Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 07:57 am GMT

PDB ID	:	4ACS
Title	:	Crystal structure of mutant GST A2-2 with enhanced catalytic efficiency with azathioprine
Authors	:	Zhang, W.; Moden, O.; Tars, K.; Mannervik, B.
Deposited on	:	2011-12-19
Resolution	:	2.10 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

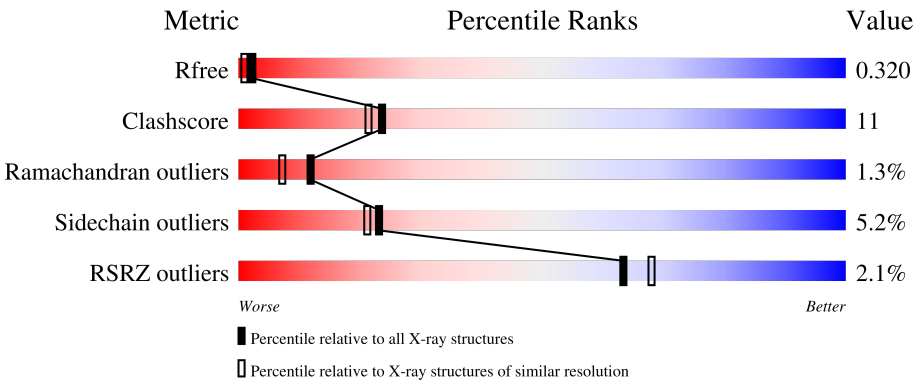
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	75% 22% • •
1	B	222	69% 27% • •
1	C	222	3% 64% 31% • •
1	D	222	5% 70% 26% • •

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GSH	A	230	X	-	-	-
2	GSH	B	230	X	-	-	-
2	GSH	C	230	X	-	-	-
2	GSH	D	230	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7665 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.

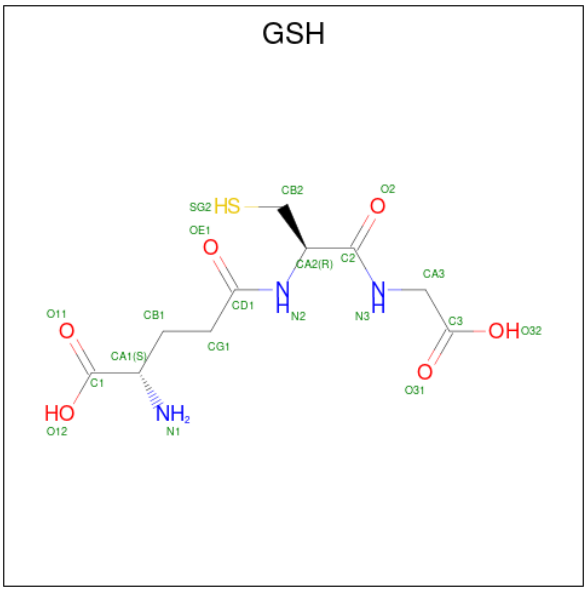
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	219	1778	1144	299	328	7	0	0	0
1	B	217	1757	1132	292	326	7	0	0	0
1	C	219	1778	1144	299	328	7	0	0	0
1	D	217	1757	1132	292	326	7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	GLY	LEU	engineered mutation	UNP P09210
A	108	ASP	LEU	engineered mutation	UNP P09210
A	110	SER	PRO	conflict	UNP P09210
A	222	HIS	PHE	engineered mutation	UNP P09210
B	107	GLY	LEU	engineered mutation	UNP P09210
B	108	ASP	LEU	engineered mutation	UNP P09210
B	110	SER	PRO	conflict	UNP P09210
B	222	HIS	PHE	engineered mutation	UNP P09210
C	107	GLY	LEU	engineered mutation	UNP P09210
C	108	ASP	LEU	engineered mutation	UNP P09210
C	110	SER	PRO	conflict	UNP P09210
C	222	HIS	PHE	engineered mutation	UNP P09210
D	107	GLY	LEU	engineered mutation	UNP P09210
D	108	ASP	LEU	engineered mutation	UNP P09210
D	110	SER	PRO	conflict	UNP P09210
D	222	HIS	PHE	engineered mutation	UNP P09210

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



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

- Molecule 3 is water.

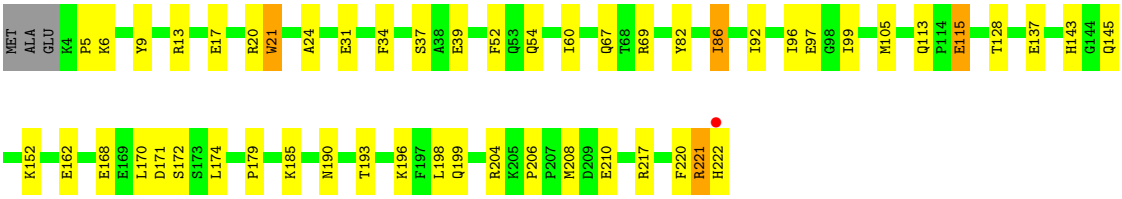
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	180	180	180	0	0
			Total	O		
3	B	110	110	110	0	0
			Total	O		
3	C	118	118	118	0	0
			Total	O		
3	D	107	107	107	0	0

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.

