D:44:GLU:HG3	3:D:922:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ASN:HD22	1:D:35:ASN:C	2.24	0.46
1:A:44:GLU:HG2	1:A:48:LYS:HE2	1.99	0.45
1:C:191:SER:HB3	3:C:948:HOH:O	2.17	0.45
1:C:37:PHE:CZ	1:C:212:MET:HE1	2.52	0.44
1:C:190:LYS:HA	1:C:193:GLN:HE21	1.83	0.44
1:B:16:ARG:HD2	1:B:202:ASN:ND2	2.33	0.44
1:D:49:LYS:HA	1:D:64:LEU:HD13	1.98	0.44
1:A:32:LYS:NZ	3:A:736:HOH:O	2.42	0.44
1:A:91:LEU:HD21	3:D:1081:HOH:O	2.16	0.44
1:A:16:ARG:HD2	1:A:202:ASN:HD22	1.82	0.44
1:B:165:VAL:CG2	1:B:192:LEU:HD23	2.48	0.43
1:A:150:LYS:HG2	1:A:151:TYR:CD1	2.53	0.43
1:D:3:LYS:HE3	1:D:30:GLU:CG	2.42	0.43
1:C:5:VAL:HG11	1:C:32:LYS:HE2	2.00	0.43
1:D:162:PHE:O	1:D:166:THR:HG23	2.19	0.42
1:B:92:LYS:HD3	3:B:910:HOH:O	2.19	0.42
1:B:165:VAL:HG21	1:B:192:LEU:HD23	2.02	0.41
1:A:9:ILE:HD12	1:A:35:ASN:HA	2.02	0.41
1:A:114:ASN:ND2	1:A:131:GLN:OE1	2.53	0.41
1:D:23:LYS:HD2	1:D:23:LYS:HA	1.71	0.41
1:D:37:PHE:CE1	1:D:212:MET:HE1	2.56	0.41
1:B:127:ILE:HG23	1:B:131:GLN:HE21	1.86	0.41
1:B:128:PRO:HB2	1:B:130:HIS:CE1	2.56	0.41
1:D:8:GLY:O	1:D:33:VAL:HA	2.21	0.41
1:A:19:LEU:O	1:A:23:LYS:HG2	2.21	0.41
1:D:16:ARG:HD2	1:D:202:ASN:ND2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/222 (97%)	210 (97%)	6 (3%)	0	100	100
1	B	216/222 (97%)	211 (98%)	4 (2%)	1 (0%)	24	14
1	C	218/222 (98%)	212 (97%)	6 (3%)	0	100	100
1	D	218/222 (98%)	211 (97%)	7 (3%)	0	100	100
All	All	868/888 (98%)	844 (97%)	23 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	ASP

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	191/194 (98%)	186 (97%)	5 (3%)	40	28
1	B	191/194 (98%)	185 (97%)	6 (3%)	35	23
1	C	193/194 (100%)	190 (98%)	3 (2%)	55	47
1	D	193/194 (100%)	189 (98%)	4 (2%)	47	36
All	All	768/776 (99%)	750 (98%)	18 (2%)	44	33

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	113	ARG
1	A	150	LYS
1	A	164	ILE
1	A	167	SER
1	B	81	LYS
1	B	113	ARG
1	B	124	GLN
1	B	126	GLN
1	B	150	LYS

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Mol	Chain	Res	Type
1	B	167	SER
1	C	3	LYS
1	C	23	LYS
1	C	42	LEU
1	D	23	LYS
1	D	81	LYS
1	D	167	SER
1	D	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	114	ASN
1	A	126	GLN
1	A	130	HIS
1	A	149	ASN
1	A	193	GLN
1	A	202	ASN
1	B	63	HIS
1	B	98	GLN
1	B	126	GLN
1	B	129	GLN
1	B	131	GLN
1	B	149	ASN
1	B	193	GLN
1	B	202	ASN
1	B	208	GLN
1	C	98	GLN
1	C	109	GLN
1	C	114	ASN
1	C	148	ASN
1	C	156	HIS
1	C	179	GLN
1	C	193	GLN
1	C	202	ASN
1	D	35	ASN
1	D	53	HIS
1	D	98	GLN
1	D	114	ASN
1	D	129	GLN
1	D	193	GLN

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Mol	Chain	Res	Type
1	D	202	ASN

