Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:35 am BST

PDB ID	:	1R4W
Title	:	Crystal structure of Mitochondrial class kappa glutathione transferase
Authors	:	Ladner, J.E.; Parsons, J.F.; Rife, C.L.; Gilliland, G.L.; Armstrong, R.N.
Deposited on	:	2003-10-08
Resolution	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

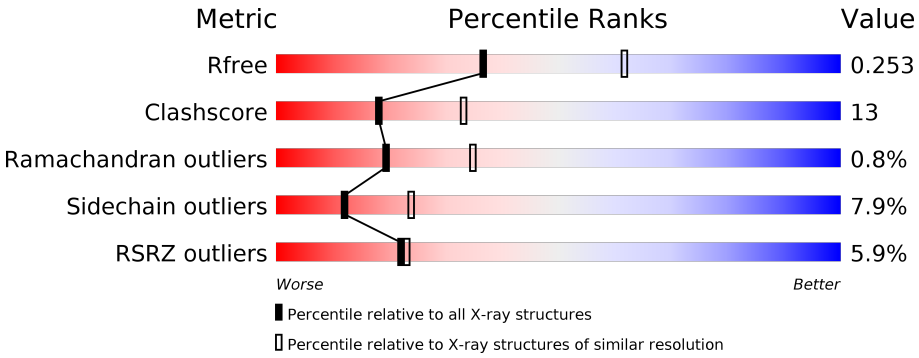
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	226	8% 71% 21% 5%
1	B	226	9% 65% 29%
1	C	226	4% 66% 27%
1	D	226	3% 68% 25% 5%

2 Entry composition

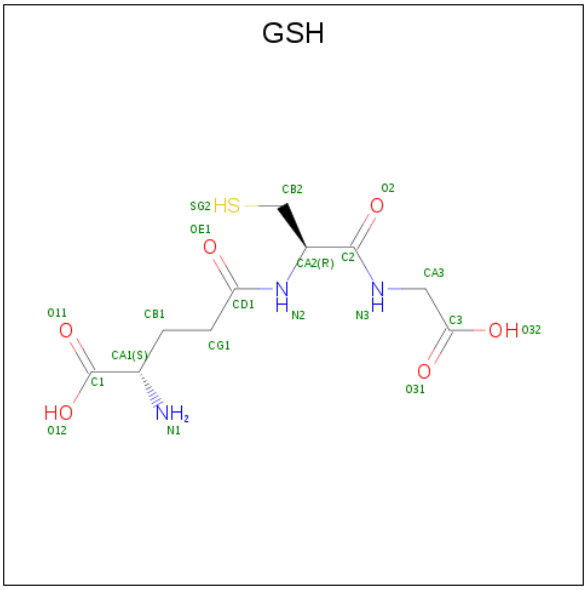
There are 3 unique types of molecules in this entry. The entry contains 7342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1749	1133	294	309	13			
1	B	221	Total	C	N	O	S	0	0	0
			1749	1133	294	309	13			
1	C	221	Total	C	N	O	S	0	0	0
			1749	1133	294	309	13			
1	D	221	Total	C	N	O	S	0	0	0
			1749	1133	294	309	13			

- Molecule 2 is GLUTATHIONE (three-letter code: 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		

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

- Molecule 3 is water.

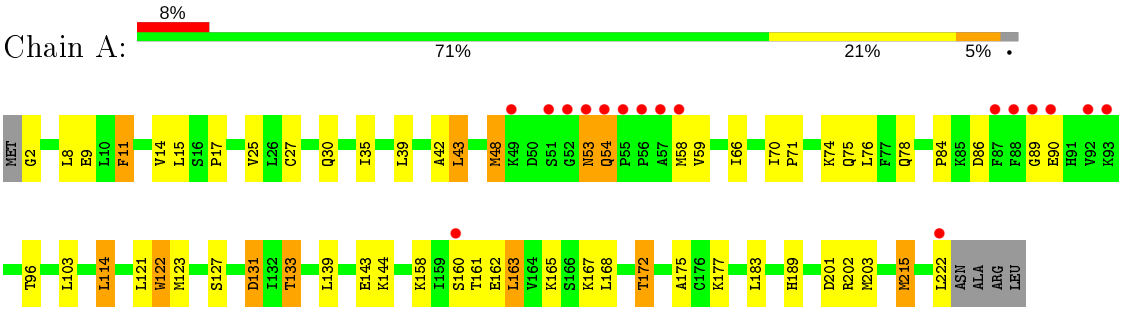
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	B	69	Total	O	0	0
			69	69		
3	C	54	Total	O	0	0
			54	54		
3	D	67	Total	O	0	0
			67	67		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

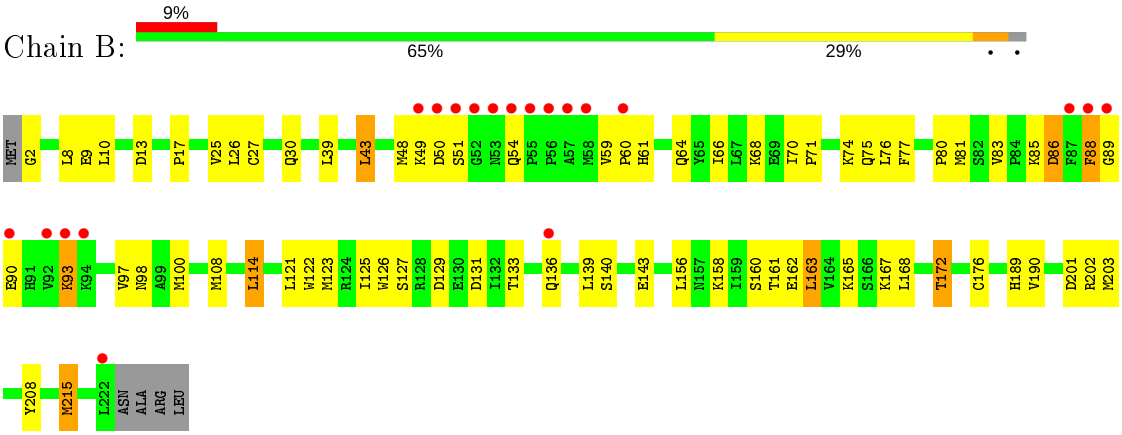
- Molecule 1: Glutathione S-transferase, mitochondrial

Chain A:



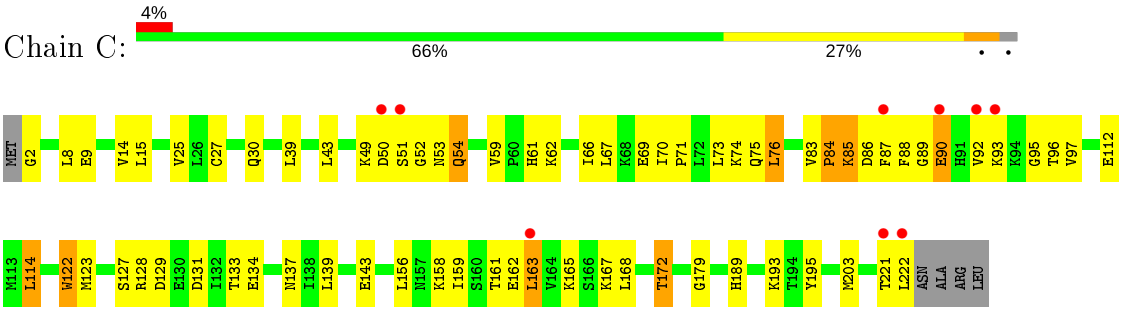
- Molecule 1: Glutathione S-transferase, mitochondrial