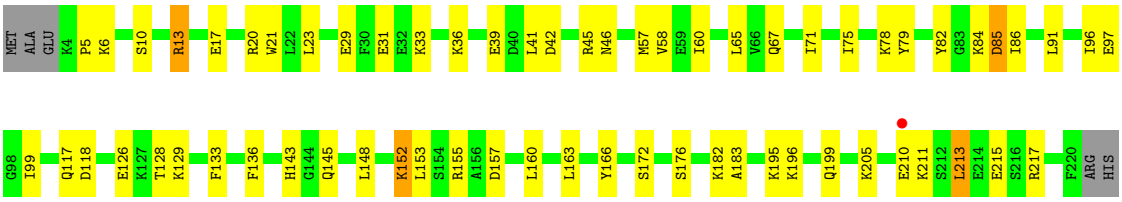
• Molecule 1: GLUTATHIONE S-TRANSFERASE A2

Chain A:



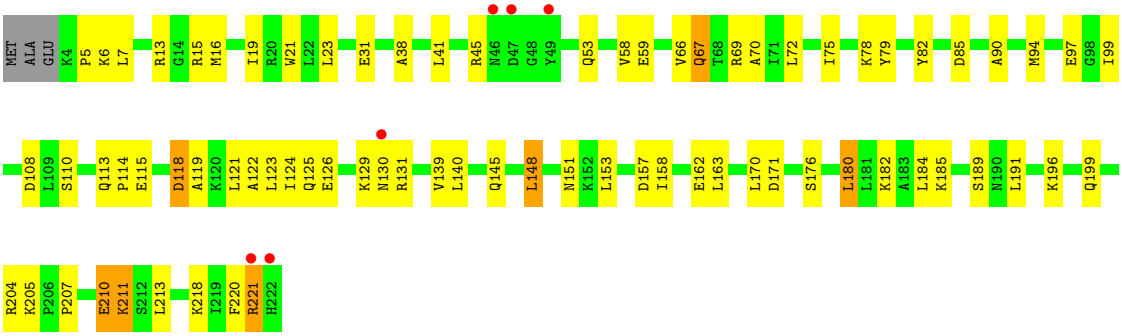
• Molecule 1: GLUTATHIONE S-TRANSFERASE A2

Chain B:



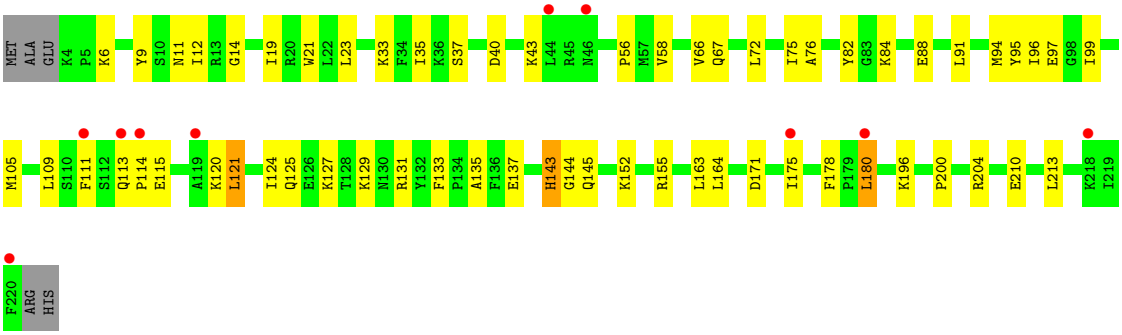
• Molecule 1: GLUTATHIONE S-TRANSFERASE A2

Chain C:



• Molecule 1: GLUTATHIONE S-TRANSFERASE A2

Chain D:


MET
ALA
GLU
K4
P5
K6
Y9
S10
N11
I12
R13
G14
I19
R20
W21
L22
L23
K33
F34
I35
K36
S37
D40
K43
L44
R45
N46
P56
M57
V58
V66
Q67
L72
I75
A76
Y82
G83
K84
E88
L91
M94
Y95
I96
E97
G98
I99
M105
L109
S110
F111
S112
Q113
P114
E115
A119
K120
L121
I124
Q125
E126
K127
T128
K129
N130
R131
Y132
F133
P134
A135
F136
E137
H143
G144
Q145
K152
R155
L163
L164
D171
I175
F178
P179
L180
K196
P200
R204
E210
L213
K218
I219
F220
ARG
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.66Å 94.80Å 113.72Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 37.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (40.00-2.10) 80.4 (37.84-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.261 , 0.321 0.261 , 0.320	Depositor DCC
R_{free} test set	2821 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 11.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.229 for h,-k,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	7665	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.68% 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 (i)

5.1 Standard geometry (i)

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	0.60	1/1812 (0.1%)	0.77	0/2433
1	B	0.56	1/1790 (0.1%)	0.75	0/2404
1	C	0.56	0/1812	0.75	0/2433
1	D	0.53	1/1790 (0.1%)	0.71	0/2404
All	All	0.56	3/7204 (0.0%)	0.75	0/9674

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	21	TRP	CD2-CE2	5.44	1.47	1.41
1	B	21	TRP	CD2-CE2	5.22	1.47	1.41
1	A	21	TRP	CD2-CE2	5.09	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1778	0	1826	34	0
1	B	1757	0	1806	40	0
1	C	1778	0	1826	53	0
1	D	1757	0	1806	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	15	2	0
2	B	20	0	15	0	0
2	C	20	0	15	0	0
2	D	20	0	15	1	0
3	A	180	0	0	7	0
3	B	110	0	0	6	0
3	C	118	0	0	9	0
3	D	107	0	0	8	0
All	All	7665	0	7324	162	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 11.