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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GSH	B	600	-	18,19,19	1.32	2 (11%)	21,24,24	0.92	0
2	GSH	A	500	-	18,19,19	1.68	5 (27%)	21,24,24	0.91	0
2	GSH	D	800	-	18,19,19	1.19	3 (16%)	21,24,24	0.86	0
2	GSH	C	700	-	18,19,19	1.15	3 (16%)	21,24,24	1.02	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	B	600	-	-	1/24/24/24	-
2	GSH	A	500	-	-	1/24/24/24	-
2	GSH	D	800	-	-	0/24/24/24	-
2	GSH	C	700	-	-	1/24/24/24	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	GSH	CA2-N2	3.38	1.52	1.45
2	B	600	GSH	CA2-N2	3.06	1.52	1.45
2	A	500	GSH	O2-C2	3.02	1.29	1.23
2	B	600	GSH	O2-C2	2.83	1.28	1.23
2	A	500	GSH	O12-C1	2.57	1.29	1.22
2	A	500	GSH	CB2-CA2	-2.55	1.50	1.53
2	A	500	GSH	CA2-C2	-2.47	1.46	1.52
2	C	700	GSH	O2-C2	2.24	1.27	1.23
2	D	800	GSH	CA2-C2	-2.23	1.47	1.52
2	D	800	GSH	O11-C1	-2.14	1.23	1.30
2	C	700	GSH	CA2-C2	-2.12	1.47	1.52
2	C	700	GSH	O11-C1	-2.12	1.23	1.30
2	D	800	GSH	O2-C2	2.00	1.27	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	GSH	O11-C1-CA1-N1
2	B	600	GSH	O11-C1-CA1-N1
2	C	700	GSH	O11-C1-CA1-N1

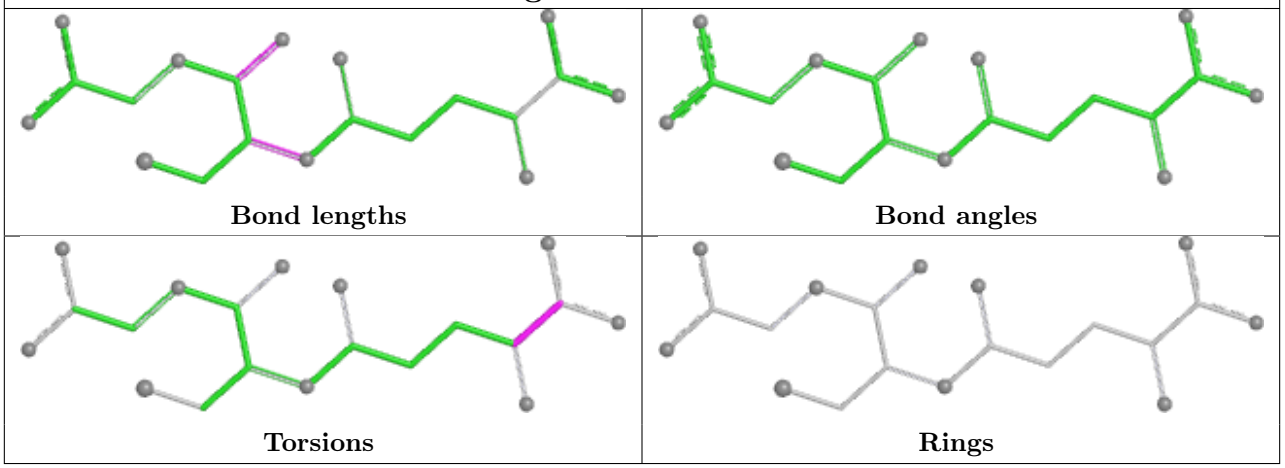
There are no ring outliers.

No monomer is involved in short contacts.

