



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:49 pm BST

PDB ID : 4NHZ  
Title : Crystal structure of glutathione transferase BBTA-3750 from Bradyrhizobium sp., Target EFI-507290, with one glutathione bound  
Authors : Patskovsky, Y.; Vetting, M.W.; Toro, R.; Bhosle, R.; Al Obaidi, N.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Stead, M.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Hillerich, B.; Love, J.; Seidel, R.D.; Imker, H.J.; Gerlt, J.A.; Armstrong, R.N.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2013-11-05  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

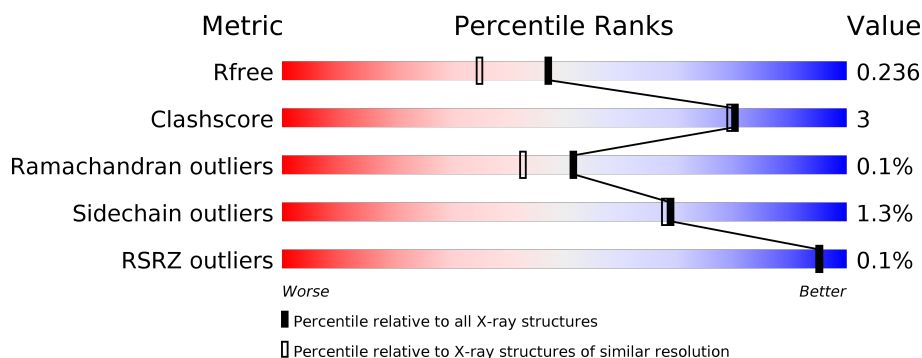
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	256	
1	B	256	
1	C	256	
1	D	256	
1	E	256	

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Mol	Chain	Length	Quality of chain
1	F	256	 82%8%10%
1	G	256	 83%7%10%
1	H	256	 92%. .
1	I	256	 80%11%9%
1	J	256	 84%5%.10%
1	K	256	 87%.10%
1	L	256	 87%.9%
1	M	256	 87%.10%
1	N	256	 85%5%9%
1	O	256	 86%.10%
1	P	256	 84%7%9%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32619 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 Putative glutathione S-transferase enzyme with thioredoxin-like domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1859	1201	326	328	4			
1	B	244	Total	C	N	O	S	0	2	0
			1967	1270	342	350	5			
1	C	233	Total	C	N	O	S	0	1	0
			1871	1208	328	331	4			
1	D	232	Total	C	N	O	S	0	3	0
			1874	1212	328	330	4			
1	E	232	Total	C	N	O	S	0	1	0
			1862	1204	327	327	4			
1	F	231	Total	C	N	O	S	0	2	0
			1863	1206	327	326	4			
1	G	231	Total	C	N	O	S	0	0	0
			1851	1197	325	325	4			
1	H	246	Total	C	N	O	S	0	4	0
			1995	1287	347	356	5			
1	I	232	Total	C	N	O	S	0	2	0
			1873	1210	329	330	4			
1	J	231	Total	C	N	O	S	0	3	0
			1869	1210	328	327	4			
1	K	231	Total	C	N	O	S	0	3	0
			1869	1210	328	327	4			
1	L	233	Total	C	N	O	S	0	0	0
			1865	1204	327	330	4			
1	M	231	Total	C	N	O	S	0	1	0
			1857	1201	326	326	4			
1	N	232	Total	C	N	O	S	0	4	0
			1885	1220	332	329	4			
1	O	231	Total	C	N	O	S	0	1	0
			1857	1201	326	326	4			
1	P	232	Total	C	N	O	S	0	2	0
			1873	1210	330	329	4			

There are 352 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP A5EI34
A	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
A	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
A	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
A	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
A	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
A	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
A	-14	SER	-	EXPRESSION TAG	UNP A5EI34
A	-13	SER	-	EXPRESSION TAG	UNP A5EI34
A	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
A	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
A	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
A	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
A	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
A	-7	THR	-	EXPRESSION TAG	UNP A5EI34
A	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
A	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
A	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
A	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
A	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
A	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
A	0	SER	-	EXPRESSION TAG	UNP A5EI34
B	-21	MET	-	EXPRESSION TAG	UNP A5EI34
B	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
B	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
B	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
B	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
B	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
B	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
B	-14	SER	-	EXPRESSION TAG	UNP A5EI34
B	-13	SER	-	EXPRESSION TAG	UNP A5EI34
B	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
B	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
B	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
B	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
B	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
B	-7	THR	-	EXPRESSION TAG	UNP A5EI34
B	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
B	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
B	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
B	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
B	-2	PHE	-	EXPRESSION TAG	UNP A5EI34

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
B	0	SER	-	EXPRESSION TAG	UNP A5EI34
C	-21	MET	-	EXPRESSION TAG	UNP A5EI34
C	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
C	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
C	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
C	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
C	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
C	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
C	-14	SER	-	EXPRESSION TAG	UNP A5EI34
C	-13	SER	-	EXPRESSION TAG	UNP A5EI34
C	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
C	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
C	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
C	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
C	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
C	-7	THR	-	EXPRESSION TAG	UNP A5EI34
C	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
C	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
C	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
C	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
C	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
C	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
C	0	SER	-	EXPRESSION TAG	UNP A5EI34
D	-20	MET	-	EXPRESSION TAG	UNP A5EI34
D	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
D	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
D	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
D	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
D	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
D	-14	HIS	-	EXPRESSION TAG	UNP A5EI34
D	-13	SER	-	EXPRESSION TAG	UNP A5EI34
D	-12	SER	-	EXPRESSION TAG	UNP A5EI34
D	-11	GLY	-	EXPRESSION TAG	UNP A5EI34
D	-10	VAL	-	EXPRESSION TAG	UNP A5EI34
D	-9	ASP	-	EXPRESSION TAG	UNP A5EI34
D	-8	LEU	-	EXPRESSION TAG	UNP A5EI34
D	-7	GLY	-	EXPRESSION TAG	UNP A5EI34
D	-6	THR	-	EXPRESSION TAG	UNP A5EI34
D	-5	GLU	-	EXPRESSION TAG	UNP A5EI34
D	-4	ASN	-	EXPRESSION TAG	UNP A5EI34
D	-3	LEU	-	EXPRESSION TAG	UNP A5EI34

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	TYR	-	EXPRESSION TAG	UNP A5EI34
D	-1	PHE	-	EXPRESSION TAG	UNP A5EI34
D	0	GLN	-	EXPRESSION TAG	UNP A5EI34
D	1	SER	-	EXPRESSION TAG	UNP A5EI34
E	-20	MET	-	EXPRESSION TAG	UNP A5EI34
E	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
E	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
E	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
E	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
E	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
E	-14	HIS	-	EXPRESSION TAG	UNP A5EI34
E	-13	SER	-	EXPRESSION TAG	UNP A5EI34
E	-12	SER	-	EXPRESSION TAG	UNP A5EI34
E	-11	GLY	-	EXPRESSION TAG	UNP A5EI34
E	-10	VAL	-	EXPRESSION TAG	UNP A5EI34
E	-9	ASP	-	EXPRESSION TAG	UNP A5EI34
E	-8	LEU	-	EXPRESSION TAG	UNP A5EI34
E	-7	GLY	-	EXPRESSION TAG	UNP A5EI34
E	-6	THR	-	EXPRESSION TAG	UNP A5EI34
E	-5	GLU	-	EXPRESSION TAG	UNP A5EI34
E	-4	ASN	-	EXPRESSION TAG	UNP A5EI34
E	-3	LEU	-	EXPRESSION TAG	UNP A5EI34
E	-2	TYR	-	EXPRESSION TAG	UNP A5EI34
E	-1	PHE	-	EXPRESSION TAG	UNP A5EI34
E	0	GLN	-	EXPRESSION TAG	UNP A5EI34
E	1	SER	-	EXPRESSION TAG	UNP A5EI34
F	-21	MET	-	EXPRESSION TAG	UNP A5EI34
F	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
F	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
F	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
F	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
F	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
F	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
F	-14	SER	-	EXPRESSION TAG	UNP A5EI34
F	-13	SER	-	EXPRESSION TAG	UNP A5EI34
F	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
F	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
F	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
F	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
F	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
F	-7	THR	-	EXPRESSION TAG	UNP A5EI34
F	-6	GLU	-	EXPRESSION TAG	UNP A5EI34

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
F	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
F	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
F	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
F	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
F	0	SER	-	EXPRESSION TAG	UNP A5EI34
G	-21	MET	-	EXPRESSION TAG	UNP A5EI34
G	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
G	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
G	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
G	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
G	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
G	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
G	-14	SER	-	EXPRESSION TAG	UNP A5EI34
G	-13	SER	-	EXPRESSION TAG	UNP A5EI34
G	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
G	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
G	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
G	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
G	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
G	-7	THR	-	EXPRESSION TAG	UNP A5EI34
G	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
G	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
G	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
G	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
G	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
G	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
G	0	SER	-	EXPRESSION TAG	UNP A5EI34
H	-21	MET	-	EXPRESSION TAG	UNP A5EI34
H	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
H	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
H	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
H	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
H	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
H	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
H	-14	SER	-	EXPRESSION TAG	UNP A5EI34
H	-13	SER	-	EXPRESSION TAG	UNP A5EI34
H	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
H	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
H	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
H	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
H	-8	GLY	-	EXPRESSION TAG	UNP A5EI34

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	THR	-	EXPRESSION TAG	UNP A5EI34
H	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
H	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
H	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
H	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
H	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
H	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
H	0	SER	-	EXPRESSION TAG	UNP A5EI34
I	-21	MET	-	EXPRESSION TAG	UNP A5EI34
I	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
I	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
I	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
I	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
I	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
I	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
I	-14	SER	-	EXPRESSION TAG	UNP A5EI34
I	-13	SER	-	EXPRESSION TAG	UNP A5EI34
I	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
I	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
I	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
I	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
I	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
I	-7	THR	-	EXPRESSION TAG	UNP A5EI34
I	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
I	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
I	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
I	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
I	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
I	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
I	0	SER	-	EXPRESSION TAG	UNP A5EI34
J	-21	MET	-	EXPRESSION TAG	UNP A5EI34
J	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
J	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
J	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
J	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
J	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
J	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
J	-14	SER	-	EXPRESSION TAG	UNP A5EI34
J	-13	SER	-	EXPRESSION TAG	UNP A5EI34
J	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
J	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
J	-10	ASP	-	EXPRESSION TAG	UNP A5EI34

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
J	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
J	-7	THR	-	EXPRESSION TAG	UNP A5EI34
J	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
J	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
J	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
J	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
J	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
J	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
J	0	SER	-	EXPRESSION TAG	UNP A5EI34
K	-21	MET	-	EXPRESSION TAG	UNP A5EI34
K	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
K	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
K	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
K	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
K	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
K	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
K	-14	SER	-	EXPRESSION TAG	UNP A5EI34
K	-13	SER	-	EXPRESSION TAG	UNP A5EI34
K	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
K	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
K	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
K	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
K	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
K	-7	THR	-	EXPRESSION TAG	UNP A5EI34
K	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
K	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
K	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
K	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
K	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
K	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
K	0	SER	-	EXPRESSION TAG	UNP A5EI34
L	-21	MET	-	EXPRESSION TAG	UNP A5EI34
L	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
L	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
L	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
L	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
L	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
L	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
L	-14	SER	-	EXPRESSION TAG	UNP A5EI34
L	-13	SER	-	EXPRESSION TAG	UNP A5EI34
L	-12	GLY	-	EXPRESSION TAG	UNP A5EI34

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
L	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
L	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
L	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
L	-7	THR	-	EXPRESSION TAG	UNP A5EI34
L	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
L	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
L	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
L	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
L	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
L	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
L	0	SER	-	EXPRESSION TAG	UNP A5EI34
M	-21	MET	-	EXPRESSION TAG	UNP A5EI34
M	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
M	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
M	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
M	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
M	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
M	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
M	-14	SER	-	EXPRESSION TAG	UNP A5EI34
M	-13	SER	-	EXPRESSION TAG	UNP A5EI34
M	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
M	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
M	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
M	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
M	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
M	-7	THR	-	EXPRESSION TAG	UNP A5EI34
M	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
M	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
M	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
M	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
M	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
M	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
M	0	SER	-	EXPRESSION TAG	UNP A5EI34
N	-21	MET	-	EXPRESSION TAG	UNP A5EI34
N	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
N	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
N	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
N	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
N	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
N	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
N	-14	SER	-	EXPRESSION TAG	UNP A5EI34

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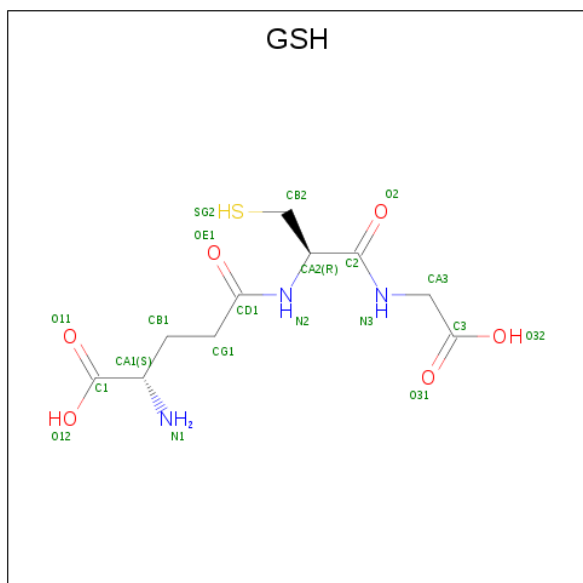
Chain	Residue	Modelled	Actual	Comment	Reference
N	-13	SER	-	EXPRESSION TAG	UNP A5EI34
N	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
N	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
N	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
N	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
N	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
N	-7	THR	-	EXPRESSION TAG	UNP A5EI34
N	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
N	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
N	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
N	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
N	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
N	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
N	0	SER	-	EXPRESSION TAG	UNP A5EI34
O	-21	MET	-	EXPRESSION TAG	UNP A5EI34
O	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
O	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
O	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
O	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
O	-16	HIS	-	EXPRESSION TAG	UNP A5EI34
O	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
O	-14	SER	-	EXPRESSION TAG	UNP A5EI34
O	-13	SER	-	EXPRESSION TAG	UNP A5EI34
O	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
O	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
O	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
O	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
O	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
O	-7	THR	-	EXPRESSION TAG	UNP A5EI34
O	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
O	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
O	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
O	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
O	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
O	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
O	0	SER	-	EXPRESSION TAG	UNP A5EI34
P	-21	MET	-	EXPRESSION TAG	UNP A5EI34
P	-20	HIS	-	EXPRESSION TAG	UNP A5EI34
P	-19	HIS	-	EXPRESSION TAG	UNP A5EI34
P	-18	HIS	-	EXPRESSION TAG	UNP A5EI34
P	-17	HIS	-	EXPRESSION TAG	UNP A5EI34
P	-16	HIS	-	EXPRESSION TAG	UNP A5EI34