All (162) 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:D:105:MET:HG3	3:D:2056:HOH:O	1.65	0.96
1:C:15:ARG:HG2	1:C:15:ARG:HH11	1.42	0.84
1:D:121:LEU:O	1:D:125:GLN:HG3	1.78	0.83
1:A:217:ARG:HA	1:A:222:HIS:CE1	2.15	0.82
1:B:36:LYS:HD3	3:B:2032:HOH:O	1.80	0.81
1:C:140:LEU:HB3	1:C:180:LEU:HD12	1.63	0.80
1:B:46:ASN:ND2	3:B:2039:HOH:O	2.14	0.80
1:C:53:GLN:HB2	1:D:131:ARG:HE	1.50	0.76
1:C:145:GLN:OE1	1:C:151:ASN:HB2	1.87	0.74
1:B:143:HIS:CD2	1:B:145:GLN:HB2	2.25	0.71
1:D:196:LYS:HG3	3:D:2094:HOH:O	1.89	0.70
1:C:6:LYS:HE2	1:C:31:GLU:OE1	1.90	0.70
1:D:143:HIS:CE1	1:D:145:GLN:HB2	2.27	0.69
1:B:183:ALA:HA	3:B:2093:HOH:O	1.91	0.69
1:B:39:GLU:HA	1:B:42:ASP:HB2	1.77	0.66
1:A:96:ILE:HA	1:A:99:ILE:HD12	1.78	0.66
1:D:111:PHE:HA	1:D:213:LEU:HD21	1.79	0.64
1:B:143:HIS:HD2	1:B:145:GLN:H	1.45	0.64
1:A:69:ARG:HD2	1:B:97:GLU:OE1	1.99	0.63
1:A:198:LEU:O	1:A:204:ARG:NH2	2.30	0.63
1:A:96:ILE:HG21	3:A:2082:HOH:O	1.98	0.62
1:A:152:LYS:HE2	3:A:2074:HOH:O	1.99	0.62
1:D:175:ILE:HG22	3:D:2080:HOH:O	1.99	0.62
1:B:13:ARG:HG2	1:B:205:LYS:HB2	1.81	0.62
1:C:115:GLU:HA	3:C:2073:HOH:O	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LYS:O	1:C:58:VAL:HA	2.01	0.61
1:D:19:ILE:HG13	1:D:72:LEU:HD21	1.83	0.61
1:A:6:LYS:HE2	1:A:31:GLU:OE2	2.02	0.60
1:C:21:TRP:NE1	1:C:162:GLU:HG3	2.17	0.60
1:C:7:LEU:HG	1:C:58:VAL:HG22	1.83	0.59
1:D:43:LYS:HD3	3:D:2032:HOH:O	2.02	0.59
1:D:113:GLN:O	1:D:115:GLU:N	2.36	0.59
1:A:92:ILE:O	1:A:96:ILE:HG23	2.03	0.58
1:A:96:ILE:HG13	1:A:97:GLU:N	2.19	0.57
1:C:23:LEU:HG	1:C:75:ILE:HD13	1.85	0.57
1:D:23:LEU:HD21	1:D:75:ILE:HD13	1.87	0.57
1:D:109:LEU:HD22	1:D:124:ILE:HD12	1.86	0.57
1:A:21:TRP:NE1	1:A:162:GLU:HG3	2.20	0.57
1:C:6:LYS:HG2	1:C:31:GLU:HB3	1.86	0.57
1:A:105:MET:HA	3:A:2093:HOH:O	2.06	0.56
1:B:118:ASP:HA	3:B:2069:HOH:O	2.06	0.55
1:B:143:HIS:CD2	1:B:145:GLN:H	2.25	0.54
1:D:19:ILE:HG13	1:D:72:LEU:CD2	2.38	0.54
1:A:24:ALA:O	1:A:193:THR:HB	2.08	0.54
1:B:57:MET:HA	1:B:65:LEU:O	2.08	0.54
1:D:33:LYS:HE3	3:D:2030:HOH:O	2.09	0.53
1:A:21:TRP:CD1	1:A:162:GLU:HG3	2.43	0.52
1:C:15:ARG:HG2	1:C:15:ARG:NH1	2.17	0.52
1:B:6:LYS:HG2	1:B:31:GLU:HB2	1.91	0.52
1:C:220:PHE:O	1:C:221:ARG:C	2.47	0.52
1:C:121:LEU:HG	1:C:125:GLN:OE1	2.10	0.52
1:C:210:GLU:HA	1:C:213:LEU:HD12	1.91	0.52
1:B:23:LEU:HG	1:B:75:ILE:HD13	1.91	0.52
1:D:204:ARG:NH1	3:D:2009:HOH:O	2.34	0.51
1:D:35:ILE:HG23	1:D:40:ASP:HB2	1.92	0.51
1:C:118:ASP:OD1	1:C:118:ASP:N	2.44	0.51
1:C:94:MET:SD	1:D:66:VAL:HG22	2.51	0.51
1:B:33:LYS:HD3	3:B:2006:HOH:O	2.09	0.51
1:C:69:ARG:HB2	1:D:97:GLU:HG3	1.91	0.51
3:A:2059:HOH:O	1:B:91:LEU:HG	2.10	0.50
1:C:41:LEU:HD21	1:C:45:ARG:NH2	2.27	0.50
1:A:190:ASN:ND2	3:A:2155:HOH:O	2.43	0.50
1:A:137:GLU:OE2	1:A:179:PRO:HD2	2.12	0.49
1:C:196:LYS:O	1:C:199:GLN:HG2	2.12	0.49
1:C:85:ASP:HB2	3:C:2056:HOH:O	2.12	0.49
1:C:7:LEU:HB3	1:C:16:MET:HE3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:SER:O	1:C:182:LYS:NZ	2.42	0.48
1:B:5:PRO:HB3	1:B:60:ILE:HG13	1.95	0.48
1:D:129:LYS:HG2	1:D:178:PHE:HE2	1.79	0.48
1:A:21:TRP:CE2	1:A:162:GLU:HG3	2.49	0.48
1:B:29:GLU:HB3	3:B:2021:HOH:O	2.14	0.48
1:C:78:LYS:HE2	1:C:79:TYR:CZ	2.48	0.48
1:D:127:LYS:NZ	1:D:131:ARG:NH1	2.62	0.48
1:B:78:LYS:HD3	1:B:79:TYR:CE2	2.49	0.48
1:C:53:GLN:HB2	1:D:131:ARG:NE	2.24	0.48
1:C:158:ILE:HG22	3:C:2014:HOH:O	2.13	0.47
1:D:127:LYS:HZ2	1:D:131:ARG:NH1	2.12	0.47
1:A:9:TYR:O	1:A:34:PHE:HA	2.14	0.47
1:B:211:LYS:HB2	1:B:211:LYS:HE2	1.40	0.47
1:C:21:TRP:CE2	1:C:162:GLU:HG3	2.49	0.47
1:D:33:LYS:CE	3:D:2030:HOH:O	2.62	0.47
1:A:220:PHE:O	1:A:221:ARG:C	2.53	0.47
1:B:143:HIS:HE1	1:B:148:LEU:O	1.97	0.47
1:D:109:LEU:HD13	1:D:120:LYS:HB2	1.97	0.47
1:C:140:LEU:HD11	1:C:184:LEU:HD22	1.96	0.47
1:A:5:PRO:HB3	1:A:60:ILE:HB	1.96	0.47