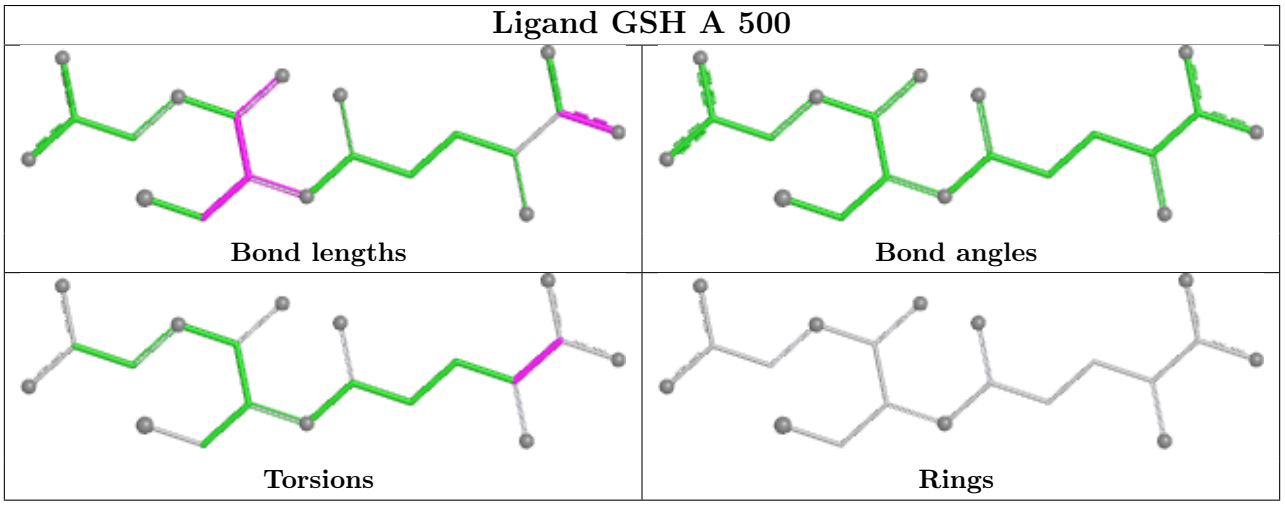
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