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-15	HIS	-	EXPRESSION TAG	UNP A5EI34
P	-14	SER	-	EXPRESSION TAG	UNP A5EI34
P	-13	SER	-	EXPRESSION TAG	UNP A5EI34
P	-12	GLY	-	EXPRESSION TAG	UNP A5EI34
P	-11	VAL	-	EXPRESSION TAG	UNP A5EI34
P	-10	ASP	-	EXPRESSION TAG	UNP A5EI34
P	-9	LEU	-	EXPRESSION TAG	UNP A5EI34
P	-8	GLY	-	EXPRESSION TAG	UNP A5EI34
P	-7	THR	-	EXPRESSION TAG	UNP A5EI34
P	-6	GLU	-	EXPRESSION TAG	UNP A5EI34
P	-5	ASN	-	EXPRESSION TAG	UNP A5EI34
P	-4	LEU	-	EXPRESSION TAG	UNP A5EI34
P	-3	TYR	-	EXPRESSION TAG	UNP A5EI34
P	-2	PHE	-	EXPRESSION TAG	UNP A5EI34
P	-1	GLN	-	EXPRESSION TAG	UNP A5EI34
P	0	SER	-	EXPRESSION TAG	UNP A5EI34

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	G	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	H	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	I	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	J	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	K	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	L	1	Total	C	N	O	S	0	0
			14	7	2	4	1		
2	M	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	N	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	O	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	P	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	132	Total	O	0	0
			132	132		
3	B	148	Total	O	0	0
			148	148		
3	C	139	Total	O	0	0
			139	139		
3	D	136	Total	O	0	0
			136	136		
3	E	146	Total	O	0	0
			146	146		
3	F	124	Total	O	0	0
			124	124		

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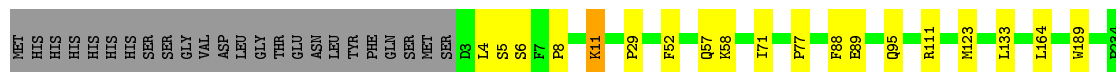
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	121	Total 121	O 121	0	0
3	H	144	Total 144	O 144	0	0
3	I	159	Total 159	O 159	0	0
3	J	137	Total 137	O 137	0	0
3	K	108	Total 108	O 108	0	0
3	L	154	Total 154	O 154	0	0
3	M	132	Total 133	O 133	0	1
3	N	161	Total 161	O 161	0	0
3	O	130	Total 130	O 130	0	0
3	P	143	Total 143	O 143	0	0

### 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: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain A: 




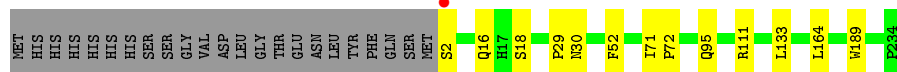
- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain B: 




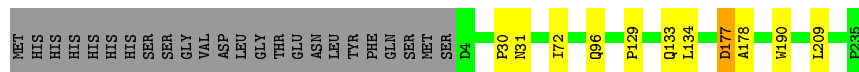
- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain C: 




- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain D: 




- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

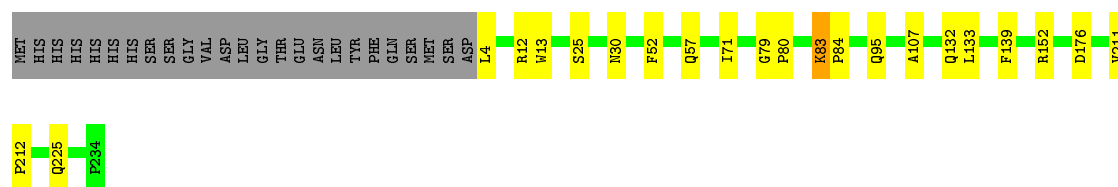
Chain E: 




- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain



Chain F: 



- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain G: 




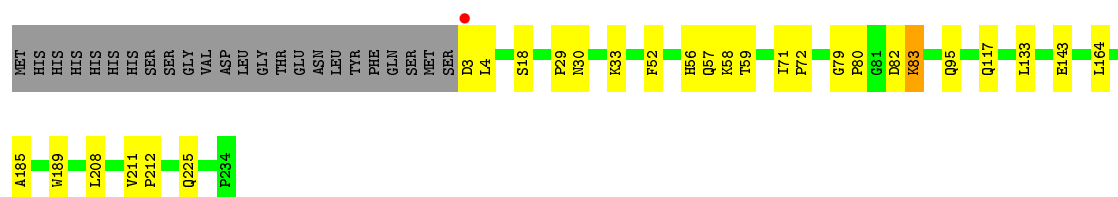
- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain H: 




- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain I: 




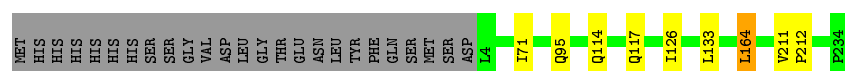
- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain J: 




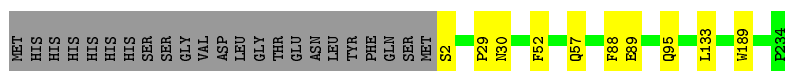
- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain K: 



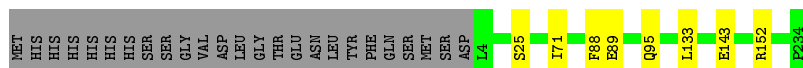
- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain L: 



- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain M: 87% 10%



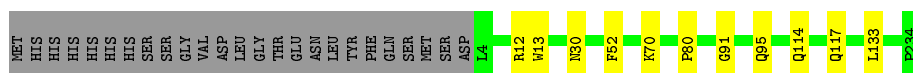
- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain N: 85% 5% 9%



- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain O: 86% 10%



- Molecule 1: Putative glutathione S-transferase enzyme with thioredoxin-like domain