1:C:13:ARG:NH2	1:C:207:PRO:HD3	2.29	0.47
1:C:97:GLU:HB3	1:D:67:GLN:OE1	2.14	0.47
1:D:135:ALA:N	3:D:2065:HOH:O	2.47	0.47
1:B:84:LYS:HD2	1:B:85:ASP:OD2	2.15	0.46
1:B:17:GLU:HG2	1:B:166:TYR:OH	2.16	0.46
1:A:143:HIS:ND1	1:A:145:GLN:HB2	2.30	0.46
1:C:110:SER:HB3	3:C:2066:HOH:O	2.15	0.46
1:C:113:GLN:HB3	1:C:115:GLU:OE1	2.16	0.46
1:D:6:LYS:O	1:D:58:VAL:HA	2.16	0.46
1:B:153:LEU:HD12	1:B:157:ASP:HB2	1.98	0.46
1:A:196:LYS:O	1:A:199:GLN:HG2	2.16	0.46
1:C:21:TRP:CD1	1:C:162:GLU:HG3	2.52	0.45
1:C:45:ARG:HB3	1:C:53:GLN:OE1	2.16	0.45
1:C:70:ALA:HB2	1:D:94:MET:N	2.31	0.45
1:D:76:ALA:CB	1:D:155:ARG:HD2	2.46	0.45
1:C:131:ARG:HH12	2:D:230:GSH:C3	2.30	0.45
1:A:168:GLU:OE1	1:A:185:LYS:NZ	2.50	0.45
1:A:220:PHE:CE1	2:A:230:GSH:HB22	2.52	0.45
1:C:124:ILE:HG13	3:C:2075:HOH:O	2.16	0.45
1:D:9:TYR:HE1	1:D:56:PRO:HD3	1.81	0.45
1:C:139:VAL:HG11	1:C:148:LEU:HD23	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ILE:HA	1:D:99:ILE:HD12	1.99	0.45
1:C:148:LEU:HD12	1:C:157:ASP:OD1	2.17	0.45
1:D:143:HIS:O	1:D:145:GLN:N	2.50	0.45
1:B:195:LYS:O	1:B:199:GLN:HG2	2.17	0.44
1:C:205:LYS:HD3	3:C:2107:HOH:O	2.17	0.44
1:A:54:GLN:NE2	2:A:230:GSH:HB13	2.32	0.44
1:B:117:GLN:O	1:B:118:ASP:C	2.55	0.44
1:C:38:ALA:HB1	3:C:2025:HOH:O	2.17	0.44
1:C:99:ILE:HG23	1:C:163:LEU:HD22	2.00	0.44
1:B:176:SER:O	1:B:182:LYS:NZ	2.51	0.44
1:B:20:ARG:NE	1:B:205:LYS:HE2	2.32	0.44
1:C:129:LYS:HG3	1:C:130:ASN:OD1	2.17	0.44
1:A:96:ILE:HD13	3:A:2082:HOH:O	2.16	0.43
1:A:52:PHE:HZ	1:B:136:PHE:CZ	2.36	0.43
1:A:128:THR:HG21	1:A:174:LEU:HD13	1.99	0.43
1:B:6:LYS:HB3	1:B:6:LYS:NZ	2.33	0.43
1:D:12:ILE:HD12	1:D:14:GLY:CA	2.48	0.43
1:D:40:ASP:O	1:D:43:LYS:HB3	2.18	0.43
1:A:204:ARG:NH1	1:D:200:PRO:HG3	2.33	0.43
1:A:13:ARG:NH1	3:A:2011:HOH:O	2.50	0.43
1:D:9:TYR:CE1	1:D:56:PRO:HD3	2.54	0.43
1:D:23:LEU:HD21	1:D:75:ILE:CD1	2.48	0.43
1:A:206:PRO:HB3	1:D:200:PRO:O	2.19	0.43
1:D:12:ILE:HD12	1:D:14:GLY:HA3	2.00	0.43
1:A:37:SER:HB2	1:A:39:GLU:OE1	2.19	0.43
1:B:58:VAL:HG21	1:B:71:ILE:HG21	1.99	0.43
1:C:185:LYS:O	1:C:189:SER:HB2	2.18	0.43
1:D:6:LYS:HB3	1:D:6:LYS:HE2	1.86	0.43
1:D:84:LYS:HG2	1:D:88:GLU:OE1	2.19	0.43
1:C:66:VAL:O	1:C:67:GLN:HB2	2.18	0.43
1:D:95:TYR:O	1:D:99:ILE:HG13	2.18	0.43
1:D:137:GLU:CD	1:D:180:LEU:HB2	2.40	0.43
1:A:113:GLN:HB3	1:A:115:GLU:HG3	2.01	0.42
1:C:5:PRO:HA	1:C:59:GLU:O	2.19	0.42
1:B:96:ILE:HD12	1:B:155:ARG:CZ	2.49	0.42
1:C:90:ALA:HB2	3:C:2057:HOH:O	2.18	0.42
1:A:17:GLU:OE1	1:A:20:ARG:HD2	2.19	0.42
1:B:196:LYS:O	1:B:199:GLN:HB2	2.19	0.42
1:C:153:LEU:HD21	1:C:191:LEU:HD13	2.00	0.42
1:B:13:ARG:NE	1:B:205:LYS:O	2.47	0.42
1:C:204:ARG:NH1	3:C:2008:HOH:O	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:HD12	1:B:157:ASP:HA	2.02	0.42
1:D:143:HIS:ND1	1:D:145:GLN:HB2	2.34	0.42
1:C:119:ALA:O	1:C:122:ALA:HB3	2.20	0.41
1:C:113:GLN:HB3	1:C:114:PRO:HD2	2.02	0.41
1:D:133:PHE:CZ	1:D:164:LEU:HD23	2.55	0.41
1:B:99:ILE:HD11	1:B:160:LEU:HB2	2.02	0.41
1:B:152:LYS:HG2	1:B:153:LEU:N	2.35	0.41
1:D:23:LEU:CD2	1:D:75:ILE:HD13	2.50	0.41
1:B:128:THR:O	1:B:133:PHE:HB2	2.21	0.40
1:B:41:LEU:HD21	1:B:45:ARG:NH2	2.36	0.40
1:C:211:LYS:HB2	1:C:211:LYS:NZ	2.35	0.40
1:C:19:ILE:HA	1:C:72:LEU:HD21	2.02	0.40
1:A:86:ILE:HD11	1:B:78:LYS:N	2.36	0.40
1:B:213:LEU:O	1:B:217:ARG:HG3	2.21	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	217/222 (98%)	204 (94%)	10 (5%)	3 (1%)	11 6
1	B	215/222 (97%)	200 (93%)	13 (6%)	2 (1%)	17 12
1	C	217/222 (98%)	205 (94%)	9 (4%)	3 (1%)	11 6
1	D	215/222 (97%)	193 (90%)	19 (9%)	3 (1%)	11 6
All	All	864/888 (97%)	802 (93%)	51 (6%)	11 (1%)	12 7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	221	ARG
1	D	144	GLY
1	D	171	ASP
1	B	13	ARG
1	D	114	PRO
1	A	67	GLN
1	C	171	ASP
1	A	171	ASP
1	C	67	GLN
1	B	67	GLN