Chain B:



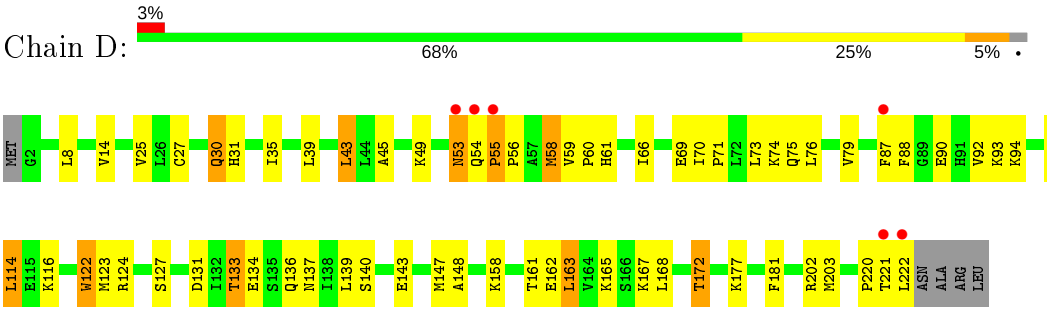
- Molecule 1: Glutathione S-transferase, mitochondrial

Chain C:



- Molecule 1: Glutathione S-transferase, mitochondrial

Chain D:


3%
68%
25%
5%
MET G2 L8 V14 V25 L26 C27 Q30 R31 I35 L39 L43 L44 A45 K49 N53 Q54 P55 P56 A57 M58 V59 P60 H61 I66 E69 I70 P71 L72 L73 K74 Q75 L76 V79 F87 F88 G89 E90 H91 V92 K93 K94 R101 E112 M113
L114 E115 K116 W122 M123 R124 S127 D131 I132 T133 E134 S135 Q136 N137 I138 L139 S140 E143 M147 A148 K158 T161 E162 L163 V164 K165 S166 K167 L168 T172 K177 F181 R202 M203 P220 T221 L222 ASN ALA ARG LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.90Å 110.79Å 74.74Å 90.00° 101.96° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 38.76 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.5 (30.00-2.50) 96.2 (38.76-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.19 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.256 0.203 , 0.253	Depositor DCC
R_{free} test set	3241 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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	1.05	3/1793 (0.2%)	0.88	0/2427
1	B	1.04	1/1793 (0.1%)	0.89	1/2427 (0.0%)
1	C	1.00	1/1793 (0.1%)	0.88	2/2427 (0.1%)
1	D	0.99	0/1793	0.88	1/2427 (0.0%)
All	All	1.02	5/7172 (0.1%)	0.88	4/9708 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	MET	SD-CE	7.18	2.18	1.77
1	A	2	GLY	N-CA	7.01	1.56	1.46
1	C	2	GLY	N-CA	6.55	1.55	1.46
1	B	215	MET	SD-CE	5.73	2.10	1.77
1	A	11	PHE	CG-CD2	-5.49	1.30	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	190	VAL	CB-CA-C	-5.37	101.19	111.40
1	C	76	LEU	CA-CB-CG	5.23	127.32	115.30
1	C	128	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	D	101	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1749	0	1791	40	0
1	B	1749	0	1791	58	0
1	C	1749	0	1791	48	0
1	D	1749	0	1791	56	0
2	A	20	0	15	1	0
2	B	20	0	16	0	0
2	C	20	0	15	1	0
2	D	20	0	15	1	0
3	A	76	0	0	3	0
3	B	69	0	0	6	0
3	C	54	0	0	4	0
3	D	67	0	0	5	0
All	All	7342	0	7225	192	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 13.