Chain P: 84% 7% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.00Å 99.36Å 108.73Å 89.98° 89.97° 89.99°	Depositor
Resolution (Å)	50.00 – 1.90 49.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-1.90) 96.9 (49.68-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.186 , 0.225 0.199 , 0.236	Depositor DCC
$R_{free}$ test set	6282 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.835	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for k,-h,l 0.000 for -k,h,l 0.467 for h,-k,-l 0.124 for -h,k,-l 0.123 for -h,-k,l 0.000 for k,h,-l 0.000 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	32619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3688e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 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	0.53	0/1915	0.68	0/2599
1	B	0.53	0/2031	0.70	0/2755
1	C	0.53	0/1930	0.68	0/2619
1	D	0.51	0/1939	0.69	0/2631
1	E	0.52	0/1921	0.66	0/2607
1	F	0.54	2/1925 (0.1%)	0.69	2/2611 (0.1%)
1	G	0.53	1/1907 (0.1%)	0.68	1/2588 (0.0%)
1	H	0.51	0/2065	0.67	0/2801
1	I	0.54	1/1935 (0.1%)	0.68	1/2625 (0.0%)
1	J	0.51	0/1934	0.66	0/2623
1	K	0.48	0/1934	0.67	0/2623
1	L	0.50	0/1921	0.66	0/2607
1	M	0.53	0/1916	0.69	0/2600
1	N	0.53	0/1953	0.68	0/2647
1	O	0.51	0/1916	0.66	0/2600
1	P	0.49	0/1935	0.65	0/2625
All	All	0.52	4/31077 (0.0%)	0.67	4/42161 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	80	PRO	N-CD	5.28	1.55	1.47
1	I	80	PRO	N-CD	5.26	1.55	1.47
1	F	80	PRO	N-CD	5.11	1.55	1.47
1	F	84	PRO	N-CD	5.05	1.54	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	83	LYS	C-N-CD	5.71	140.39	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	79	GLY	C-N-CD	5.57	140.10	128.40
1	F	79	GLY	C-N-CD	5.52	140.00	128.40
1	G	79	GLY	C-N-CD	5.52	139.99	128.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	1859	0	1843	11	0
1	B	1967	0	1951	10	0
1	C	1871	0	1856	10	0
1	D	1874	0	1863	7	0
1	E	1862	0	1849	11	0
1	F	1863	0	1860	21	0
1	G	1851	0	1839	10	0
1	H	1995	0	1981	8	0
1	I	1873	0	1862	16	0
1	J	1869	0	1868	14	0
1	K	1869	0	1868	6	0
1	L	1865	0	1848	10	0
1	M	1857	0	1847	6	0
1	N	1885	0	1890	12	0
1	O	1857	0	1847	10	0
1	P	1873	0	1864	14	0
2	A	20	0	15	2	0
2	B	20	0	15	2	0
2	C	20	0	15	2	0
2	D	20	0	15	1	0
2	E	20	0	15	3	0
2	F	20	0	15	4	0
2	G	20	0	15	3	0
2	H	20	0	15	3	0
2	I	20	0	15	1	0
2	J	20	0	15	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	20	0	15	0	0
2	L	14	0	8	4	0
2	M	20	0	15	0	0
2	N	20	0	15	3	0
2	O	20	0	15	4	0
2	P	20	0	15	1	0
3	A	132	0	0	0	0
3	B	148	0	0	4	0
3	C	139	0	0	1	0
3	D	136	0	0	0	0
3	E	146	0	0	0	0
3	F	124	0	0	6	0
3	G	121	0	0	1	0
3	H	144	0	0	2	0
3	I	159	0	0	1	0
3	J	137	0	0	0	0
3	K	108	0	0	0	0
3	L	154	0	0	0	0
3	M	133	0	0	0	0
3	N	161	0	0	1	0
3	O	130	0	0	1	0
3	P	143	0	0	0	0
All	All	32619	0	30169	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:95:GLN:HE22	1:J:95[A]:GLN:HE22	1.15	0.91
1:I:83:LYS:HA	1:I:83:LYS:HE3	1.54	0.89
1:J:52:PHE:HE2	2:J:301:GSH:HA32	1.36	0.89
1:K:95[A]:GLN:HE22	1:L:95:GLN:HE22	1.14	0.89
1:P:112[B]:ARG:CG	1:P:112[B]:ARG:HH11	1.87	0.88
1:J:52:PHE:CE2	2:J:301:GSH:HA32	2.10	0.87
1:O:95[A]:GLN:HE22	1:P:95:GLN:HE22	1.24	0.86
1:C:95:GLN:HE22	1:D:96[A]:GLN:HE22	1.23	0.86
1:E:96:GLN:HE22	1:F:95[A]:GLN:HE22	1.22	0.84
1:L:52:PHE:CE2	2:L:301:GSH:HA32	2.14	0.83
1:M:95[B]:GLN:HE22	1:N:95:GLN:HE22	1.24	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HE22	1:B:95[A]:GLN:HE22	1.26	0.80
1:P:112[B]:ARG:HH11	1:P:112[B]:ARG:HG3	1.50	0.77
1:G:52:PHE:CE2	2:G:301:GSH:HA32	2.23	0.74
1:G:132:GLN:HE22	1:H:152:ARG:HH21	1.36	0.74
1:E:133:GLN:HE22	1:F:152:ARG:HH21	1.37	0.72
1:L:52:PHE:CE2	2:L:301:GSH:CA3	2.74	0.71
1:J:52:PHE:HE2	2:J:301:GSH:CA3	2.04	0.70
1:H:52:PHE:CE2	2:H:301:GSH:HA31	2.29	0.67
1:O:114:GLN:O	1:O:117:GLN:HB3	1.95	0.66
1:F:52:PHE:CE2	2:F:301:GSH:HA32	2.34	0.63
1:M:152:ARG:HH21	1:N:132:GLN:HE22	1.47	0.62
1:O:30:ASN:HD22	2:O:301:GSH:CD1	2.15	0.60
1:B:52:PHE:CE2	2:B:301:GSH:HA31	2.37	0.59
1:A:52:PHE:CE2	2:A:301:GSH:HA32	2.38	0.58
1:F:107:ALA:N	3:F:497:HOH:O	2.36	0.57
1:G:52:PHE:HE2	2:G:301:GSH:HA32	1.70	0.56
1:H:12:ARG:HD3	1:H:13:TRP:CH2	2.40	0.56
1:E:153:ARG:HH21	1:F:132:GLN:HE22	1.53	0.56
1:F:52:PHE:CE2	1:F:57:GLN:HG3	2.41	0.55
1:O:70:LYS:HG2	2:O:301:GSH:HA31	1.88	0.55
1:P:112[B]:ARG:HG2	1:P:112[B]:ARG:HH11	1.71	0.55
1:O:52:PHE:CE2	2:O:301:GSH:HA32	2.41	0.55
1:A:8:PRO:O	1:A:11:LYS:HG3	2.07	0.55
1:H:52:PHE:CE2	2:H:301:GSH:CA3	2.90	0.54
1:B:52:PHE:CE2	2:B:301:GSH:CA3	2.91	0.54
1:F:133:LEU:C	1:F:133:LEU:HD23	2.29	0.53
1:F:4:LEU:N	3:F:475:HOH:O	2.40	0.53
1:I:4:LEU:HD13	1:I:18:SER:HB2	1.90	0.53
1:J:30:ASN:HD22	2:J:301:GSH:CD1	2.22	0.53
1:K:133:LEU:C	1:K:133:LEU:HD23	2.29	0.53
1:P:29:PRO:HB2	1:P:189:TRP:CE2	2.44	0.52
1:L:133:LEU:C	1:L:133:LEU:HD23	2.29	0.52
1:P:112[B]:ARG:NH1	1:P:112[B]:ARG:CG	2.57	0.51
1:D:31:ASN:HD22	2:D:301:GSH:CD1	2.24	0.51
1:E:31:ASN:HD22	2:E:301:GSH:CD1	2.24	0.51
1:L:30:ASN:HD22	2:L:301:GSH:CD1	2.23	0.51
1:I:83:LYS:CA	1:I:83:LYS:HE3	2.31	0.51
1:D:134:LEU:HD23	1:D:134:LEU:C	2.31	0.51
1:E:53:PHE:CE2	2:E:301:GSH:HA32	2.46	0.50
1:N:52:PHE:HE2	2:N:301:GSH:CA3	2.24	0.50
1:M:133:LEU:HD23	1:M:133:LEU:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:52:PHE:HE2	2:O:301:GSH:HA32	1.77	0.50
1:O:80:PRO:HD2	3:O:436:HOH:O	2.11	0.50
1:F:52:PHE:CE2	2:F:301:GSH:CA3	2.95	0.49
1:H:133:LEU:HD23	1:H:133:LEU:C	2.33	0.49
1:I:133:LEU:C	1:I:133:LEU:HD23	2.32	0.49
1:C:2:SER:N	1:C:18:SER:HG	2.11	0.49
1:P:133:LEU:C	1:P:133:LEU:HD23	2.32	0.49
1:B:29:PRO:HB2	1:B:189:TRP:CE2	2.48	0.49
1:C:16:GLN:HG3	3:C:437:HOH:O	2.13	0.49
1:D:129:PRO:O	1:D:133:GLN:HG2	2.12	0.49
1:E:53:PHE:CE2	2:E:301:GSH:CA3	2.96	0.48
1:C:52:PHE:CE2	2:C:301:GSH:HA32	2.48	0.48
1:D:30:PRO:HB2	1:D:190:TRP:CE2	2.48	0.48
1:F:71:ILE:C	1:F:71:ILE:HD12	2.34	0.48
1:K:71:ILE:C	1:K:71:ILE:HD12	2.34	0.48
1:B:133:LEU:HD23	1:B:133:LEU:C	2.34	0.48
1:E:53:PHE:CE2	1:E:58:GLN:HG3	2.48	0.48
1:E:13:ARG:HB3	1:E:14:TRP:CE3	2.48	0.48
1:C:71:ILE:HD12	1:C:71:ILE:C	2.34	0.48
1:M:71:ILE:C	1:M:71:ILE:HD12	2.34	0.48
1:B:3:ASP:HA	3:B:524:HOH:O	2.13	0.48
1:J:83:LYS:HA	1:J:83:LYS:HE2	1.96	0.48
1:G:112:ARG:HB2	3:G:450:HOH:O	2.14	0.48
1:K:114:GLN:O	1:K:117:GLN:HB3	2.14	0.48
1:A:88:PHE:O	1:A:89:GLU:HB2	2.14	0.47
1:N:71:ILE:C	1:N:71:ILE:HD12	2.34	0.47
1:A:29:PRO:HB2	1:A:189:TRP:CE2	2.50	0.47
1:C:133:LEU:HD23	1:C:133:LEU:O	2.15	0.47
1:E:89:PHE:O	1:E:90:GLU:HB2	2.14	0.47
1:G:88:PHE:O	1:G:89:GLU:HB2	2.15	0.47
1:I:29:PRO:HB2	1:I:189:TRP:CE2	2.50	0.47
1:L:88:PHE:O	1:L:89:GLU:HB2	2.14	0.47
1:N:52:PHE:CE2	2:N:301:GSH:HA32	2.49	0.47
1:N:29:PRO:HB2	1:N:189:TRP:CE2	2.50	0.47
1:F:211:VAL:HB	1:F:212:PRO:HD3	1.95	0.47
1:N:52:PHE:HE2	2:N:301:GSH:HA32	1.80	0.47
1:N:112[A]:ARG:CZ	3:N:497:HOH:O	2.62	0.46
1:H:52:PHE:HE2	2:H:301:GSH:HA31	1.78	0.46
1:F:30:ASN:HD22	2:F:301:GSH:CD1	2.29	0.46
1:E:30:PRO:HB2	1:E:190:TRP:CE2	2.51	0.46
1:O:12:ARG:HD2	1:O:13:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ARG:HD3	3:B:540:HOH:O	2.15	0.46
1:I:30:ASN:HD22	2:I:301:GSH:CD1	2.29	0.46
1:B:3:ASP:HB3	3:B:475:HOH:O	2.16	0.46
1:C:133:LEU:HD23	1:C:133:LEU:C	2.36	0.46
1:D:177:ASP:HB3	1:D:178:ALA:H	1.62	0.46
1:G:71:ILE:HD12	1:G:71:ILE:C	2.37	0.45
1:O:91:GLY:O	1:O:95[A]:GLN:HG3	2.17	0.45
1:A:58:LYS:NZ	2:A:301:GSH:O31	2.49	0.45
1:G:70:LYS:HG2	2:G:301:GSH:HA31	1.99	0.45
1:I:52:PHE:CE2	1:I:57:GLN:HG3	2.52	0.45
1:O:133:LEU:HD23	1:O:133:LEU:C	2.37	0.45
1:P:33:LYS:HG2	1:P:185:ALA:HA	1.99	0.45
1:F:57:GLN:N	1:F:57:GLN:OE1	2.49	0.45
1:F:52:PHE:HE2	2:F:301:GSH:CA3	2.31	0.44
1:J:111:ARG:HA	1:J:114:GLN:HE21	1.83	0.44
1:J:128:PRO:O	1:J:132:GLN:HG2	2.18	0.44
1:N:133:LEU:HD23	1:N:133:LEU:C	2.38	0.44
1:J:133:LEU:C	1:J:133:LEU:HD23	2.38	0.44
1:M:88:PHE:O	1:M:89:GLU:HB2	2.18	0.44
1:B:81:GLY:O	1:B:83:LYS:HG2	2.17	0.43
1:F:52:PHE:CD2	1:F:57:GLN:NE2	2.86	0.43
1:N:106:PRO:O	1:N:112[A]:ARG:CG	2.66	0.43
1:A:4:LEU:HD21	1:A:77:PRO:HB3	2.01	0.43
1:F:139:PHE:HB3	3:F:434:HOH:O	2.18	0.43
1:I:211:VAL:HB	1:I:212:PRO:HD3	2.00	0.43
1:F:4:LEU:HA	3:F:475:HOH:O	2.18	0.43
1:G:123:MET:HB3	3:H:456:HOH:O	2.18	0.43
1:K:211:VAL:HB	1:K:212:PRO:HD3	1.99	0.43
1:E:134:LEU:HD23	1:E:134:LEU:C	2.38	0.43
1:G:29:PRO:HB2	1:G:189:TRP:CE2	2.54	0.43
1:L:133:LEU:HD23	1:L:133:LEU:O	2.19	0.43
1:I:56:HIS:HA	1:I:59:THR:HG23	2.01	0.42
1:J:25:SER:HA	1:J:71:ILE:HB	2.00	0.42
1:J:108:ASP:OD2	1:J:111:ARG:HG3	2.19	0.42
1:D:72:ILE:HD12	1:D:72:ILE:C	2.39	0.42
1:P:194:ILE:HD12	1:P:200:ARG:NH1	2.34	0.42
1:I:225:GLN:NE2	3:I:440:HOH:O	2.50	0.42
1:J:29:PRO:HB2	1:J:189:TRP:CE2	2.55	0.42
1:L:52:PHE:CE2	1:L:57:GLN:HG3	2.54	0.42
1:P:30:ASN:HD22	2:P:301:GSH:CD1	2.33	0.42
1:A:71:ILE:C	1:A:71:ILE:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:PRO:HB2	1:C:189:TRP:CE2	2.54	0.42
1:I:57:GLN:N	1:I:57:GLN:OE1	2.50	0.42
1:P:12:ARG:HD2	1:P:13:TRP:CH2	2.54	0.42
1:A:133:LEU:HD23	1:A:133:LEU:C	2.40	0.41
1:F:4:LEU:CA	3:F:475:HOH:O	2.67	0.41
1:H:211:VAL:HB	1:H:212:PRO:HD3	2.01	0.41
1:P:112[B]:ARG:HG2	1:P:112[B]:ARG:NH1	2.30	0.41
1:A:57:GLN:OE1	1:A:57:GLN:N	2.50	0.41
1:C:71:ILE:HB	1:C:72:PRO:HA	2.01	0.41
1:M:25:SER:HA	1:M:71:ILE:HB	2.02	0.41
1:A:123:MET:HB3	3:B:422:HOH:O	2.19	0.41
1:C:30:ASN:HD22	2:C:301:GSH:CD1	2.34	0.41
1:F:25:SER:HA	1:F:71:ILE:HB	2.03	0.41
1:I:83:LYS:HA	1:I:83:LYS:CE	2.36	0.41
1:F:225:GLN:HG2	3:F:436:HOH:O	2.21	0.41
1:F:12:ARG:HD2	1:F:13:TRP:CZ3	2.55	0.41
1:J:71:ILE:HD12	1:J:71:ILE:C	2.40	0.41
1:P:128:PRO:O	1:P:132:GLN:HG2	2.20	0.41
1:I:117:GLN:OE1	1:J:87:LEU:HA	2.21	0.41
1:L:52:PHE:HE2	2:L:301:GSH:CA3	2.26	0.41
1:N:211:VAL:HB	1:N:212:PRO:HD3	2.03	0.41
1:K:126:ILE:HD11	1:K:164:LEU:HD21	2.03	0.41
1:G:57:GLN:OE1	1:G:57:GLN:N	2.50	0.40
1:P:133:LEU:O	1:P:133:LEU:HD23	2.21	0.40
1:B:76:ASP:O	1:B:84:PRO:HA	2.22	0.40
1:H:3:ASP:HA	3:H:539:HOH:O	2.20	0.40
1:I:33:LYS:HG2	1:I:185:ALA:HA	2.04	0.40
1:L:29:PRO:HB2	1:L:189:TRP:CE2	2.56	0.40
1:N:194:ILE:HD12	1:N:200:ARG:NH1	2.36	0.40
1:I:71:ILE:HB	1:I:72:PRO:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	230/256 (90%)	222 (96%)	8 (4%)	0	100	100
1	B	244/256 (95%)	237 (97%)	6 (2%)	1 (0%)	34	24
1	C	232/256 (91%)	223 (96%)	9 (4%)	0	100	100
1	D	233/256 (91%)	225 (97%)	8 (3%)	0	100	100
1	E	231/256 (90%)	223 (96%)	8 (4%)	0	100	100
1	F	231/256 (90%)	225 (97%)	6 (3%)	0	100	100
1	G	229/256 (90%)	222 (97%)	7 (3%)	0	100	100
1	H	248/256 (97%)	238 (96%)	10 (4%)	0	100	100
1	I	232/256 (91%)	225 (97%)	7 (3%)	0	100	100
1	J	232/256 (91%)	224 (97%)	7 (3%)	1 (0%)	34	24
1	K	232/256 (91%)	224 (97%)	8 (3%)	0	100	100
1	L	231/256 (90%)	222 (96%)	9 (4%)	0	100	100
1	M	230/256 (90%)	222 (96%)	8 (4%)	0	100	100
1	N	234/256 (91%)	226 (97%)	8 (3%)	0	100	100
1	O	230/256 (90%)	223 (97%)	7 (3%)	0	100	100
1	P	232/256 (91%)	226 (97%)	5 (2%)	1 (0%)	34	24
All	All	3731/4096 (91%)	3607 (97%)	121 (3%)	3 (0%)	51	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	176	ASP
1	P	89	GLU
1	B	176	ASP

### 5.3.2 Protein sidechains ⓘ

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	192/214 (90%)	187 (97%)	5 (3%)	46	39
1	B	205/214 (96%)	201 (98%)	4 (2%)	55	51
1	C	194/214 (91%)	192 (99%)	2 (1%)	76	76
1	D	194/214 (91%)	192 (99%)	2 (1%)	76	76
1	E	192/214 (90%)	189 (98%)	3 (2%)	62	60
1	F	193/214 (90%)	191 (99%)	2 (1%)	76	76
1	G	191/214 (89%)	186 (97%)	5 (3%)	46	39
1	H	209/214 (98%)	207 (99%)	2 (1%)	76	76
1	I	194/214 (91%)	186 (96%)	8 (4%)	30	21
1	J	194/214 (91%)	192 (99%)	2 (1%)	76	76
1	K	194/214 (91%)	193 (100%)	1 (0%)	88	89
1	L	193/214 (90%)	192 (100%)	1 (0%)	88	89
1	M	192/214 (90%)	191 (100%)	1 (0%)	88	89
1	N	196/214 (92%)	195 (100%)	1 (0%)	88	89
1	O	192/214 (90%)	192 (100%)	0	100	100
1	P	194/214 (91%)	192 (99%)	2 (1%)	76	76
All	All	3119/3424 (91%)	3078 (99%)	41 (1%)	69	68

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	SER
1	A	11	LYS
1	A	111	ARG
1	A	164	LEU
1	B	82	ASP
1	B	99	GLU
1	B	164	LEU
1	B	208	LEU
1	C	111	ARG
1	C	164	LEU
1	D	177	ASP
1	D	209	LEU
1	E	17	GLN
1	E	165	LEU
1	E	209	LEU

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Mol	Chain	Res	Type
1	F	83	LYS
1	F	176	ASP
1	G	58	LYS
1	G	82	ASP
1	G	83	LYS
1	G	164	LEU
1	G	208	LEU
1	H	82	ASP
1	H	117	GLN
1	I	3	ASP
1	I	58	LYS
1	I	82	ASP
1	I	83	LYS
1	I	143[A]	GLU
1	I	143[B]	GLU
1	I	164	LEU
1	I	208	LEU
1	J	111	ARG
1	J	176	ASP
1	K	164	LEU
1	L	2	SER
1	M	143	GLU
1	N	164	LEU
1	P	3	ASP
1	P	82	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	B	122	GLN
1	E	17	GLN
1	E	133	GLN
1	F	132	GLN
1	F	151	GLN
1	G	132	GLN
1	I	114	GLN
1	I	151	GLN
1	I	225	GLN
1	J	114	GLN
1	K	210	HIS
1	L	95	GLN