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	195/197 (99%)	188 (96%)	7 (4%)	35	36
1	B	193/197 (98%)	181 (94%)	12 (6%)	18	15
1	C	195/197 (99%)	184 (94%)	11 (6%)	21	18
1	D	193/197 (98%)	183 (95%)	10 (5%)	23	21
All	All	776/788 (98%)	736 (95%)	40 (5%)	23	21

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	TYR
1	A	86	ILE
1	A	115	GLU
1	A	170	LEU
1	A	172	SER
1	A	208	MET
1	A	210	GLU
1	B	10	SER
1	B	82	TYR
1	B	85	ASP
1	B	86	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	126	GLU
1	B	129	LYS
1	B	152	LYS
1	B	163	LEU
1	B	172	SER
1	B	210	GLU
1	B	213	LEU
1	B	215	GLU
1	C	82	TYR
1	C	108	ASP
1	C	118	ASP
1	C	123	LEU
1	C	126	GLU
1	C	148	LEU
1	C	170	LEU
1	C	180	LEU
1	C	210	GLU
1	C	211	LYS
1	C	218	LYS
1	D	11	ASN
1	D	37	SER
1	D	82	TYR
1	D	91	LEU
1	D	121	LEU
1	D	143	HIS
1	D	152	LYS
1	D	163	LEU
1	D	180	LEU
1	D	210	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	190	ASN
1	A	222	HIS
1	B	54	GLN
1	B	130	ASN
1	B	143	HIS
1	C	46	ASN
1	C	54	GLN
1	C	113	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	190	ASN
1	D	113	GLN
1	D	190	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	230	-	18,19,19	0.81	0	23,24,24	1.69	4 (17%)
2	GSH	D	230	-	18,19,19	0.78	0	23,24,24	1.05	2 (8%)
2	GSH	B	230	-	18,19,19	0.73	0	23,24,24	2.06	8 (34%)
2	GSH	A	230	-	18,19,19	0.73	1 (5%)	23,24,24	1.19	5 (21%)