All (192) 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:215:MET:CE	1:B:215:MET:SD	2.09	1.39
1:A:215:MET:CE	1:A:215:MET:SD	2.18	1.32
1:A:177:LYS:HE3	3:A:710:HOH:O	1.56	1.04
1:D:54:GLN:HB3	1:D:55:PRO:HD2	1.50	0.94
1:C:52:GLY:HA3	1:D:59:VAL:HG13	1.56	0.88
1:B:70:ILE:HB	1:B:71:PRO:HD3	1.58	0.84
1:B:39:LEU:HB2	1:B:114:LEU:HD13	1.61	0.83
1:A:48:MET:HG3	1:A:53:ASN:HB3	1.59	0.83
1:C:25:VAL:HG11	1:C:203:MET:HG3	1.65	0.79
1:C:89:GLY:O	1:C:93:LYS:HB2	1.82	0.79
1:D:49:LYS:HA	1:D:53:ASN:HB3	1.66	0.76
1:A:70:ILE:HB	1:A:71:PRO:HD3	1.68	0.75
1:B:25:VAL:HG11	1:B:203:MET:HG3	1.69	0.73
1:C:59:VAL:HB	1:C:62:LYS:HB2	1.70	0.73
1:B:85:LYS:HD3	1:B:129:ASP:OD2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ASP:OD1	1:D:133:THR:HG22	1.88	0.72
1:A:161:THR:HG22	1:A:163:LEU:H	1.54	0.72
1:C:87:PHE:O	1:C:92:VAL:HG23	1.90	0.72
1:D:168:LEU:O	1:D:172:THR:HG23	1.90	0.71
1:B:161:THR:HG22	1:B:163:LEU:N	2.05	0.71
1:C:49:LYS:HG2	1:C:50:ASP:N	2.06	0.70
1:B:168:LEU:O	1:B:172:THR:HG23	1.91	0.70
1:C:66:ILE:O	1:C:70:ILE:HG12	1.93	0.69
1:A:161:THR:HG22	1:A:163:LEU:N	2.07	0.69
1:C:131:ASP:OD1	1:C:133:THR:HG22	1.93	0.69
1:A:123:MET:O	1:A:127:SER:HB3	1.92	0.68
1:A:53:ASN:ND2	1:B:59:VAL:HG21	2.09	0.67
1:D:161:THR:HG22	1:D:163:LEU:H	1.60	0.67
1:C:70:ILE:HB	1:C:71:PRO:HD3	1.77	0.66
1:B:161:THR:HG22	1:B:163:LEU:H	1.60	0.66
1:D:70:ILE:HB	1:D:71:PRO:HD3	1.77	0.65
1:C:53:ASN:ND2	1:C:54:GLN:H	1.95	0.65
1:A:168:LEU:O	1:A:172:THR:HG23	1.98	0.64
1:C:168:LEU:O	1:C:172:THR:HG23	1.98	0.64
1:D:43:LEU:HD22	3:D:620:HOH:O	1.98	0.64
1:D:161:THR:HG22	1:D:163:LEU:N	2.14	0.63
1:A:27:CYS:O	1:A:30:GLN:HG2	1.99	0.63
1:D:87:PHE:O	1:D:92:VAL:HG23	1.99	0.63
1:C:123:MET:O	1:C:127:SER:HB3	2.00	0.62
1:C:86:ASP:O	1:C:90:GLU:HG3	2.00	0.62
1:B:86:ASP:HB3	1:B:90:GLU:HB2	1.82	0.61
1:B:168:LEU:O	1:B:172:THR:CG2	2.48	0.61
1:C:9:GLU:OE1	1:C:189:HIS:HE1	1.83	0.61
1:C:62:LYS:HE2	2:D:901:GSH:O31	2.00	0.61
1:B:89:GLY:O	1:B:93:LYS:HE3	2.01	0.61
1:A:78:GLN:HE22	1:D:148:ALA:H	1.49	0.61
1:C:161:THR:HG22	1:C:163:LEU:N	2.16	0.60
1:B:136:GLN:OE1	3:B:727:HOH:O	2.15	0.59
1:A:39:LEU:HB2	1:A:114:LEU:HD13	1.82	0.59
1:D:66:ILE:O	1:D:70:ILE:HG12	2.03	0.59
1:A:131:ASP:OD1	1:A:133:THR:HG22	2.04	0.58
1:A:78:GLN:NE2	1:D:148:ALA:H	2.02	0.57
1:B:27:CYS:O	1:B:30:GLN:HG2	2.04	0.57
1:C:161:THR:HG22	1:C:163:LEU:H	1.69	0.57
1:A:66:ILE:O	1:A:70:ILE:HG12	2.05	0.57
1:B:88:PHE:O	1:B:93:LYS:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:CYS:O	1:D:30:GLN:HG2	2.05	0.57
1:A:25:VAL:HG11	1:A:203:MET:HG3	1.87	0.56
1:A:158:LYS:O	1:A:161:THR:HB	2.05	0.56
1:C:75:GLN:HG2	3:C:552:HOH:O	2.06	0.56
1:A:78:GLN:HE22	1:D:147:MET:HA	1.70	0.56
1:D:161:THR:O	1:D:165:LYS:HG3	2.06	0.55
1:B:39:LEU:HB2	1:B:114:LEU:CD1	2.34	0.55
1:C:15:LEU:HB2	1:C:96:THR:HG21	1.89	0.55
1:A:161:THR:CG2	1:A:163:LEU:H	2.18	0.55
1:D:25:VAL:HG11	1:D:203:MET:HG3	1.88	0.55
1:A:86:ASP:OD2	1:A:89:GLY:HA3	2.07	0.55
1:B:123:MET:O	1:B:127:SER:HB3	2.08	0.54
1:B:2:GLY:N	3:B:708:HOH:O	2.41	0.54
1:D:220:PRO:HG2	1:D:220:PRO:O	2.08	0.54
1:A:15:LEU:HB2	1:A:96:THR:HG21	1.90	0.53
1:B:131:ASP:OD1	1:B:133:THR:HG22	2.09	0.53
1:B:85:LYS:N	1:B:85:LYS:HD2	2.24	0.53
1:D:39:LEU:HB2	1:D:114:LEU:HD13	1.90	0.53
1:A:43:LEU:HD22	3:A:617:HOH:O	2.07	0.53
1:B:39:LEU:CB	1:B:114:LEU:HD13	2.36	0.52
1:A:168:LEU:O	1:A:172:THR:CG2	2.58	0.52
1:B:121:LEU:O	1:B:125:ILE:HG22	2.09	0.52
1:D:53:ASN:H	1:D:53:ASN:HD22	1.55	0.52
1:C:27:CYS:O	1:C:30:GLN:HG2	2.09	0.51
1:B:10:LEU:HD22	1:B:26:LEU:HD12	1.92	0.51
1:C:39:LEU:HB2	1:C:114:LEU:HD13	1.92	0.51
1:D:161:THR:CG2	1:D:162:GLU:N	2.74	0.51
1:C:61:HIS:HB2	1:D:181:PHE:HB3	1.93	0.51
1:C:74:LYS:HG3	1:C:75:GLN:N	2.24	0.50
1:D:116:LYS:HG3	3:D:518:HOH:O	2.10	0.50
1:B:161:THR:CG2	1:B:162:GLU:N	2.75	0.50
1:B:108:MET:HE2	3:B:675:HOH:O	2.11	0.50
1:C:9:GLU:OE1	1:C:189:HIS:CE1	2.64	0.49
1:D:54:GLN:O	1:D:55:PRO:C	2.50	0.49
1:C:156:LEU:O	1:C:159:ILE:HG12	2.13	0.49
1:C:158:LYS:O	1:C:161:THR:HB	2.13	0.49
1:D:161:THR:CG2	1:D:163:LEU:H	2.24	0.49
1:D:74:LYS:HG3	1:D:75:GLN:N	2.27	0.49
1:B:133:THR:HA	3:B:736:HOH:O	2.12	0.48
1:D:30:GLN:HA	1:D:35:ILE:HD11	1.95	0.48
1:A:9:GLU:OE1	1:A:189:HIS:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:PHE:O	1:D:93:LYS:HB2	2.13	0.48
1:B:74:LYS:HG3	1:B:75:GLN:N	2.28	0.48
1:C:53:ASN:CG	1:C:54:GLN:H	2.16	0.48
1:B:13:ASP:HA	1:B:100:MET:HE2	1.96	0.47
1:A:167:LYS:HA	1:A:167:LYS:HD2	1.65	0.47
1:B:125:ILE:HG23	1:B:126:TRP:N	2.29	0.47
1:B:161:THR:CG2	1:B:163:LEU:H	2.26	0.47
1:A:17:PRO:HD2	2:A:301:GSH:SG2	2.53	0.47
1:C:84:PRO:HB3	1:C:129:ASP:OD1	2.14	0.47
1:A:11:PHE:CD1	1:A:175:ALA:HB2	2.50	0.47
1:D:123:MET:O	1:D:127:SER:HB3	2.14	0.47
1:D:54:GLN:HB3	1:D:55:PRO:CD	2.35	0.47
1:A:11:PHE:O	1:A:183:LEU:HD22	2.14	0.47
1:C:25:VAL:CG1	1:C:203:MET:HG3	2.40	0.47
2:C:801:GSH:O12	1:D:202:ARG:NH2	2.40	0.47
1:D:168:LEU:O	1:D:172:THR:CG2	2.60	0.47
1:A:161:THR:CG2	1:A:162:GLU:N	2.78	0.46
1:B:66:ILE:O	1:B:70:ILE:HG12	2.14	0.46
1:D:31:HIS:HB2	3:D:707:HOH:O	2.14	0.46
1:D:69:GLU:HG2	1:D:73:LEU:CD1	2.45	0.46
1:B:17:PRO:HB2	1:B:81:MET:CE	2.46	0.46
1:C:14:VAL:HA	1:C:122:TRP:NE1	2.31	0.45
1:D:134:GLU:O	1:D:137:ASN:HB2	2.16	0.45
1:A:161:THR:O	1:A:165:LYS:HG3	2.16	0.45
1:B:139:LEU:O	1:B:143:GLU:HG3	2.16	0.45
1:C:30:GLN:NE2	3:C:555:HOH:O	2.43	0.45
1:C:67:LEU:HD22	1:C:83:VAL:HG11	1.96	0.45
1:C:67:LEU:HD21	1:C:88:PHE:CE2	2.52	0.45
1:B:89:GLY:C	1:B:93:LYS:HE3	2.37	0.45
1:B:49:LYS:C	1:B:51:SER:H	2.20	0.45
1:A:30:GLN:HA	1:A:35:ILE:HD11	1.98	0.45
1:A:54:GLN:HB2	1:A:58:MET:SD	2.57	0.45
1:D:90:GLU:O	1:D:94:LYS:HE3	2.17	0.45
1:D:88:PHE:HA	1:D:92:VAL:HB	1.98	0.44
1:B:161:THR:HG22	1:B:162:GLU:N	2.32	0.44
1:A:202:ARG:NH1	1:B:201:ASP:OD2	2.34	0.44
1:B:25:VAL:HG21	1:B:77:PHE:CE2	2.51	0.44
1:B:60:PRO:O	1:B:64:GLN:HG3	2.17	0.44
1:C:69:GLU:HG2	1:C:73:LEU:CD1	2.47	0.44
1:C:83:VAL:HA	1:C:84:PRO:HD3	1.83	0.44
1:D:55:PRO:HA	1:D:58:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLU:HG2	1:C:73:LEU:HD12	1.98	0.44
1:D:136:GLN:HB2	3:D:718:HOH:O	2.17	0.44
1:D:53:ASN:O	1:D:56:PRO:HG3	2.18	0.44
1:D:167:LYS:HA	1:D:167:LYS:HD2	1.68	0.43
1:B:68:LYS:NZ	3:B:764:HOH:O	2.50	0.43
1:C:139:LEU:O	1:C:143:GLU:HG3	2.18	0.43
1:B:43:LEU:HD11	1:B:97:VAL:HG22	2.01	0.43
1:C:62:LYS:O	1:C:66:ILE:HG12	2.17	0.43
1:D:139:LEU:O	1:D:143:GLU:HG3	2.19	0.43
1:B:9:GLU:OE1	1:B:189:HIS:HE1	2.01	0.43
1:B:208:TYR:CZ	1:D:112:GLU:HG3	2.54	0.43
1:D:74:LYS:HB2	1:D:79:VAL:O	2.19	0.43
1:B:125:ILE:HG23	1:B:126:TRP:H	1.84	0.43
1:C:97:VAL:HG23	3:C:629:HOH:O	2.19	0.43
1:D:45:ALA:O	1:D:49:LYS:HG3	2.18	0.43
1:A:103:LEU:HD11	1:A:121:LEU:HD12	2.00	0.42
1:A:201:ASP:OD2	1:B:202:ARG:NH1	2.44	0.42
1:D:158:LYS:O	1:D:161:THR:HB	2.20	0.42
1:D:124:ARG:HD2	3:D:536:HOH:O	2.19	0.42
1:B:25:VAL:HG21	1:B:77:PHE:HE2	1.84	0.42
1:B:85:LYS:N	1:B:85:LYS:CD	2.82	0.42
1:C:193:LYS:HD2	1:C:195:TYR:OH	2.18	0.42
1:B:43:LEU:HD22	3:B:502:HOH:O	2.19	0.42
1:D:70:ILE:N	1:D:71:PRO:CD	2.82	0.42
1:B:25:VAL:CG2	1:B:77:PHE:CE2	3.02	0.42
1:A:14:VAL:HA	1:A:122:TRP:NE1	2.35	0.42
1:B:70:ILE:CB	1:B:71:PRO:HD3	2.35	0.42
1:D:114:LEU:HD23	1:D:114:LEU:HA	1.80	0.42
1:B:158:LYS:O	1:B:161:THR:HB	2.20	0.42
1:B:160:SER:O	1:B:165:LYS:HE2	2.19	0.42
1:C:95:GLY:HA3	3:C:629:HOH:O	2.20	0.42
1:D:14:VAL:HA	1:D:122:TRP:NE1	2.33	0.42
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.77	0.42
1:B:70:ILE:N	1:B:71:PRO:CD	2.83	0.41
1:C:167:LYS:HD2	1:C:167:LYS:HA	1.68	0.41
1:C:134:GLU:O	1:C:137:ASN:HB2	2.21	0.41
1:C:161:THR:HG22	1:C:162:GLU:N	2.34	0.41
1:C:161:THR:O	1:C:165:LYS:HG3	2.19	0.41
1:B:50:ASP:HB2	1:B:176:CYS:SG	2.60	0.41
1:D:54:GLN:CB	1:D:55:PRO:HD2	2.30	0.41
1:A:139:LEU:O	1:A:143:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LEU:HB2	1:D:114:LEU:CD1	2.49	0.41
1:B:161:THR:O	1:B:165:LYS:HG3	2.19	0.41
1:C:179:GLY:HA2	1:D:61:HIS:HD2	1.85	0.41
1:B:17:PRO:HB2	1:B:81:MET:HE3	2.01	0.41
1:C:161:THR:CG2	1:C:162:GLU:N	2.84	0.41
1:D:177:LYS:HE2	1:D:177:LYS:HB3	1.86	0.41
1:A:42:ALA:HB1	1:A:172:THR:HB	2.03	0.41
1:D:137:ASN:HD22	1:D:137:ASN:HA	1.61	0.41
1:B:167:LYS:HD2	1:B:167:LYS:HA	1.67	0.40
1:A:144:LYS:NZ	3:A:541:HOH:O	2.54	0.40
1:C:85:LYS:HD3	1:C:85:LYS:HA	1.90	0.40
1:D:87:PHE:O	1:D:87:PHE:CG	2.74	0.40
1:A:74:LYS:HG3	1:A:75:GLN:N	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	219/226 (97%)	209 (95%)	9 (4%)	1 (0%)	29	48
1	B	219/226 (97%)	198 (90%)	20 (9%)	1 (0%)	29	48
1	C	219/226 (97%)	200 (91%)	16 (7%)	3 (1%)	11	20
1	D	219/226 (97%)	205 (94%)	12 (6%)	2 (1%)	17	31
All	All	876/904 (97%)	812 (93%)	57 (6%)	7 (1%)	19	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	SER
1	D	55	PRO