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Mol	Chain	Res	Type
1	N	132	GLN
1	N	192	ASN
1	O	172	GLN
1	P	114	GLN
1	P	151	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 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	L	301	-	10,13,19	1.56	1 (10%)	13,16,24	3.22	5 (38%)
2	GSH	N	301	-	12,19,19	0.72	1 (8%)	15,24,24	1.15	2 (13%)
2	GSH	H	301	-	12,19,19	0.69	0	15,24,24	1.57	2 (13%)
2	GSH	D	301	-	12,19,19	0.55	0	15,24,24	1.36	3 (20%)
2	GSH	F	301	-	12,19,19	0.62	0	15,24,24	1.47	3 (20%)
2	GSH	M	301	-	12,19,19	0.60	0	15,24,24	1.44	5 (33%)
2	GSH	O	301	-	12,19,19	0.45	0	15,24,24	1.60	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GSH	I	301	-	12,19,19	0.91	1 (8%)	15,24,24	2.50	6 (40%)
2	GSH	K	301	-	12,19,19	0.54	0	15,24,24	1.34	3 (20%)
2	GSH	E	301	-	12,19,19	0.68	0	15,24,24	1.56	2 (13%)
2	GSH	J	301	-	12,19,19	0.69	0	15,24,24	1.64	3 (20%)
2	GSH	G	301	-	12,19,19	1.16	1 (8%)	15,24,24	2.28	6 (40%)
2	GSH	A	301	-	12,19,19	0.99	1 (8%)	15,24,24	2.16	5 (33%)
2	GSH	C	301	-	12,19,19	0.99	1 (8%)	15,24,24	2.04	5 (33%)
2	GSH	P	301	-	12,19,19	0.78	0	15,24,24	2.70	7 (46%)
2	GSH	B	301	-	12,19,19	0.70	0	15,24,24	2.10	5 (33%)

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	L	301	-	-	2/13/15/24	-
2	GSH	N	301	-	-	2/18/24/24	-
2	GSH	H	301	-	-	0/18/24/24	-
2	GSH	D	301	-	-	1/18/24/24	-
2	GSH	F	301	-	-	0/18/24/24	-
2	GSH	M	301	-	-	1/18/24/24	-
2	GSH	O	301	-	-	0/18/24/24	-
2	GSH	I	301	-	-	3/18/24/24	-
2	GSH	K	301	-	-	0/18/24/24	-
2	GSH	E	301	-	-	1/18/24/24	-
2	GSH	J	301	-	-	0/18/24/24	-
2	GSH	G	301	-	-	0/18/24/24	-
2	GSH	A	301	-	-	0/18/24/24	-
2	GSH	C	301	-	-	0/18/24/24	-
2	GSH	P	301	-	-	3/18/24/24	-
2	GSH	B	301	-	-	4/18/24/24	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	GSH	O2-C2	-3.48	1.16	1.23
2	G	301	GSH	CB2-CA2	3.09	1.56	1.53
2	I	301	GSH	CB2-CA2	2.40	1.55	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	GSH	CB2-CA2	2.35	1.55	1.53
2	C	301	GSH	CB2-CA2	2.12	1.55	1.53
2	N	301	GSH	CB2-CA2	2.01	1.55	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	GSH	CA2-CB2-SG2	-7.02	106.31	114.19
2	L	301	GSH	CB2-CA2-C2	5.50	121.10	109.76
2	P	301	GSH	CA3-N3-C2	5.30	129.97	122.34
2	I	301	GSH	CA3-N3-C2	5.22	129.84	122.34
2	P	301	GSH	CA2-C2-N3	4.85	126.32	116.54
2	P	301	GSH	O2-C2-N3	-4.66	112.99	122.99
2	L	301	GSH	CB2-CA2-N2	-4.64	104.66	111.28
2	L	301	GSH	OE1-CD1-N2	-4.40	113.86	121.95
2	G	301	GSH	CB2-CA2-C2	4.39	118.82	109.76
2	B	301	GSH	CG1-CD1-N2	4.29	123.28	115.83
2	G	301	GSH	CA2-C2-N3	4.25	125.12	116.54
2	I	301	GSH	CA2-C2-N3	4.24	125.09	116.54
2	H	301	GSH	C3-CA3-N3	4.24	118.60	110.43
2	A	301	GSH	CA2-C2-N3	4.08	124.78	116.54
2	A	301	GSH	CB2-CA2-C2	4.07	118.16	109.76
2	I	301	GSH	CB2-CA2-C2	4.06	118.15	109.76
2	C	301	GSH	CA2-C2-N3	3.88	124.36	116.54
2	E	301	GSH	C3-CA3-N3	3.84	117.83	110.43
2	C	301	GSH	CB2-CA2-C2	3.76	117.53	109.76
2	B	301	GSH	OE1-CD1-CG1	-3.71	115.23	122.02
2	B	301	GSH	C3-CA3-N3	3.70	117.56	110.43
2	C	301	GSH	C3-CA3-N3	3.68	117.52	110.43
2	J	301	GSH	C3-CA3-N3	3.66	117.49	110.43
2	I	301	GSH	O2-C2-N3	-3.65	115.16	122.99
2	A	301	GSH	CB2-CA2-N2	-3.60	106.15	111.28
2	G	301	GSH	C3-CA3-N3	3.52	117.22	110.43
2	P	301	GSH	CB2-CA2-C2	3.43	116.85	109.76
2	O	301	GSH	C3-CA3-N3	3.43	117.03	110.43
2	H	301	GSH	CB2-CA2-C2	3.40	116.77	109.76
2	F	301	GSH	C3-CA3-N3	3.36	116.91	110.43
2	F	301	GSH	CA2-CB2-SG2	-3.09	110.72	114.19
2	G	301	GSH	CB2-CA2-N2	-3.07	106.91	111.28
2	E	301	GSH	CB2-CA2-C2	3.01	115.97	109.76
2	L	301	GSH	CG1-CD1-N2	2.98	121.15	116.10
2	K	301	GSH	C3-CA3-N3	2.80	115.83	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	301	GSH	CA2-CB2-SG2	-2.77	111.08	114.19
2	P	301	GSH	CA2-CB2-SG2	2.69	117.22	114.19
2	J	301	GSH	CA2-C2-N3	2.68	121.94	116.54
2	I	301	GSH	C2-CA2-N2	-2.66	103.92	111.16
2	D	301	GSH	CB2-CA2-C2	2.64	115.21	109.76
2	J	301	GSH	CA3-N3-C2	-2.60	118.59	122.34
2	A	301	GSH	C3-CA3-N3	2.57	115.39	110.43
2	N	301	GSH	CB2-CA2-N2	2.57	114.95	111.28
2	D	301	GSH	C3-CA3-N3	2.56	115.37	110.43
2	C	301	GSH	O2-C2-N3	-2.53	117.55	122.99
2	C	301	GSH	CB2-CA2-N2	-2.50	107.72	111.28
2	M	301	GSH	CA2-CB2-SG2	-2.49	111.39	114.19
2	P	301	GSH	CB2-CA2-N2	-2.48	107.75	111.28
2	K	301	GSH	CA2-C2-N3	2.45	121.48	116.54
2	P	301	GSH	C3-CA3-N3	-2.41	105.79	110.43
2	A	301	GSH	CA2-CB2-SG2	-2.34	111.56	114.19
2	B	301	GSH	CB2-CA2-N2	2.28	114.53	111.28
2	B	301	GSH	CB2-CA2-C2	2.26	114.42	109.76
2	M	301	GSH	CB2-CA2-C2	2.25	114.40	109.76
2	G	301	GSH	O2-C2-N3	-2.24	118.19	122.99
2	N	301	GSH	C3-CA3-N3	2.22	114.71	110.43
2	O	301	GSH	CB2-CA2-C2	2.19	114.28	109.76
2	D	301	GSH	CA2-C2-N3	2.17	120.91	116.54
2	M	301	GSH	CA2-C2-N3	2.15	120.89	116.54
2	M	301	GSH	C3-CA3-N3	2.15	114.57	110.43
2	G	301	GSH	C2-CA2-N2	-2.14	105.33	111.16
2	I	301	GSH	C3-CA3-N3	-2.14	106.30	110.43
2	F	301	GSH	CA3-N3-C2	-2.13	119.27	122.34
2	O	301	GSH	CA3-N3-C2	-2.10	119.31	122.34
2	M	301	GSH	CB2-CA2-N2	-2.08	108.31	111.28
2	K	301	GSH	CA3-N3-C2	-2.00	119.46	122.34

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	301	GSH	C2-CA2-CB2-SG2
2	B	301	GSH	N1-CA1-CB1-CG1
2	B	301	GSH	C1-CA1-CB1-CG1
2	L	301	GSH	CG1-CD1-N2-CA2
2	I	301	GSH	O2-C2-N3-CA3
2	P	301	GSH	O2-C2-N3-CA3

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Mol	Chain	Res	Type	Atoms
2	I	301	GSH	CA2-C2-N3-CA3
2	P	301	GSH	CA2-C2-N3-CA3
2	L	301	GSH	OE1-CD1-N2-CA2
2	B	301	GSH	OE1-CD1-CG1-CB1
2	B	301	GSH	N2-CD1-CG1-CB1
2	E	301	GSH	C3-CA3-N3-C2
2	D	301	GSH	C3-CA3-N3-C2
2	M	301	GSH	C3-CA3-N3-C2
2	I	301	GSH	C3-CA3-N3-C2
2	P	301	GSH	C3-CA3-N3-C2
2	N	301	GSH	C3-CA3-N3-C2

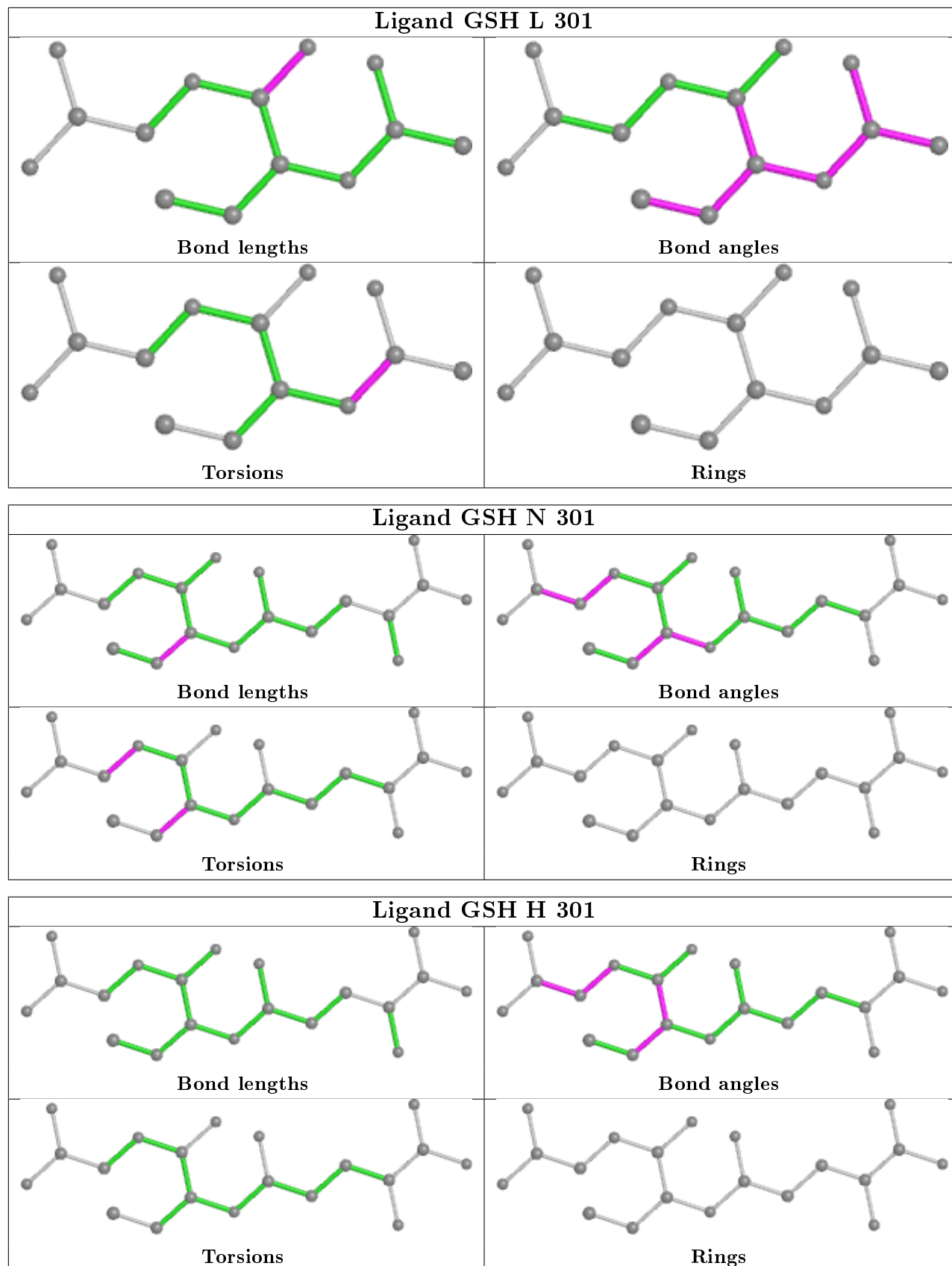
There are no ring outliers.