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	C	230	-	1/1/6/8	5/24/24/24	-
2	GSH	D	230	-	1/1/6/8	7/24/24/24	-
2	GSH	B	230	-	1/1/6/8	7/24/24/24	-
2	GSH	A	230	-	1/1/6/8	6/24/24/24	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	230	GSH	O32-C3	-2.00	1.24	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	230	GSH	CB2-CA2-N2	-4.74	104.52	111.28
2	C	230	GSH	CA2-CB2-SG2	4.58	119.34	114.19
2	B	230	GSH	CA2-CB2-SG2	-3.53	110.22	114.19
2	B	230	GSH	O12-C1-CA1	3.40	124.97	113.38
2	B	230	GSH	CB1-CA1-C1	3.23	117.98	110.30
2	C	230	GSH	O12-C1-CA1	3.09	123.92	113.38
2	B	230	GSH	CG1-CD1-N2	-2.91	110.79	115.83
2	B	230	GSH	CB2-CA2-C2	2.85	115.64	109.76
2	A	230	GSH	O12-C1-CA1	2.80	122.92	113.38
2	B	230	GSH	O11-C1-CA1	-2.79	112.30	122.14
2	D	230	GSH	O12-C1-CA1	2.63	122.33	113.38
2	C	230	GSH	O12-C1-O11	-2.53	118.35	124.09
2	C	230	GSH	O2-C2-N3	-2.45	117.72	122.99
2	D	230	GSH	CB1-CA1-C1	2.28	115.72	110.30
2	A	230	GSH	CA2-CB2-SG2	2.17	116.64	114.19
2	A	230	GSH	CB1-CA1-C1	2.12	115.34	110.30
2	B	230	GSH	O32-C3-CA3	2.11	120.08	112.74
2	A	230	GSH	O32-C3-CA3	2.06	119.90	112.74
2	A	230	GSH	O11-C1-CA1	-2.03	114.98	122.14

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	230	GSH	CA1
2	B	230	GSH	CA1
2	C	230	GSH	CA1
2	D	230	GSH	CA1

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	230	GSH	C1-CA1-CB1-CG1
2	B	230	GSH	O11-C1-CA1-N1
2	B	230	GSH	C1-CA1-CB1-CG1
2	A	230	GSH	CA1-CB1-CG1-CD1
2	C	230	GSH	CA1-CB1-CG1-CD1
2	A	230	GSH	O12-C1-CA1-N1
2	B	230	GSH	O12-C1-CA1-N1
2	C	230	GSH	O12-C1-CA1-N1
2	D	230	GSH	O12-C1-CA1-N1
2	B	230	GSH	CA1-CB1-CG1-CD1
2	D	230	GSH	CA1-CB1-CG1-CD1
2	C	230	GSH	O11-C1-CA1-CB1
2	C	230	GSH	O12-C1-CA1-CB1
2	D	230	GSH	O11-C1-CA1-CB1
2	D	230	GSH	O12-C1-CA1-CB1
2	A	230	GSH	O12-C1-CA1-CB1
2	A	230	GSH	O11-C1-CA1-CB1
2	A	230	GSH	O11-C1-CA1-N1
2	C	230	GSH	O11-C1-CA1-N1
2	D	230	GSH	O11-C1-CA1-N1
2	B	230	GSH	O11-C1-CA1-CB1
2	D	230	GSH	C1-CA1-CB1-CG1
2	B	230	GSH	O12-C1-CA1-CB1
2	B	230	GSH	N1-CA1-CB1-CG1
2	D	230	GSH	N2-CA2-CB2-SG2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	230	GSH	1	0
2	A	230	GSH	2	0

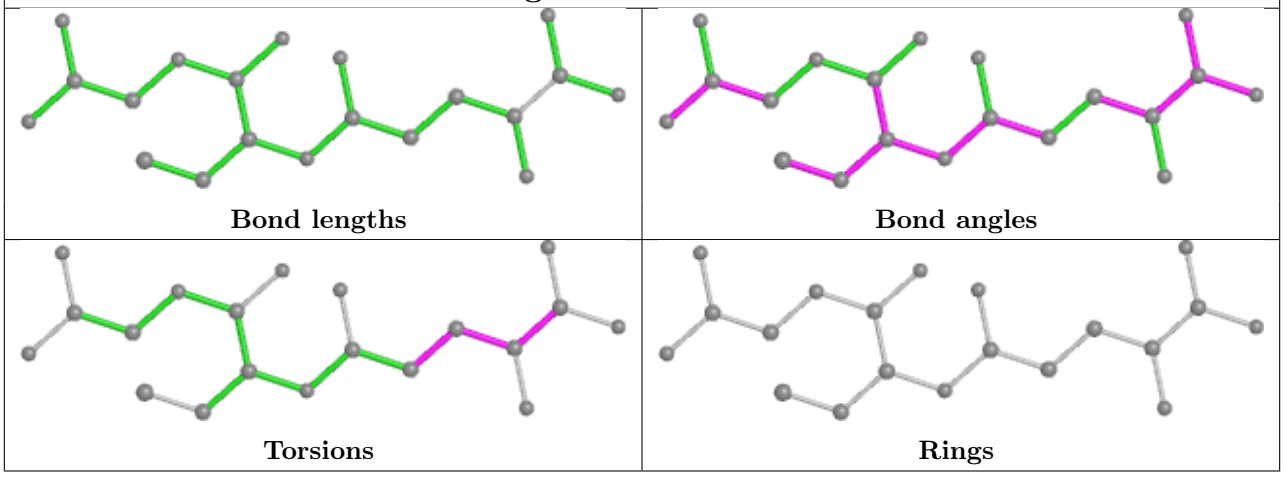
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