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Mol	Chain	Res	Type
1	A	84	PRO
1	C	54	GLN
1	D	60	PRO
1	C	84	PRO
1	B	80	PRO

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	189/193 (98%)	173 (92%)	16 (8%)	10 21
1	B	189/193 (98%)	172 (91%)	17 (9%)	9 19
1	C	189/193 (98%)	177 (94%)	12 (6%)	18 34
1	D	189/193 (98%)	174 (92%)	15 (8%)	12 24
All	All	756/772 (98%)	696 (92%)	60 (8%)	12 24

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	43	LEU
1	A	48	MET
1	A	53	ASN
1	A	54	GLN
1	A	59	VAL
1	A	76	LEU
1	A	90	GLU
1	A	114	LEU
1	A	122	TRP
1	A	131	ASP
1	A	133	THR
1	A	160	SER
1	A	163	LEU
1	A	172	THR
1	A	222	LEU

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Mol	Chain	Res	Type
1	B	8	LEU
1	B	43	LEU
1	B	48	MET
1	B	54	GLN
1	B	61	HIS
1	B	76	LEU
1	B	83	VAL
1	B	86	ASP
1	B	88	PHE
1	B	93	LYS
1	B	98	ASN
1	B	114	LEU
1	B	122	TRP
1	B	140	SER
1	B	156	LEU
1	B	163	LEU
1	B	172	THR
1	C	8	LEU
1	C	43	LEU
1	C	76	LEU
1	C	85	LYS
1	C	90	GLU
1	C	112	GLU
1	C	114	LEU
1	C	122	TRP
1	C	163	LEU
1	C	172	THR
1	C	221	THR
1	C	222	LEU
1	D	8	LEU
1	D	30	GLN
1	D	43	LEU
1	D	53	ASN
1	D	58	MET
1	D	76	LEU
1	D	112	GLU
1	D	114	LEU
1	D	122	TRP
1	D	133	THR
1	D	140	SER
1	D	163	LEU
1	D	172	THR

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Mol	Chain	Res	Type
1	D	221	THR
1	D	222	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	53	ASN
1	A	78	GLN
1	A	137	ASN
1	A	151	GLN
1	A	189	HIS
1	B	30	GLN
1	B	78	GLN
1	B	137	ASN
1	B	151	GLN
1	B	189	HIS
1	C	34	ASN
1	C	53	ASN
1	C	54	GLN
1	C	78	GLN
1	C	137	ASN
1	C	189	HIS
1	D	53	ASN
1	D	61	HIS
1	D	64	GLN
1	D	78	GLN
1	D	137	ASN
1	D	189	HIS