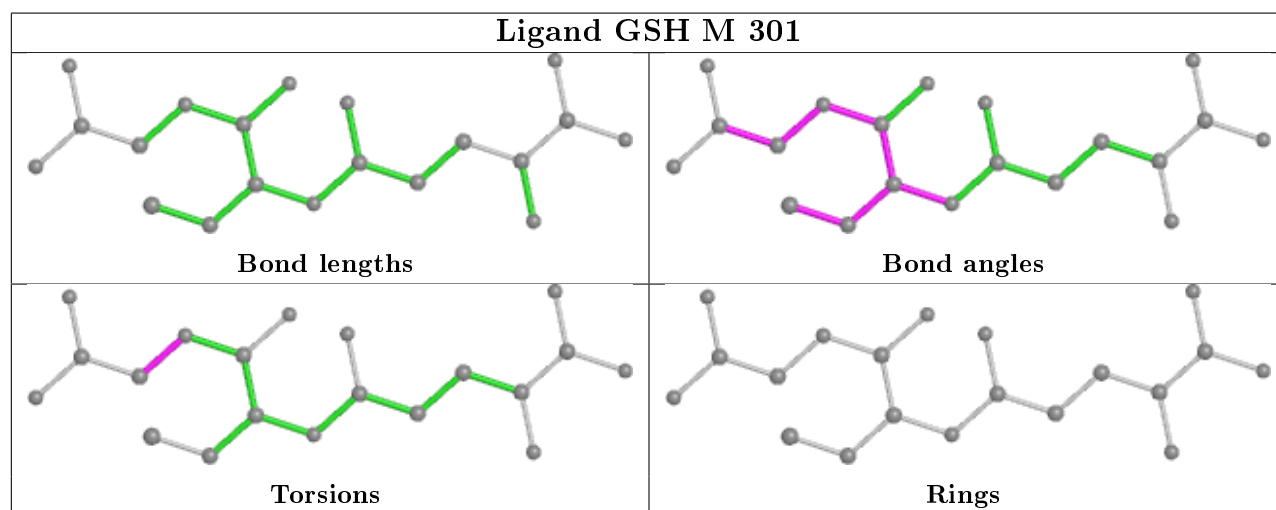
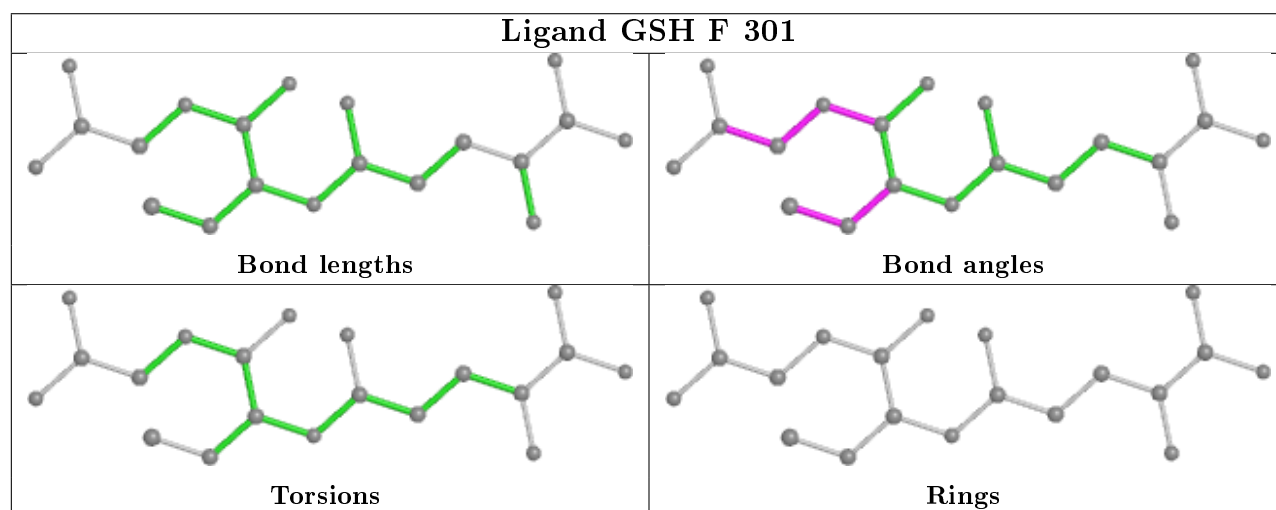
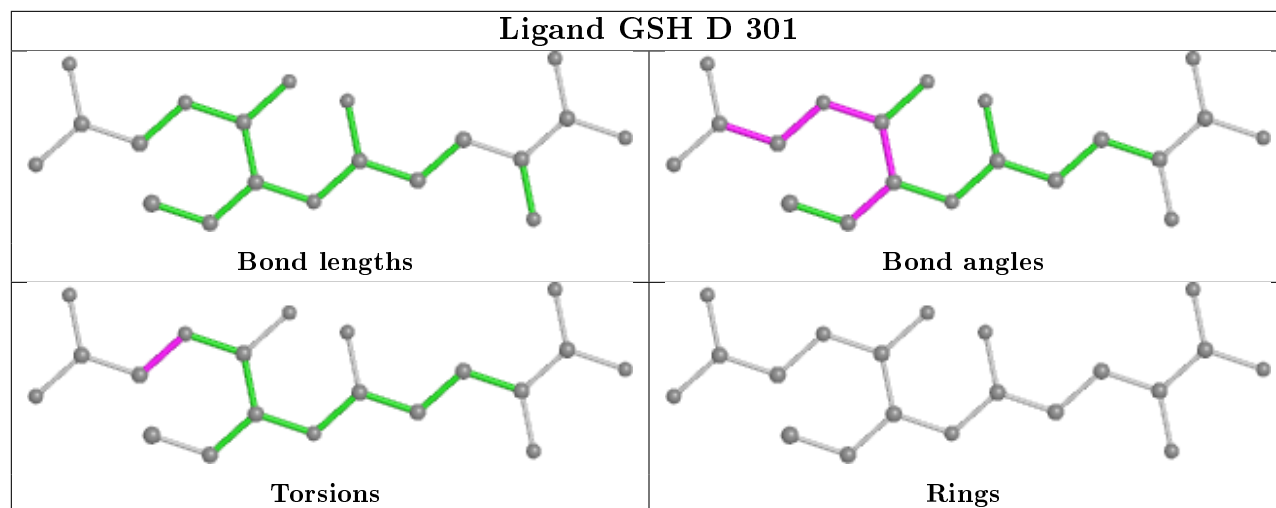
14 monomers are involved in 37 short contacts:

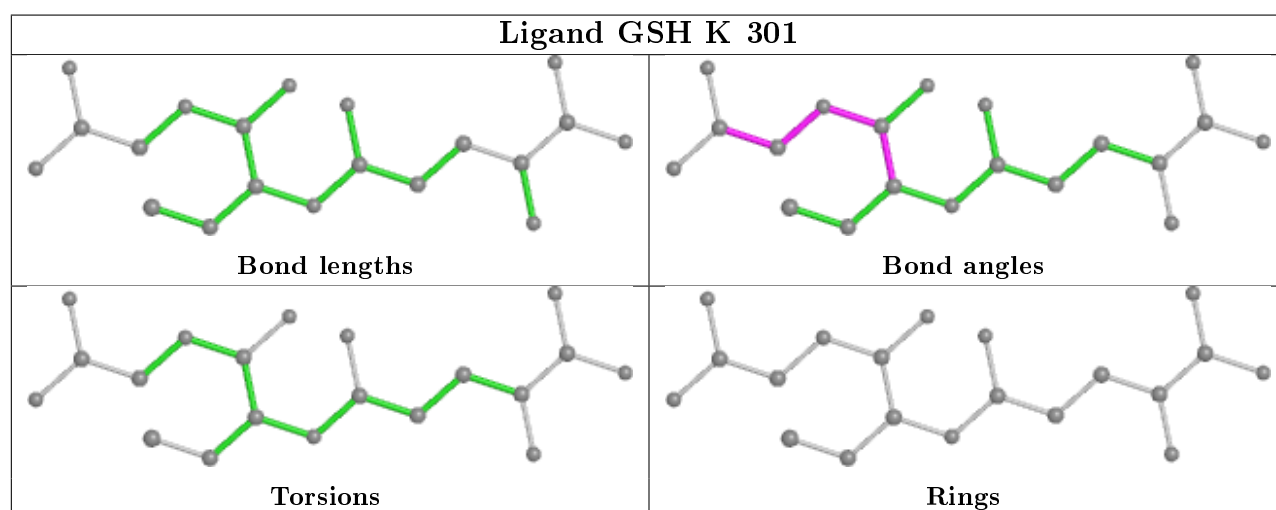
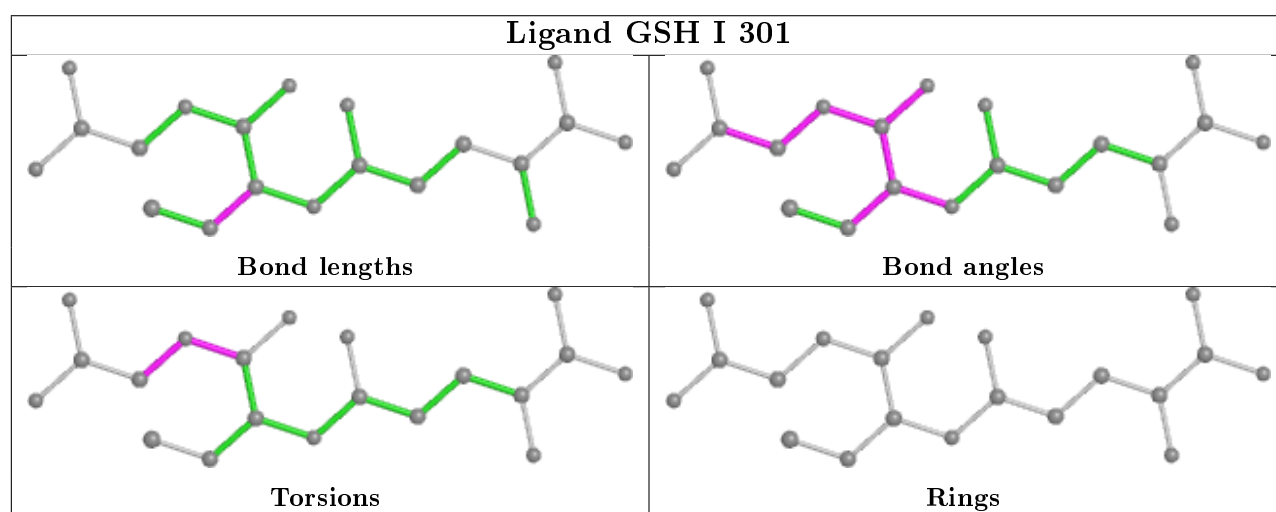
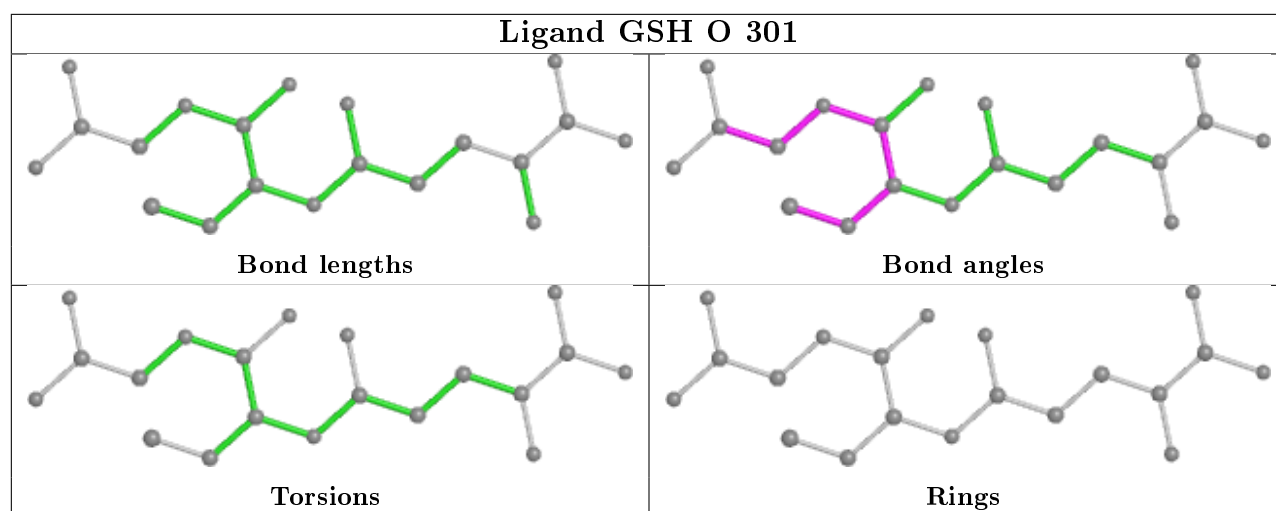
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	301	GSH	4	0
2	N	301	GSH	3	0
2	H	301	GSH	3	0
2	D	301	GSH	1	0
2	F	301	GSH	4	0
2	O	301	GSH	4	0
2	I	301	GSH	1	0
2	E	301	GSH	3	0
2	J	301	GSH	4	0
2	G	301	GSH	3	0
2	A	301	GSH	2	0
2	C	301	GSH	2	0
2	P	301	GSH	1	0
2	B	301	GSH	2	0