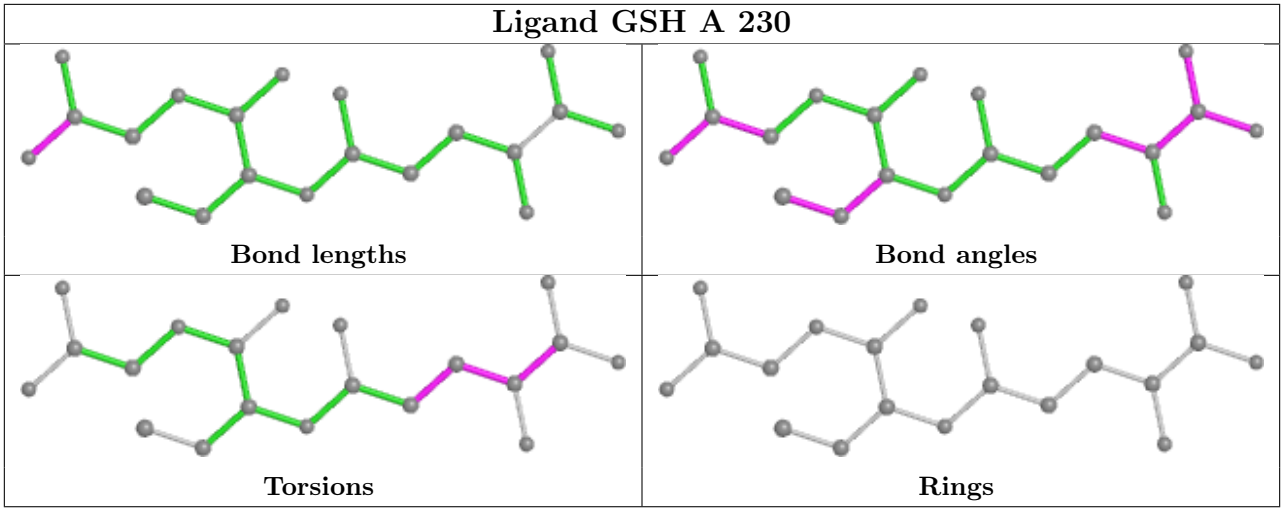
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GSH C 230

Ligand GSH D 230

Ligand GSH B 230





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	219/222 (98%)	0.03	1 (0%)	91	92	4, 10, 22, 38	0
1	B	217/222 (97%)	0.23	1 (0%)	91	92	7, 14, 28, 37	0
1	C	219/222 (98%)	0.35	6 (2%)	54	60	8, 17, 29, 55	0
1	D	217/222 (97%)	0.41	10 (4%)	32	38	8, 18, 39, 45	0
All	All	872/888 (98%)	0.25	18 (2%)	63	68	4, 14, 30, 55	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	222	HIS	4.8
1	A	222	HIS	4.1
1	D	44	LEU	3.0
1	D	113	GLN	2.9
1	C	221	ARG	2.4
1	C	47	ASP	2.3
1	D	175	ILE	2.3
1	D	220	PHE	2.3
1	C	46	ASN	2.3
1	C	49	TYR	2.2
1	B	210	GLU	2.2
1	D	46	ASN	2.2
1	D	119	ALA	2.1
1	D	114	PRO	2.1
1	D	111	PHE	2.1
1	D	180	LEU	2.0
1	C	130	ASN	2.0
1	D	218	LYS	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)

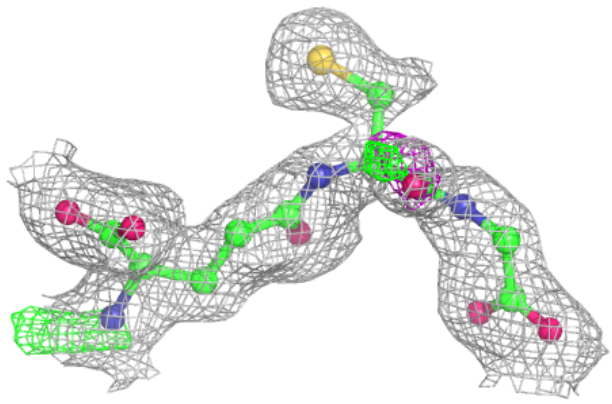
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

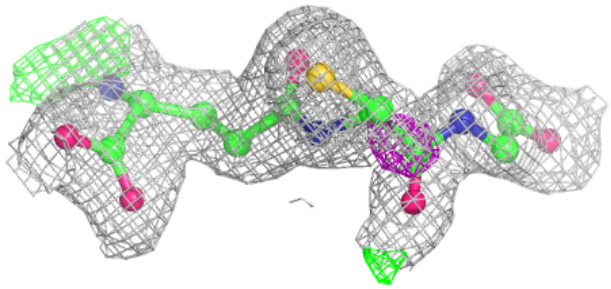
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GSH	D	230	20/20	0.85	0.17	16,21,23,23	0
2	GSH	B	230	20/20	0.92	0.14	11,14,15,16	0
2	GSH	C	230	20/20	0.93	0.14	13,15,16,16	0
2	GSH	A	230	20/20	0.93	0.12	8,10,13,15	0

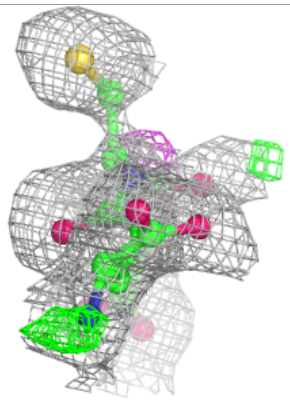
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GSH D 230:

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

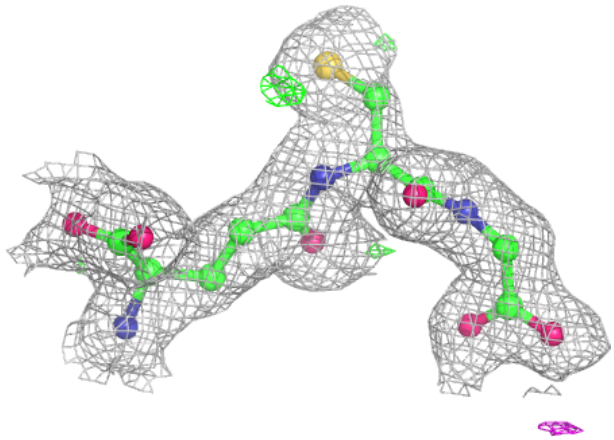


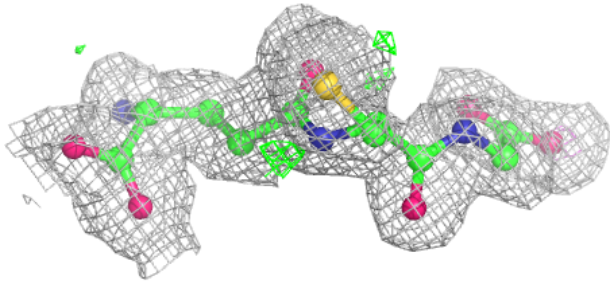


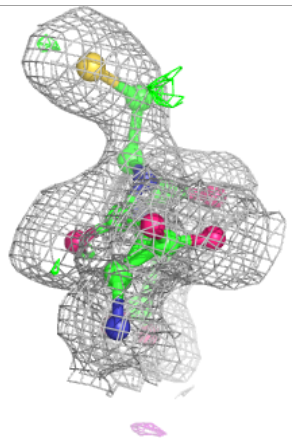


Electron density around GSH B 230:

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

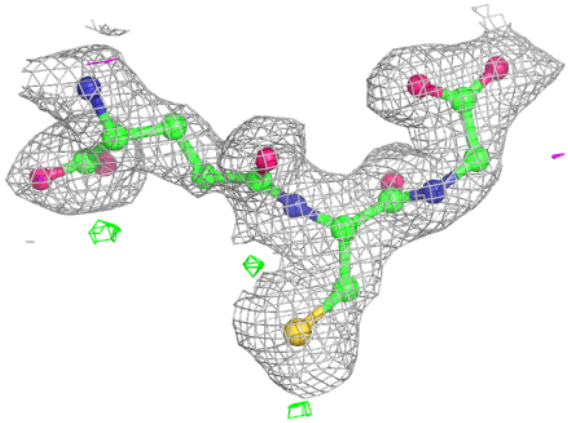


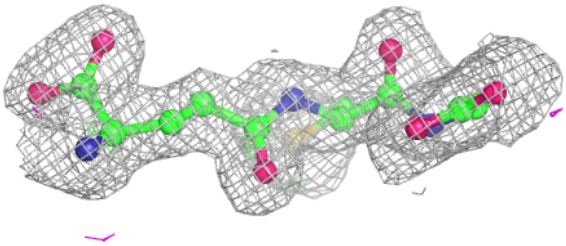


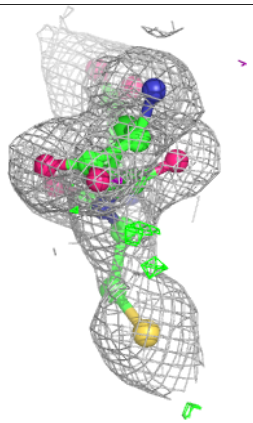


Electron density around GSH C 230:

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

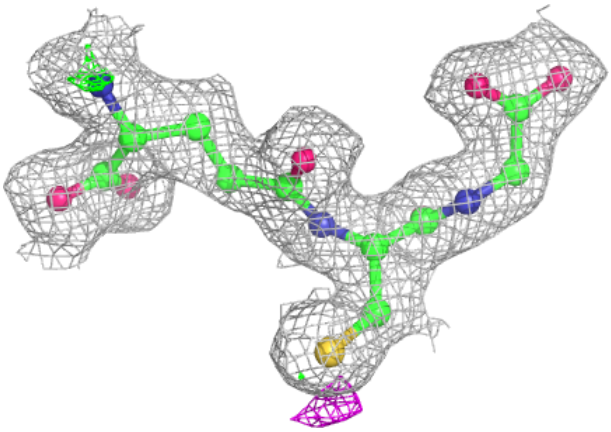


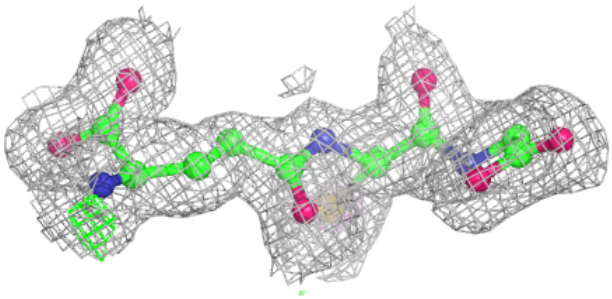


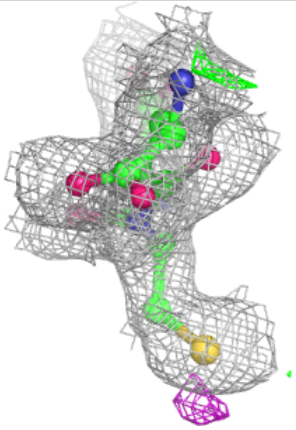


Electron density around GSH A 230:

$2mF_o$-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.