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	401	-	12,19,19	2.09	5 (41%)	15,24,24	1.20	1 (6%)
2	GSH	D	901	-	12,19,19	1.96	4 (33%)	15,24,24	1.42	1 (6%)
2	GSH	A	301	-	12,19,19	2.48	4 (33%)	15,24,24	1.45	2 (13%)
2	GSH	C	801	-	12,19,19	2.34	8 (66%)	15,24,24	1.44	2 (13%)

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	401	-	-	2/18/24/24	-
2	GSH	D	901	-	-	3/18/24/24	-
2	GSH	A	301	-	-	2/18/24/24	-
2	GSH	C	801	-	-	3/18/24/24	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	GSH	CB2-CA2	5.13	1.58	1.53
2	A	301	GSH	CG1-CD1	4.58	1.60	1.51
2	B	401	GSH	CG1-CD1	3.99	1.58	1.51
2	C	801	GSH	CG1-CD1	3.62	1.58	1.51
2	D	901	GSH	CG1-CD1	3.34	1.57	1.51
2	D	901	GSH	OE1-CD1	3.31	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	GSH	CA3-N3	3.15	1.52	1.46
2	A	301	GSH	CA3-N3	3.13	1.52	1.46
2	C	801	GSH	OE1-CD1	3.06	1.29	1.23
2	C	801	GSH	CB2-CA2	2.62	1.55	1.53
2	A	301	GSH	CB2-SG2	2.57	1.86	1.81
2	C	801	GSH	CA2-C2	2.55	1.59	1.52
2	D	901	GSH	O2-C2	2.54	1.28	1.23
2	B	401	GSH	CB2-CA2	2.51	1.55	1.53
2	B	401	GSH	CB1-CG1	2.47	1.60	1.52
2	C	801	GSH	C2-N3	2.43	1.38	1.33
2	C	801	GSH	O2-C2	2.28	1.27	1.23
2	C	801	GSH	CD1-N2	2.24	1.38	1.34
2	B	401	GSH	O2-C2	2.18	1.27	1.23
2	B	401	GSH	C2-N3	2.15	1.38	1.33
2	D	901	GSH	CD1-N2	2.13	1.38	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	GSH	C2-CA2-N2	-3.99	100.31	111.16
2	D	901	GSH	CB1-CG1-CD1	-3.78	104.59	113.04
2	C	801	GSH	CB1-CG1-CD1	-3.50	105.22	113.04
2	A	301	GSH	CA3-N3-C2	2.45	125.86	122.34
2	B	401	GSH	CB1-CG1-CD1	-2.28	107.95	113.04
2	C	801	GSH	CA3-N3-C2	2.13	125.41	122.34

There are no chirality outliers.

All (10) torsion outliers are listed below:

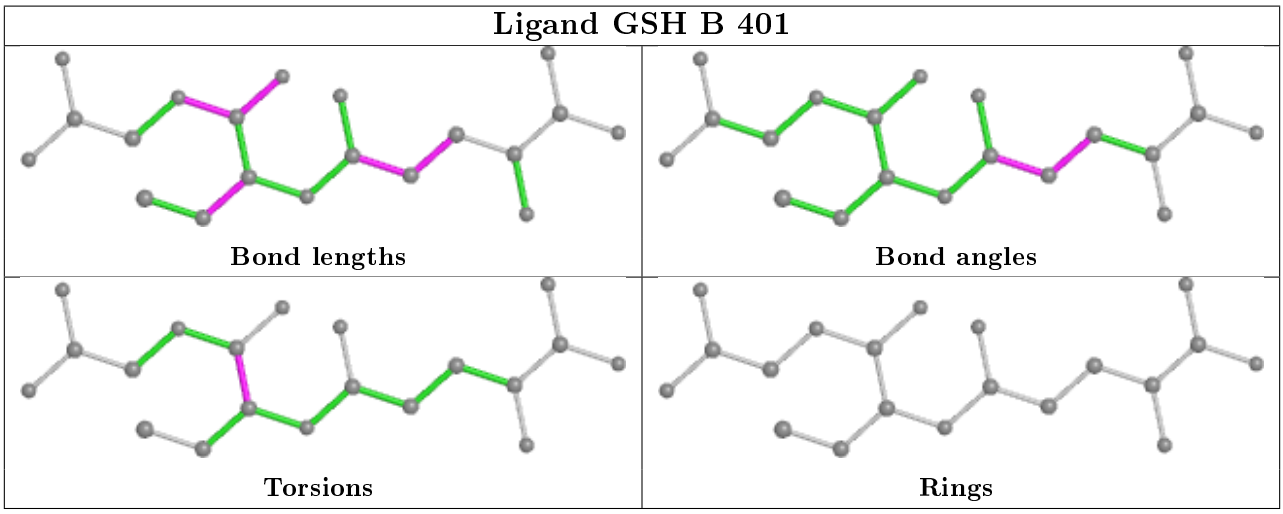
Mol	Chain	Res	Type	Atoms
2	B	401	GSH	N3-C2-CA2-N2
2	B	401	GSH	O2-C2-CA2-N2
2	D	901	GSH	O2-C2-CA2-N2
2	D	901	GSH	N3-C2-CA2-N2
2	C	801	GSH	O2-C2-CA2-N2
2	A	301	GSH	N3-C2-CA2-N2
2	C	801	GSH	N3-C2-CA2-N2
2	D	901	GSH	C3-CA3-N3-C2
2	A	301	GSH	O2-C2-CA2-N2
2	C	801	GSH	C3-CA3-N3-C2

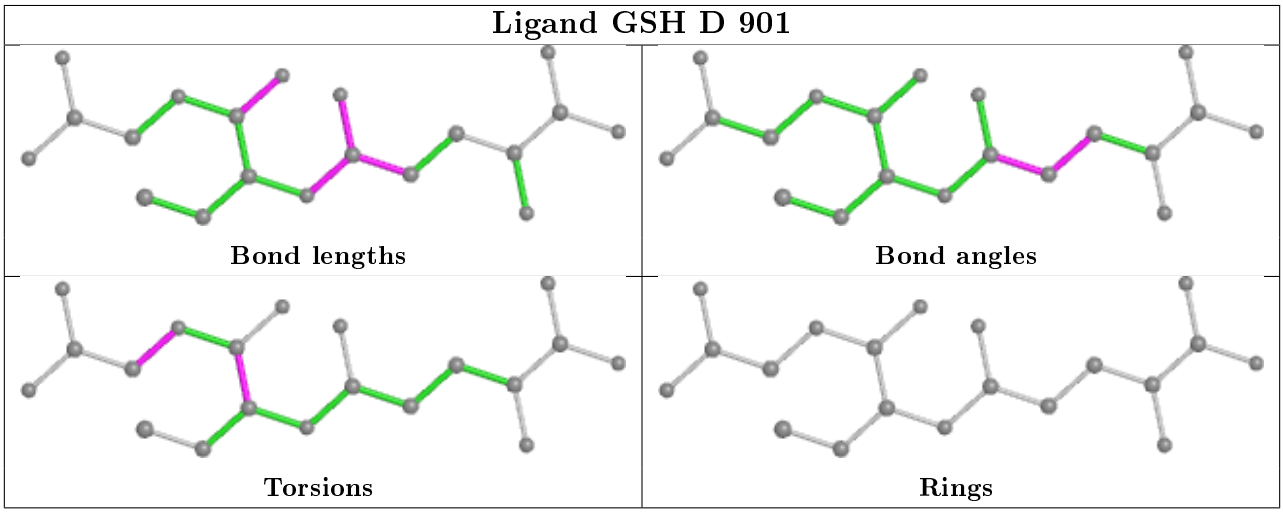
There are no ring outliers.