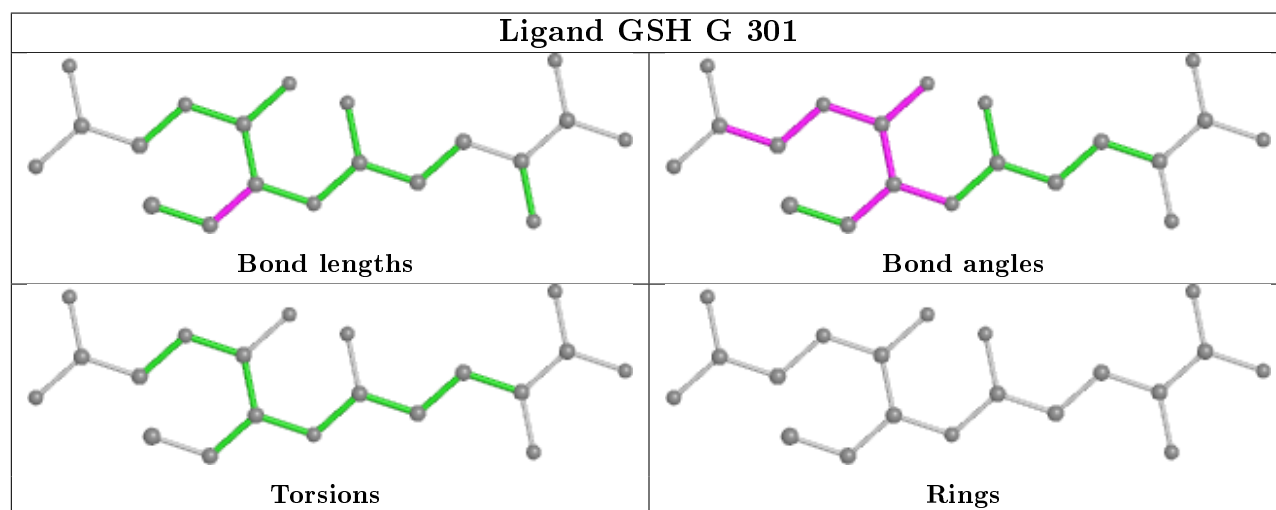
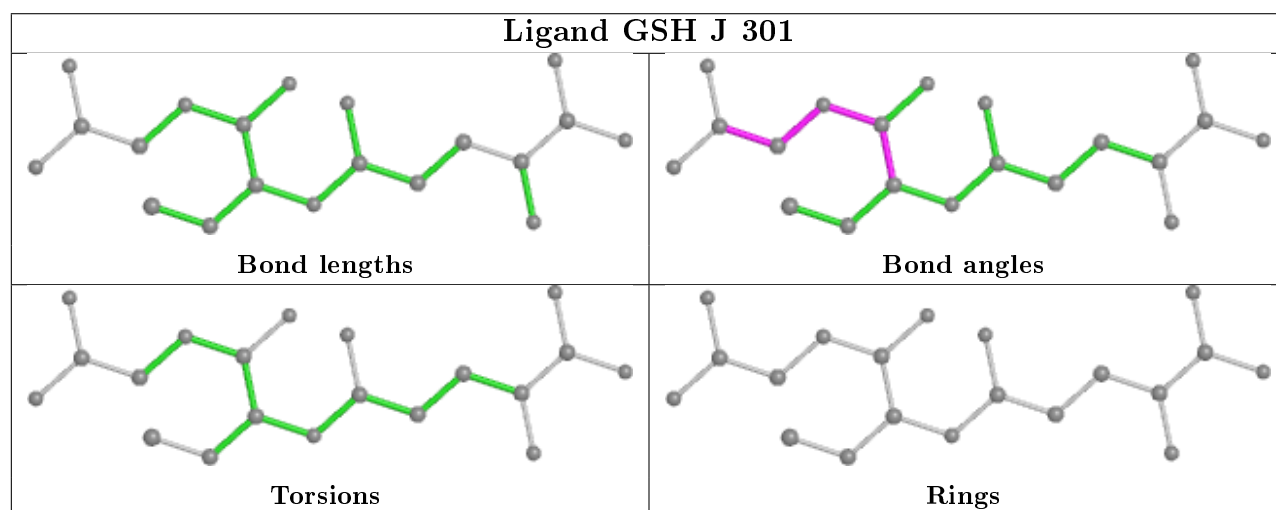
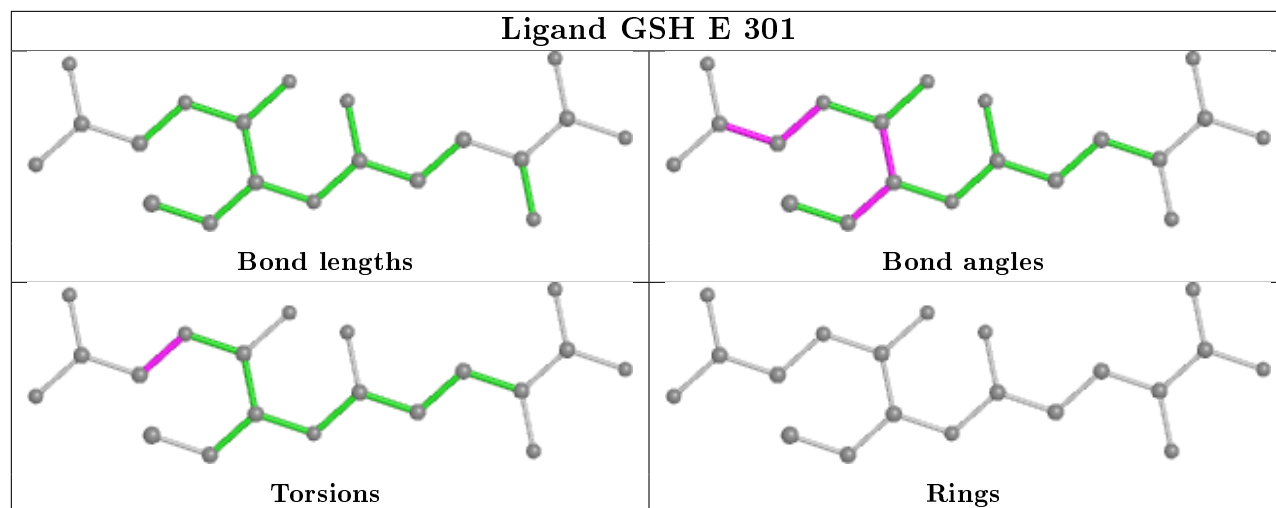
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

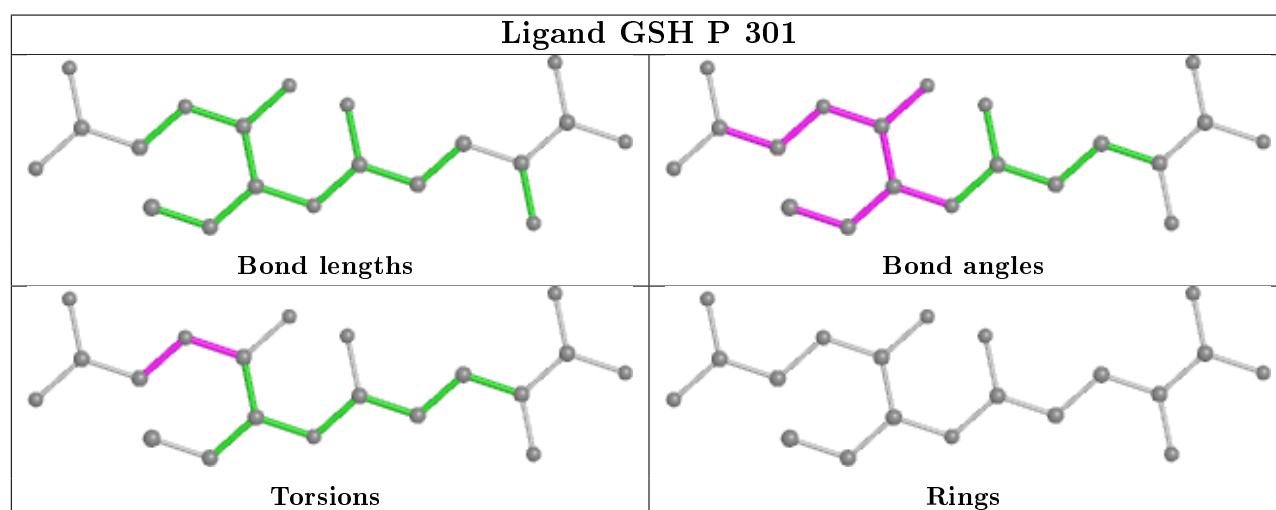
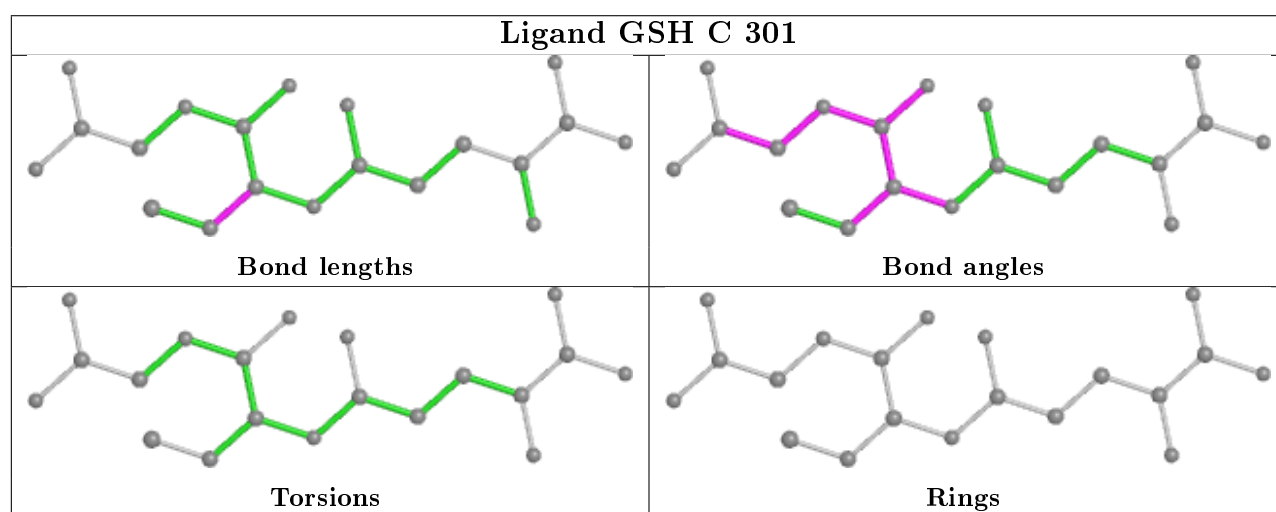
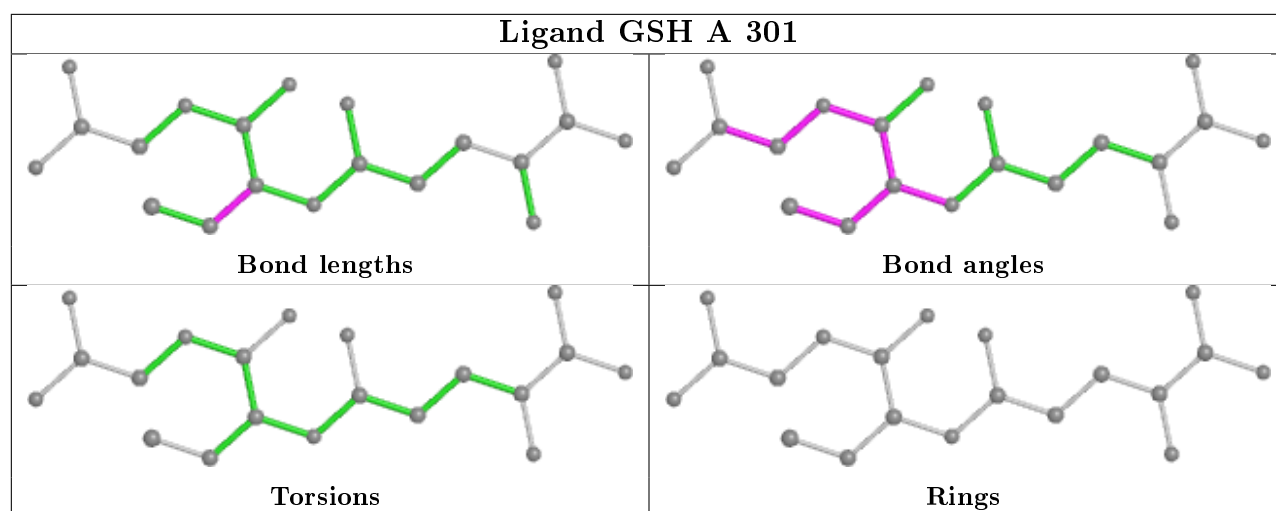
equivalents in the CSD to analyse the geometry.

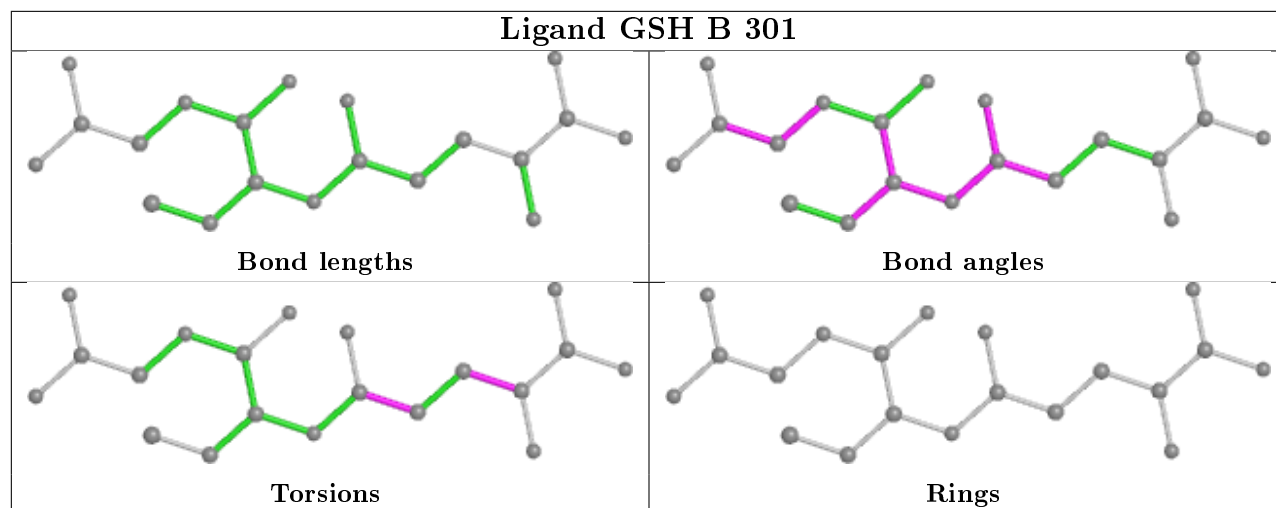












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	232/256 (90%)	-0.44	0 100 100	20, 29, 49, 90	0
1	B	244/256 (95%)	-0.40	1 (0%) 92 93	18, 28, 58, 81	0
1	C	233/256 (91%)	-0.44	1 (0%) 92 93	18, 27, 52, 96	0
1	D	232/256 (90%)	-0.51	0 100 100	19, 28, 49, 81	0
1	E	232/256 (90%)	-0.48	0 100 100	19, 28, 49, 69	0
1	F	231/256 (90%)	-0.49	0 100 100	20, 29, 51, 77	0
1	G	231/256 (90%)	-0.49	0 100 100	20, 29, 51, 69	0
1	H	246/256 (96%)	-0.41	0 100 100	19, 28, 58, 82	0
1	I	232/256 (90%)	-0.43	1 (0%) 92 93	19, 28, 52, 91	0
1	J	231/256 (90%)	-0.46	0 100 100	19, 28, 54, 79	0
1	K	231/256 (90%)	-0.47	0 100 100	21, 30, 53, 73	0
1	L	233/256 (91%)	-0.46	0 100 100	21, 29, 50, 79	0
1	M	231/256 (90%)	-0.48	0 100 100	19, 27, 48, 69	0
1	N	232/256 (90%)	-0.47	0 100 100	17, 26, 51, 86	0
1	O	231/256 (90%)	-0.45	0 100 100	20, 29, 53, 80	0
1	P	232/256 (90%)	-0.44	1 (0%) 92 93	20, 29, 53, 86	0
All	All	3734/4096 (91%)	-0.46	4 (0%) 95 95	17, 28, 53, 96	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	3	ASP	3.6
1	B	-8	GLY	2.8
1	P	3	ASP	2.7
1	C	2	SER	2.5