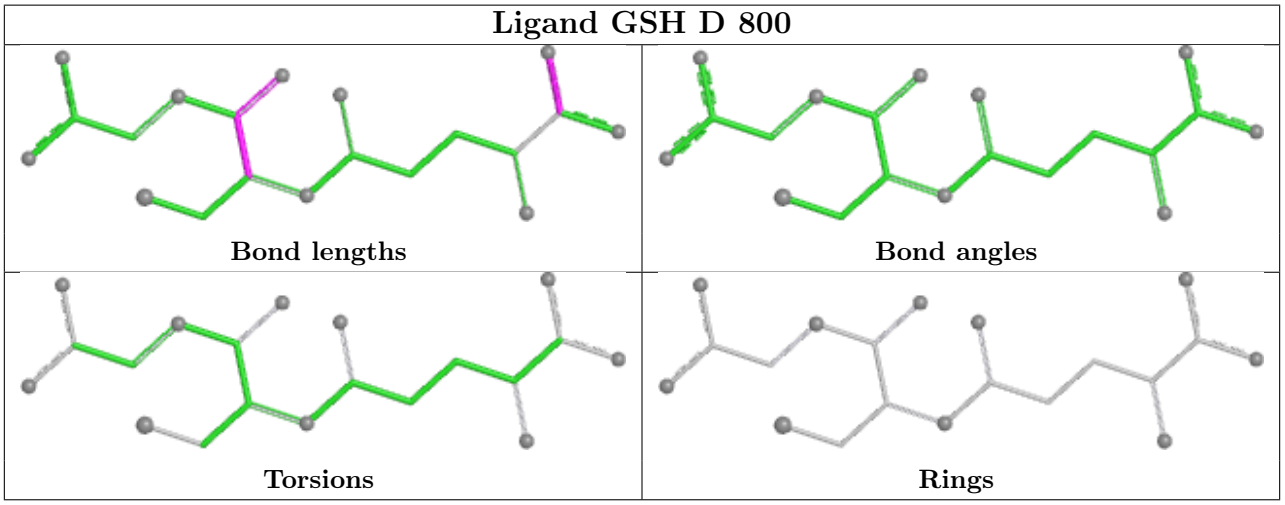
Ligand GSH B 600

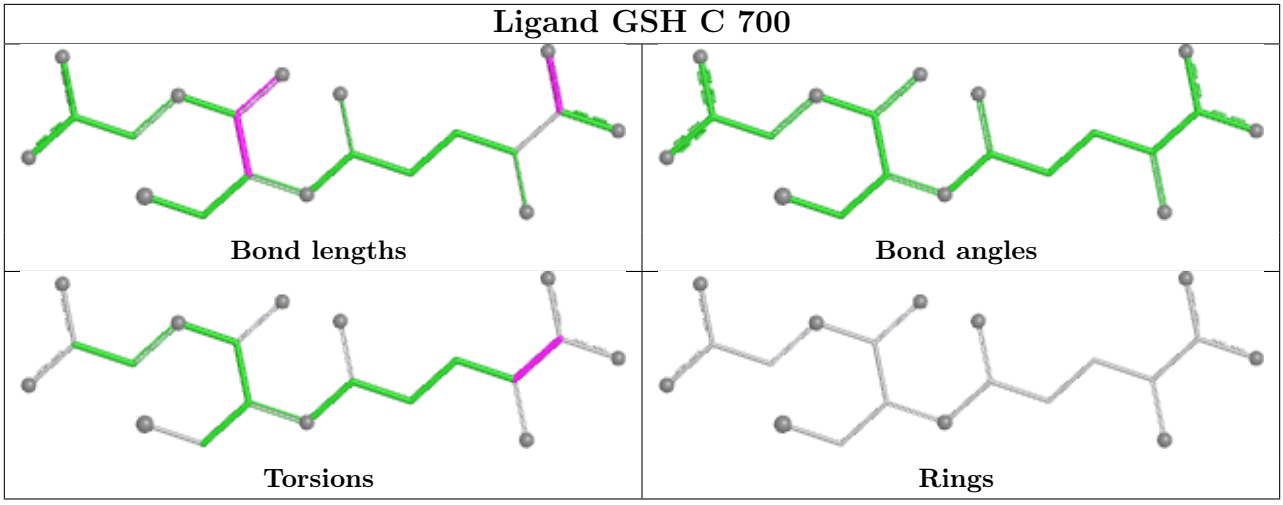


Ligand GSH A 500



Ligand GSH D 800





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	218/222 (98%)	-1.34	0	100	100	15, 23, 42, 52	0
1	B	218/222 (98%)	-1.37	0	100	100	15, 23, 42, 54	0
1	C	220/222 (99%)	-1.37	0	100	100	15, 22, 38, 45	0
1	D	220/222 (99%)	-1.36	0	100	100	15, 22, 38, 45	0
All	All	876/888 (98%)	-1.36	0	100	100	15, 23, 40, 54	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

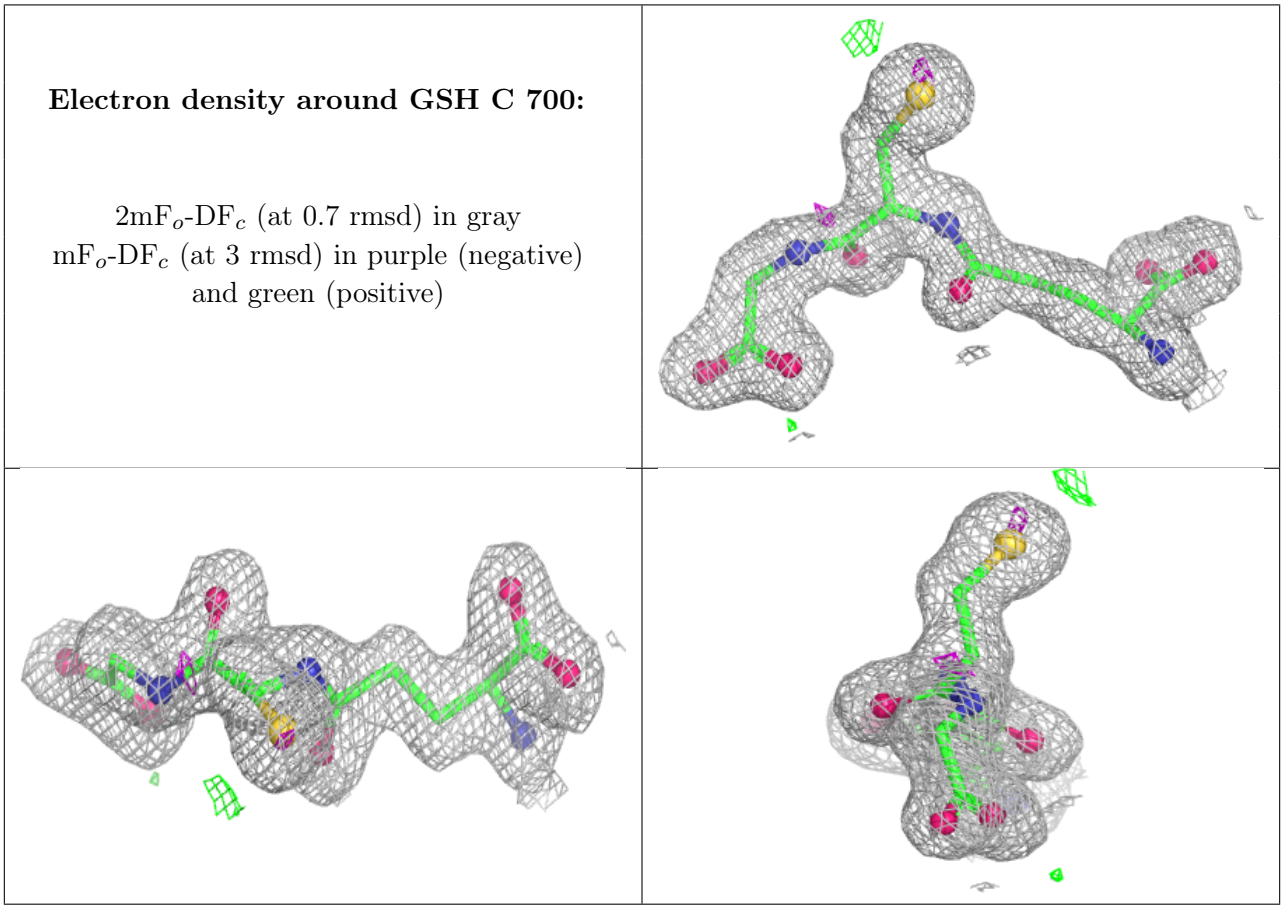
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GSH	C	700	20/20	0.99	0.03	19,20,27,27	0
2	GSH	D	800	20/20	0.99	0.03	19,21,27,28	0
2	GSH	A	500	20/20	1.00	0.02	16,19,24,26	0
2	GSH	B	600	20/20	1.00	0.02	17,19,24,26	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.