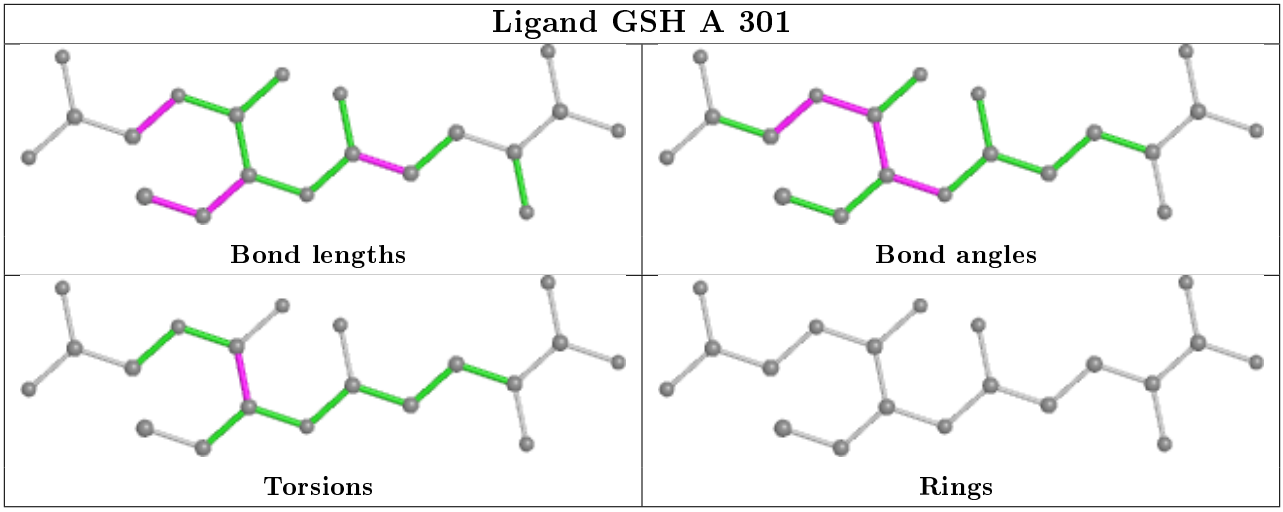
3 monomers are involved in 3 short contacts:

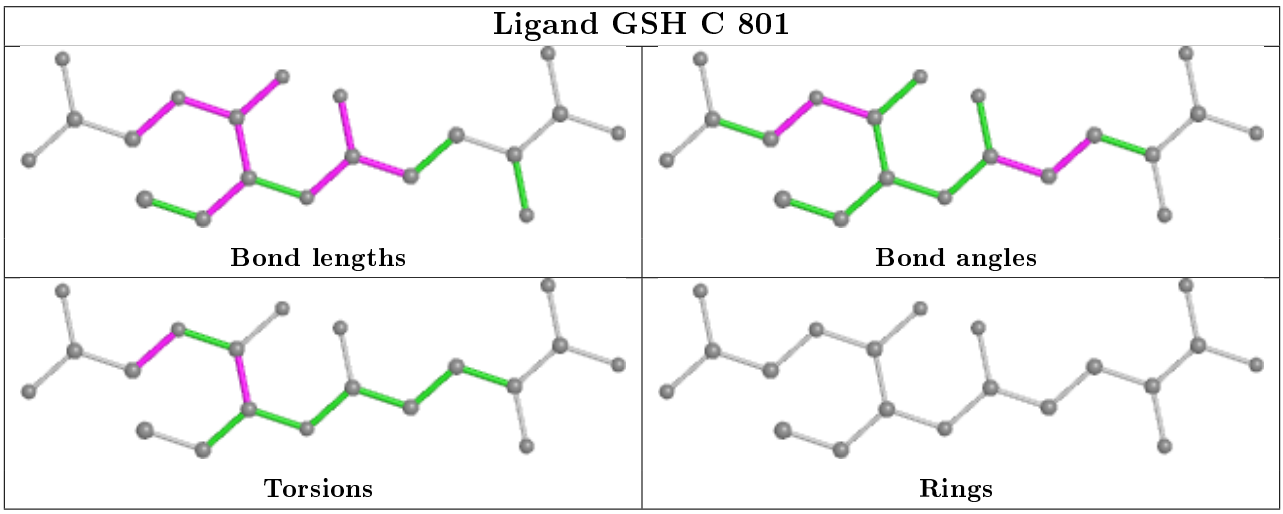
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	GSH	1	0
2	A	301	GSH	1	0
2	C	801	GSH	1	0

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









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	221/226 (97%)	0.31	17 (7%) 13 13	23, 36, 65, 82	0
1	B	221/226 (97%)	0.44	20 (9%) 9 9	21, 37, 71, 79	0
1	C	221/226 (97%)	0.13	9 (4%) 37 40	27, 40, 66, 78	0
1	D	221/226 (97%)	-0.06	6 (2%) 54 58	25, 36, 66, 82	0
All	All	884/904 (97%)	0.20	52 (5%) 22 23	21, 38, 68, 82	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	PRO	9.6
1	A	57	ALA	8.0
1	A	58	MET	7.0
1	B	89	GLY	6.8
1	B	88	PHE	6.0
1	A	56	PRO	5.6
1	D	53	ASN	5.6
1	B	55	PRO	5.3
1	B	90	GLU	5.0
1	D	54	GLN	4.8
1	A	54	GLN	4.8
1	A	52	GLY	4.5
1	D	221	THR	4.4
1	B	56	PRO	4.3
1	B	54	GLN	4.1
1	B	51	SER	4.1
1	A	88	PHE	4.0
1	A	89	GLY	3.9
1	B	93	LYS	3.8
1	A	53	ASN	3.8
1	D	55	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	87	PHE	3.7
1	B	92	VAL	3.7
1	B	94	LYS	3.6
1	A	90	GLU	3.6
1	B	222	LEU	3.5
1	B	57	ALA	3.5
1	A	222	LEU	3.4
1	C	221	THR	3.3
1	B	53	ASN	3.3
1	A	51	SER	3.1
1	D	222	LEU	3.0
1	C	163	LEU	3.0
1	C	87	PHE	2.9
1	C	51	SER	2.9
1	A	93	LYS	2.9
1	B	136	GLN	2.8
1	C	222	LEU	2.7
1	C	90	GLU	2.7
1	A	87	PHE	2.5
1	B	58	MET	2.5
1	B	52	GLY	2.5
1	B	60	PRO	2.2
1	D	87	PHE	2.2
1	C	50	ASP	2.2
1	A	160	SER	2.2
1	A	49	LYS	2.1
1	B	50	ASP	2.1
1	B	49	LYS	2.1
1	C	93	LYS	2.1
1	A	92	VAL	2.0
1	C	92	VAL	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 carbohydrates in this entry.