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

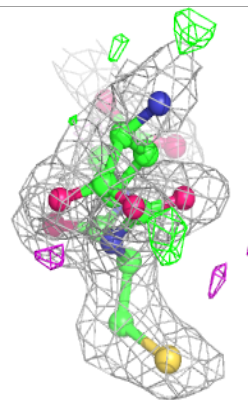
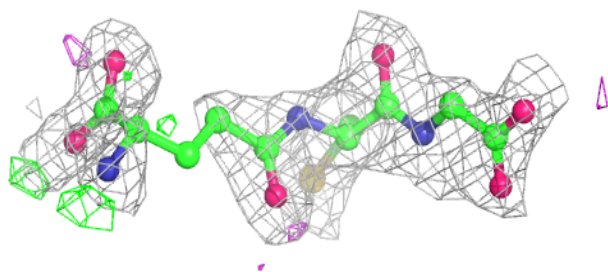
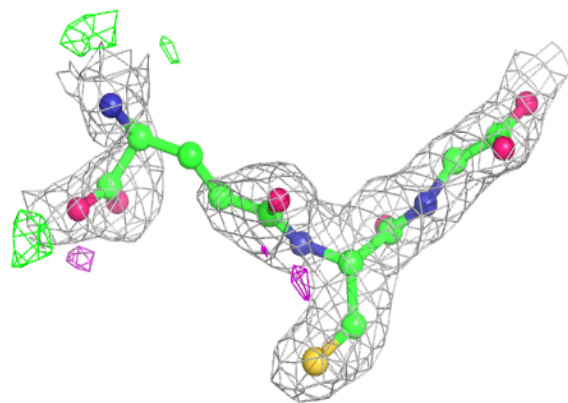
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GSH	O	301	20/20	0.89	0.15	32,53,104,116	0
2	GSH	G	301	20/20	0.89	0.17	23,50,109,117	0
2	GSH	P	301	20/20	0.89	0.20	20,58,91,98	0
2	GSH	F	301	20/20	0.90	0.15	28,47,68,79	0
2	GSH	N	301	20/20	0.90	0.22	24,57,105,107	0
2	GSH	I	301	20/20	0.91	0.23	21,58,103,108	0
2	GSH	A	301	20/20	0.91	0.14	22,46,87,125	0
2	GSH	E	301	20/20	0.91	0.19	19,51,94,98	0
2	GSH	C	301	20/20	0.92	0.16	21,52,101,118	0
2	GSH	J	301	20/20	0.92	0.15	28,52,76,105	0
2	GSH	H	301	20/20	0.93	0.17	23,49,87,100	0
2	GSH	M	301	20/20	0.93	0.15	28,46,70,87	0
2	GSH	K	301	20/20	0.93	0.14	23,46,75,109	0
2	GSH	D	301	20/20	0.94	0.12	29,45,80,96	0
2	GSH	L	301	14/20	0.94	0.20	17,56,102,123	0
2	GSH	B	301	20/20	0.94	0.14	18,48,85,91	0

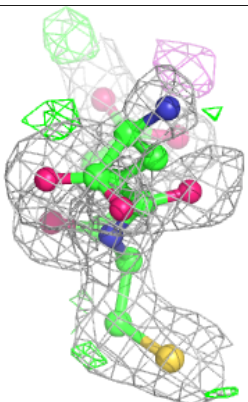
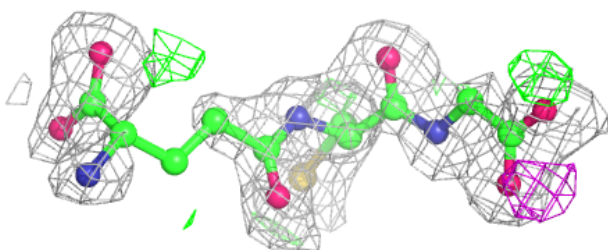
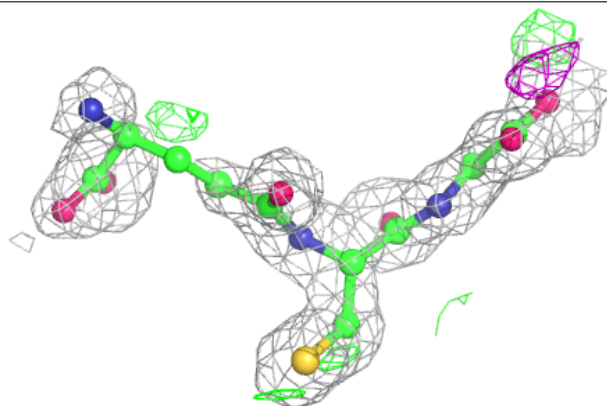
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GSH O 301:**

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

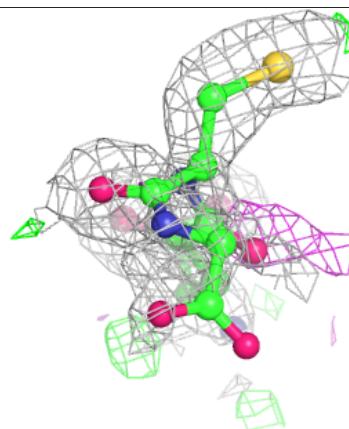
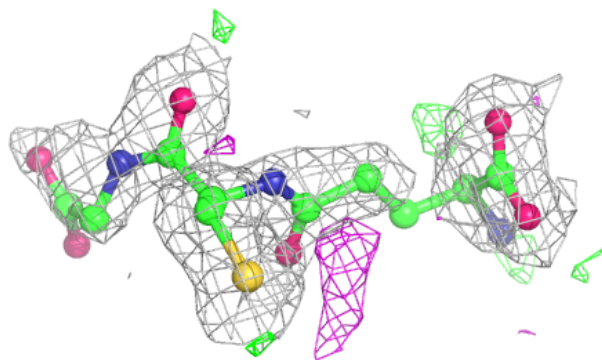
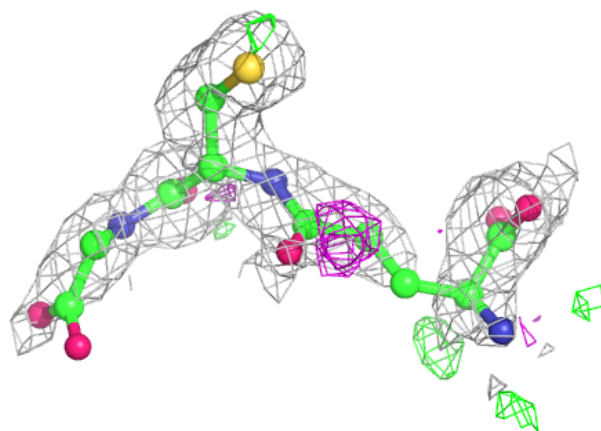
**Electron density around GSH G 301:**

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

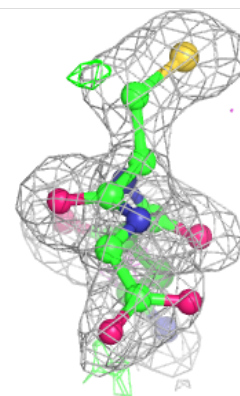
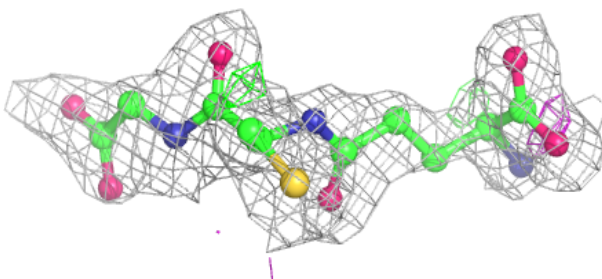
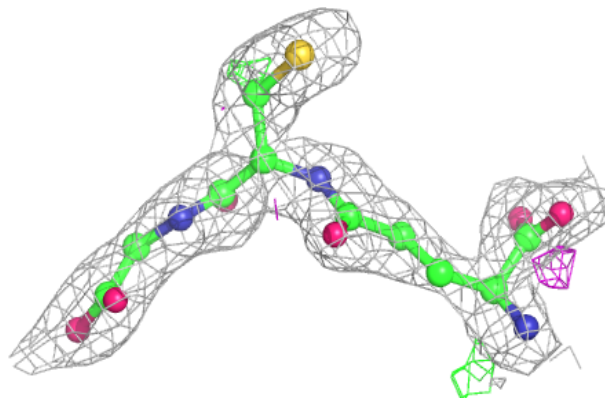


**Electron density around GSH P 301:**

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

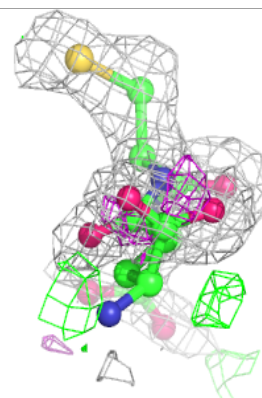
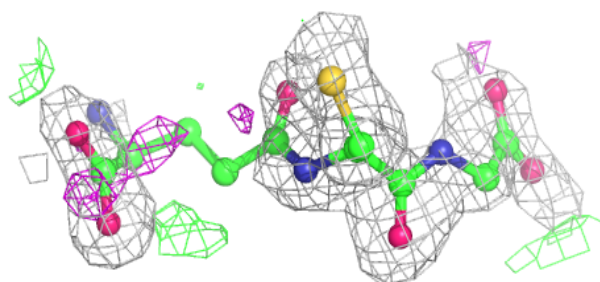
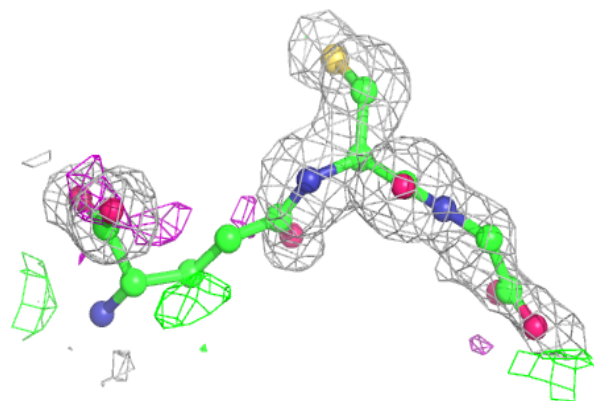
**Electron density around GSH F 301:**

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

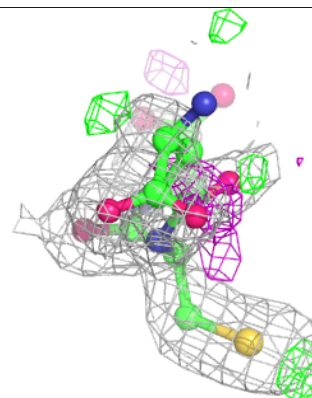
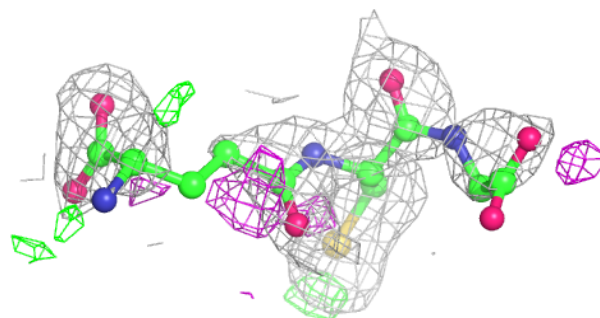
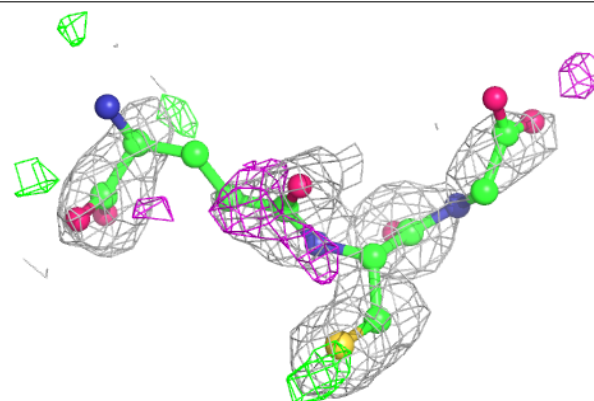