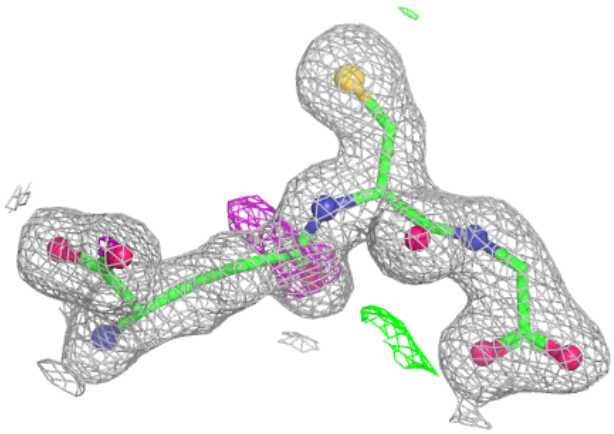
Electron density around GSH C 700:

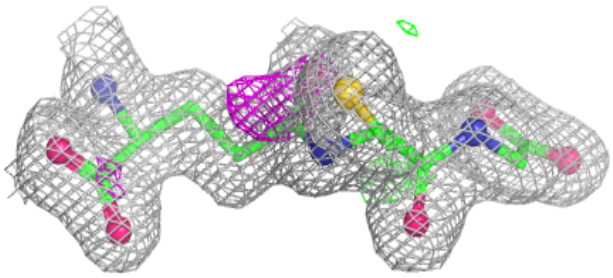
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

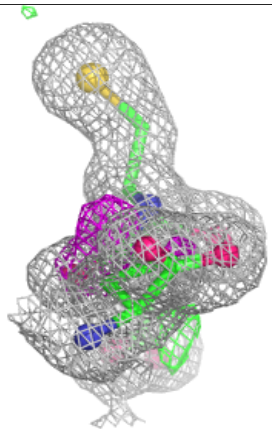


Electron density around GSH D 800:

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

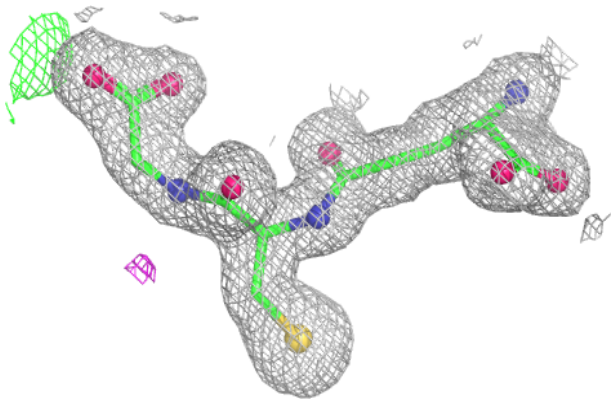


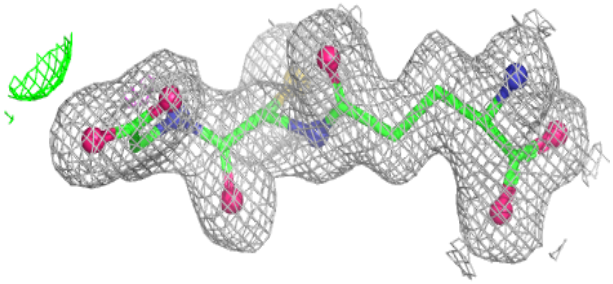


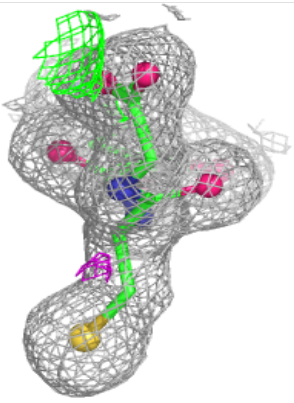


Electron density around GSH A 500:

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

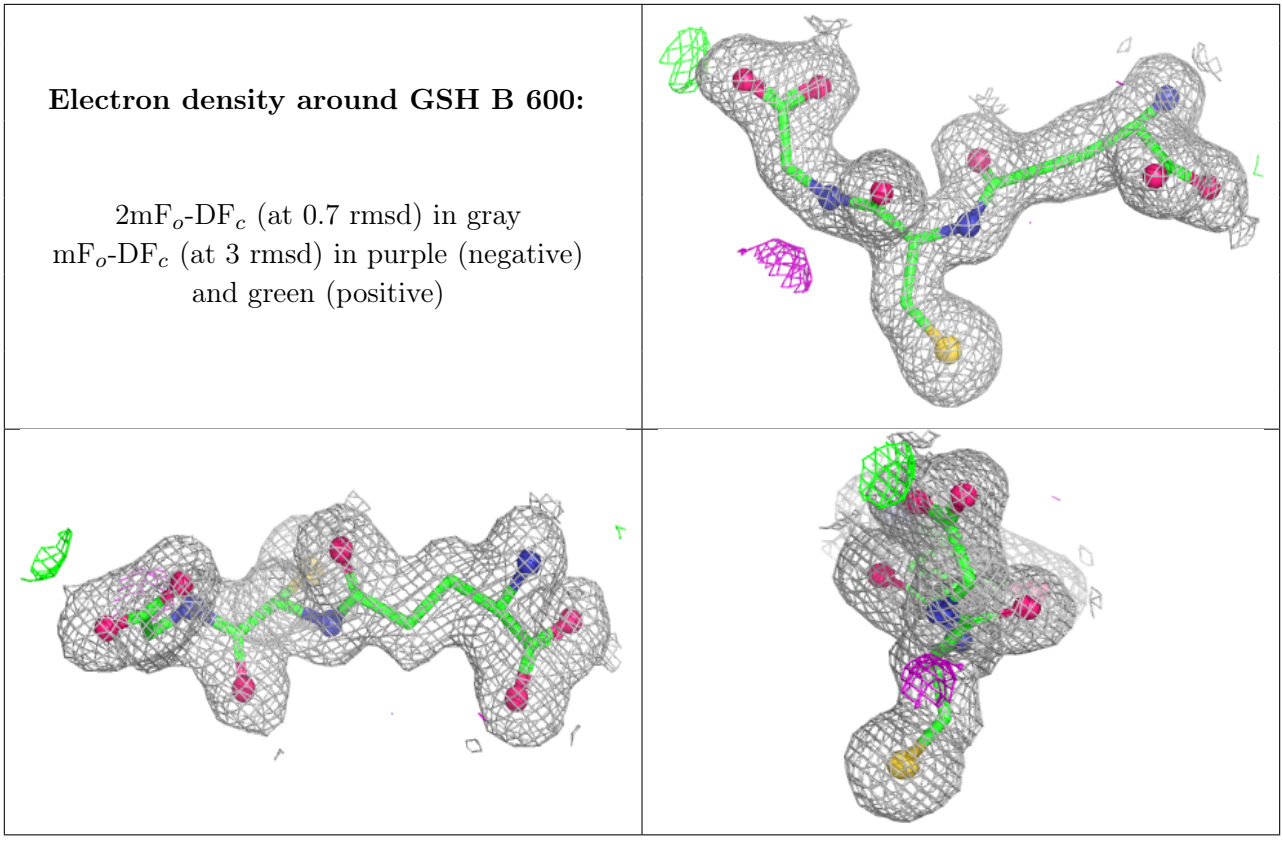






Electron density around GSH B 600:

$2mF_o$-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.