6.4 Ligands

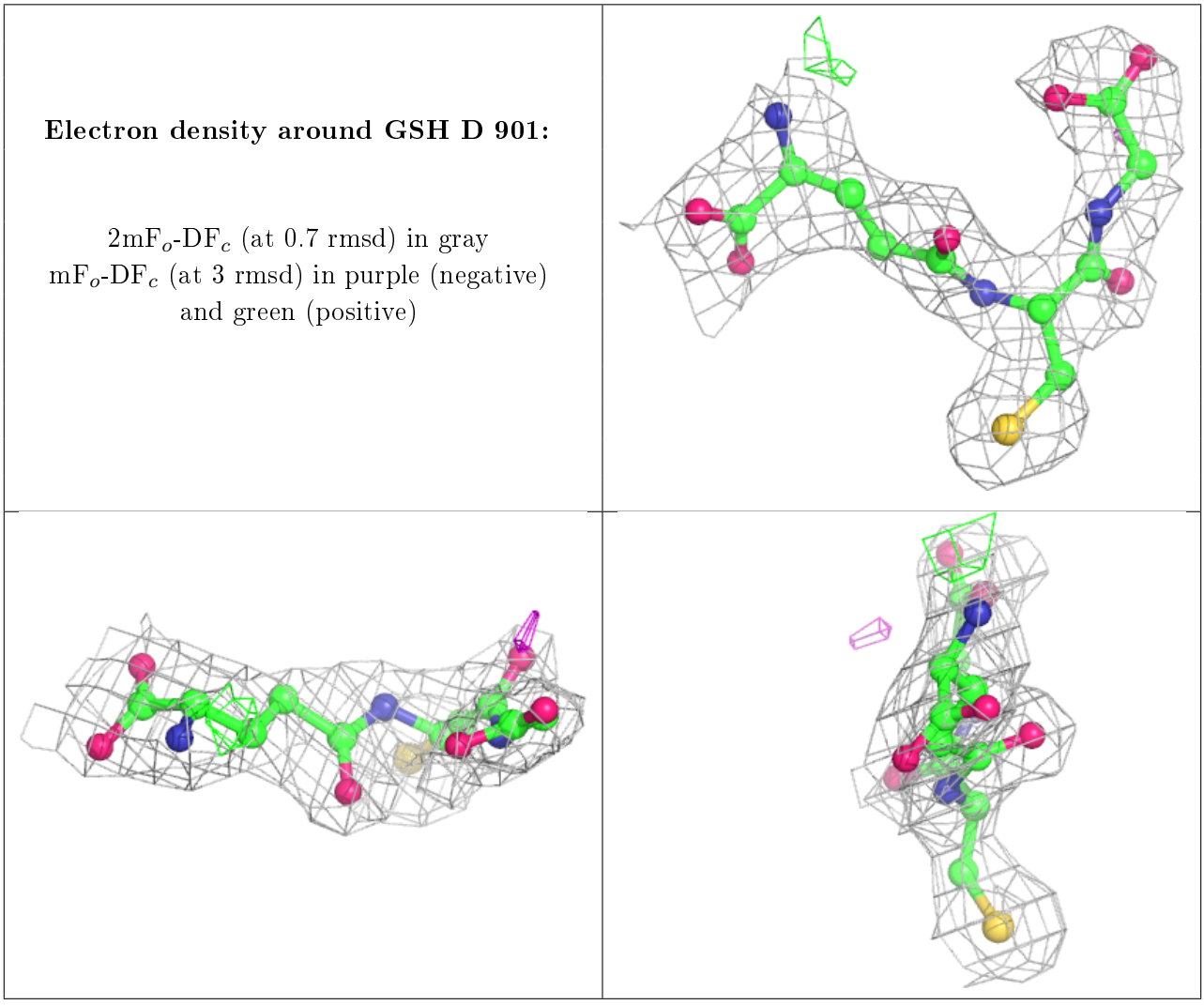
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	D	901	20/20	0.88	0.21	50,54,58,61	0
2	GSH	C	801	20/20	0.89	0.25	52,57,62,63	0
2	GSH	B	401	20/20	0.91	0.18	42,50,60,61	0
2	GSH	A	301	20/20	0.92	0.18	33,46,50,51	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.

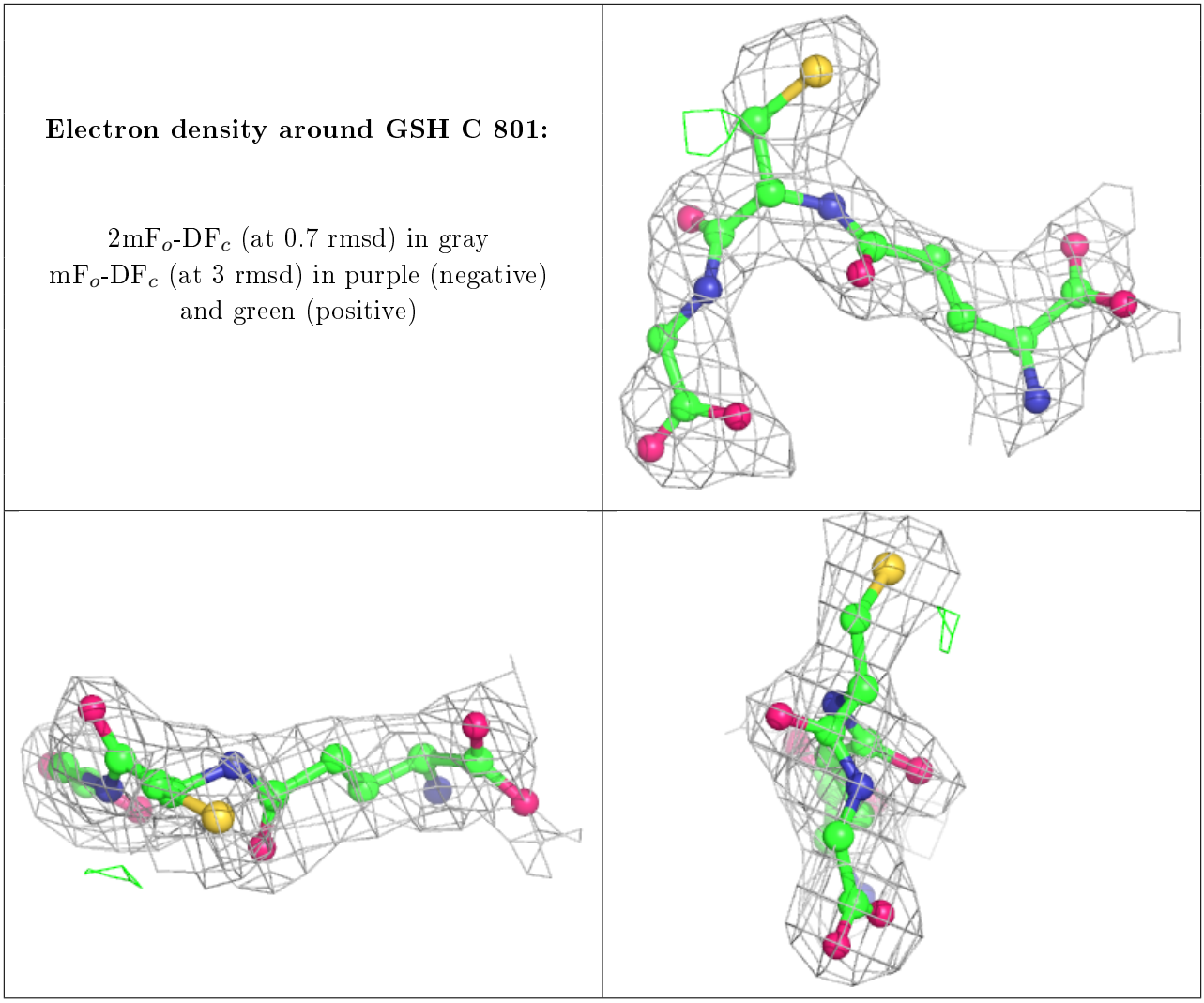
Electron density around GSH D 901:

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



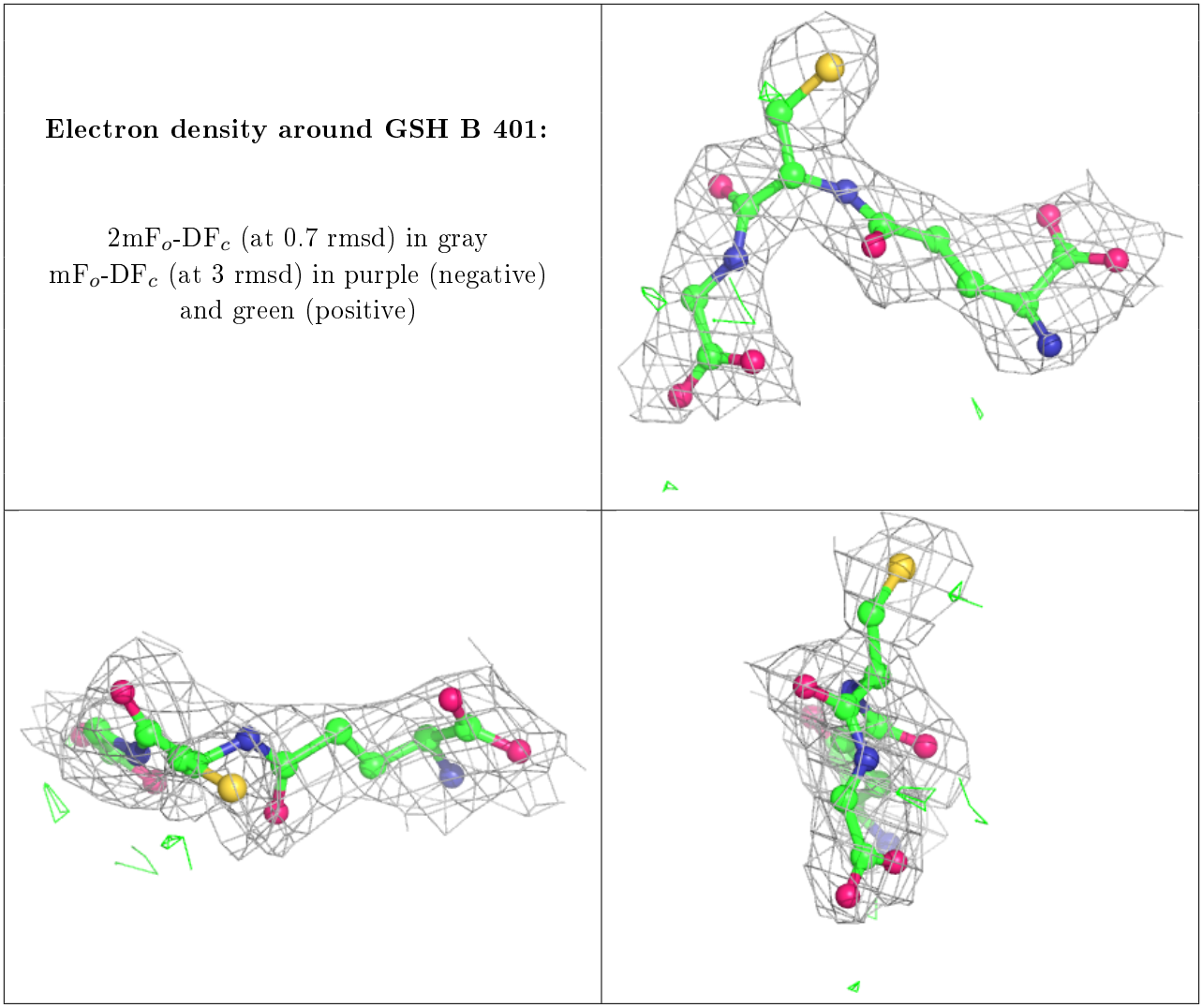
Electron density around GSH C 801:

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



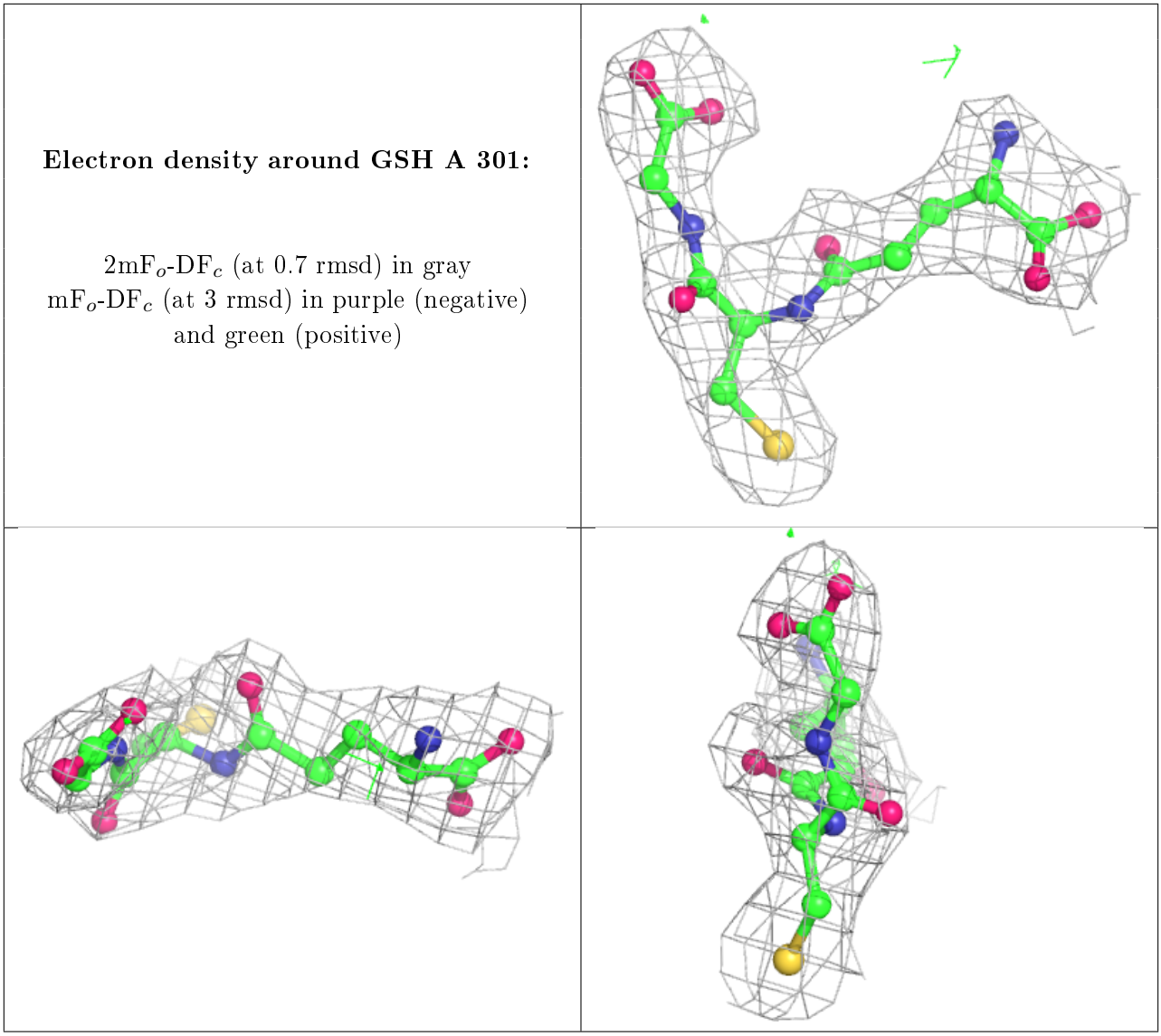
Electron density around GSH B 401:

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



Electron density around GSH A 301:

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



6.5 Other polymers

There are no such residues in this entry.