**Electron density around GSH N 301:**

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

**Electron density around GSH I 301:**

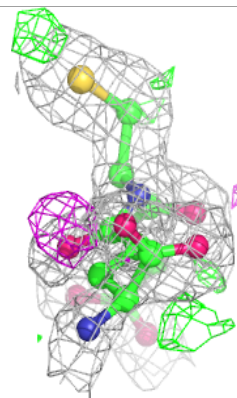
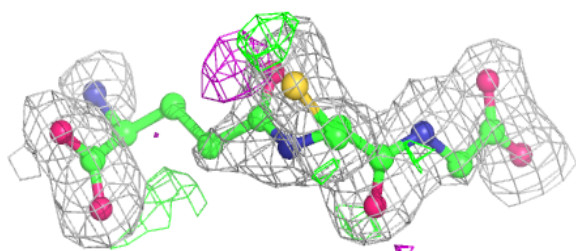
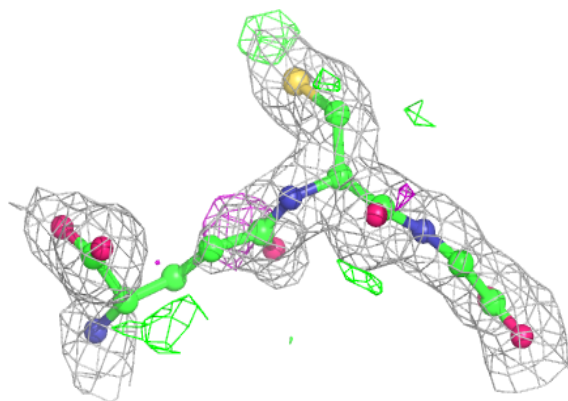
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



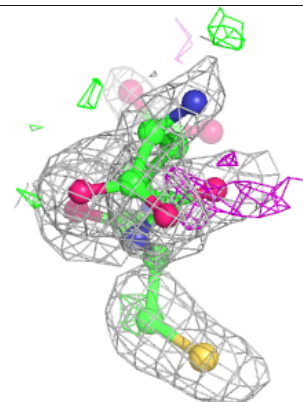
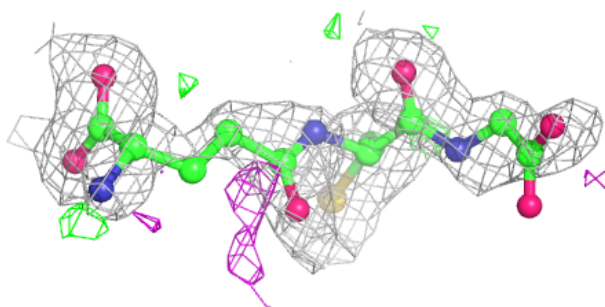
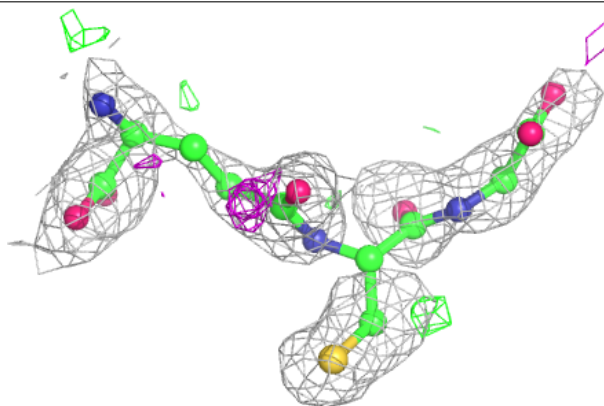


**Electron density around GSH A 301:**

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

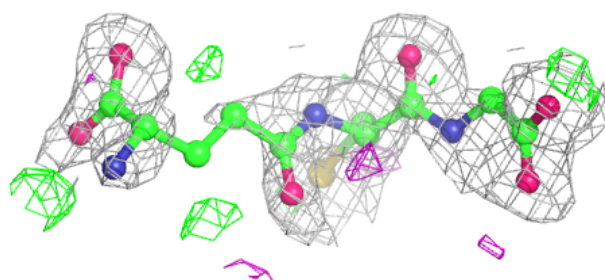
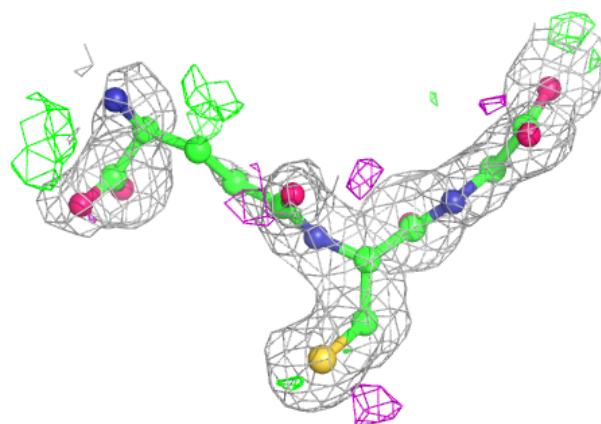
**Electron density around GSH E 301:**

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

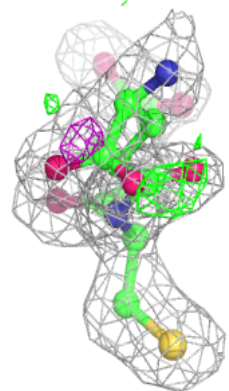
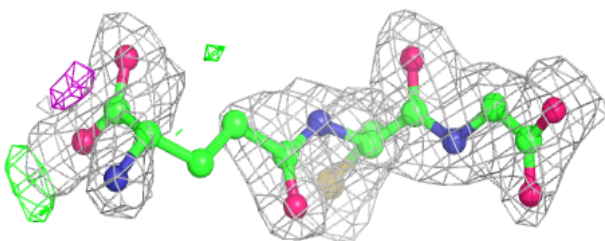
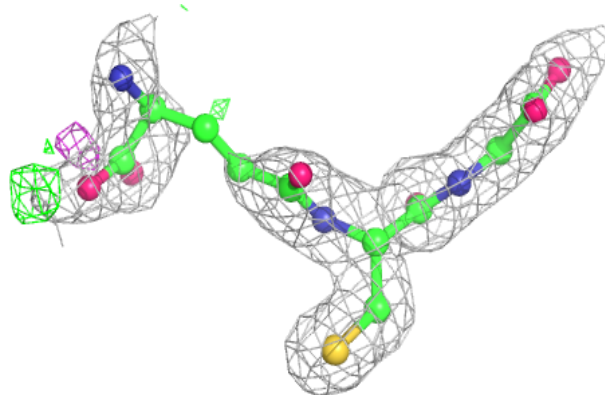


**Electron density around GSH C 301:**

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

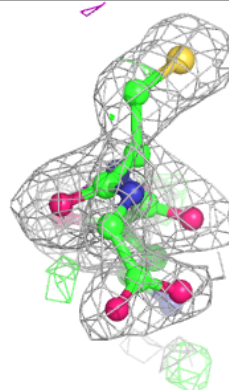
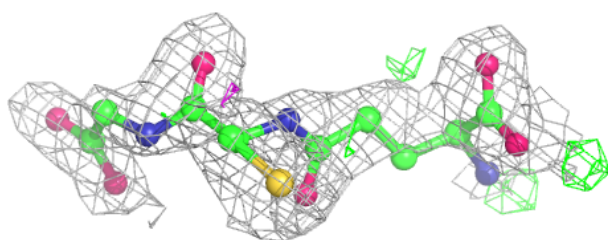
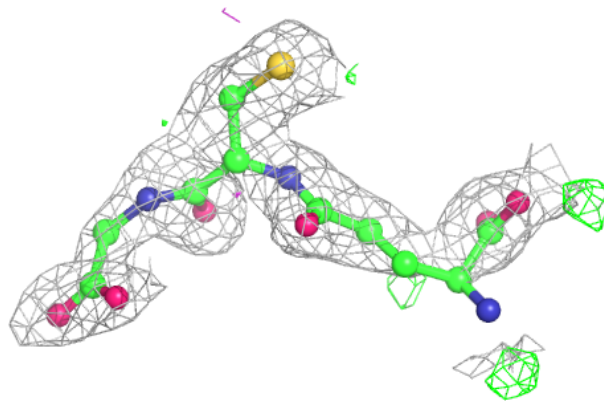
**Electron density around GSH J 301:**

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

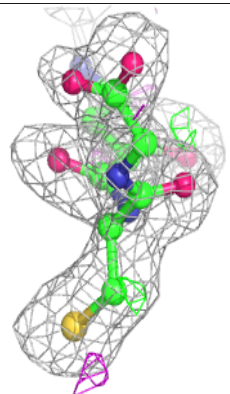
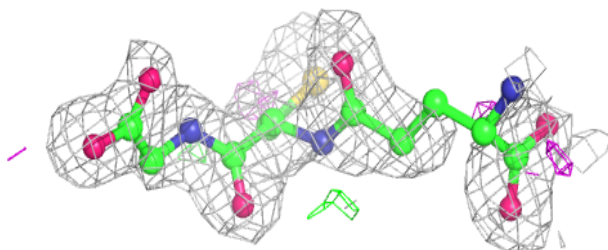
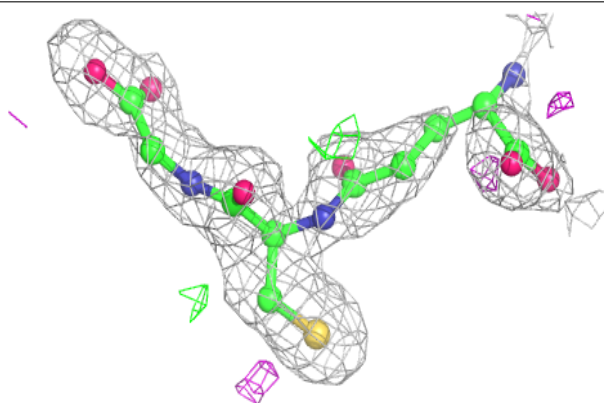


**Electron density around GSH H 301:**

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

**Electron density around GSH M 301:**

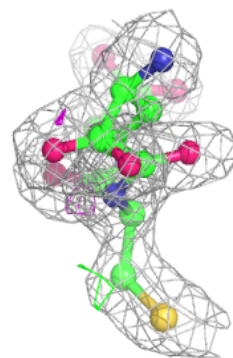
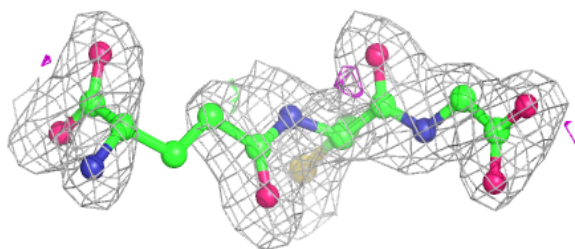
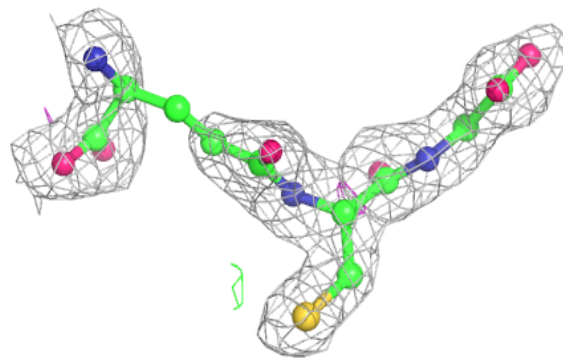
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



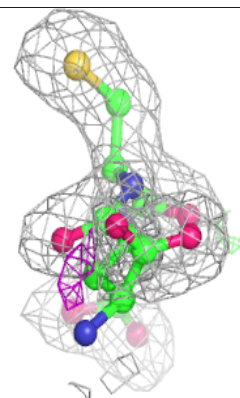
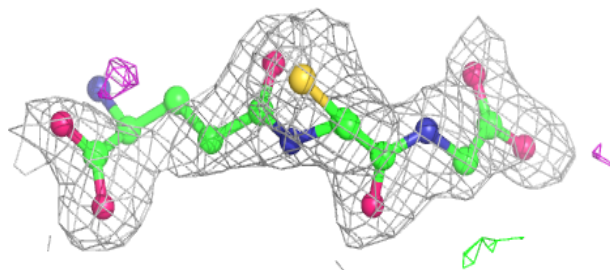
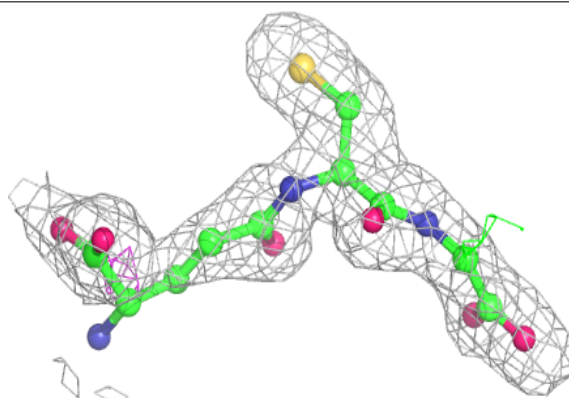


**Electron density around GSH K 301:**

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

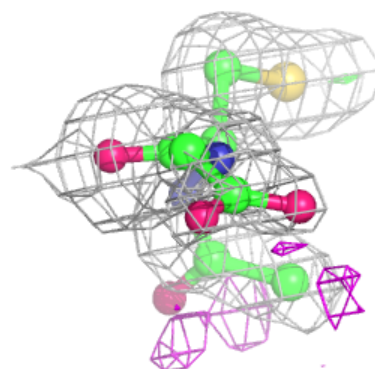
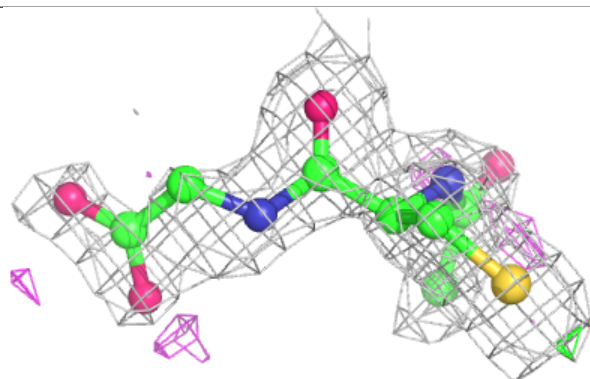
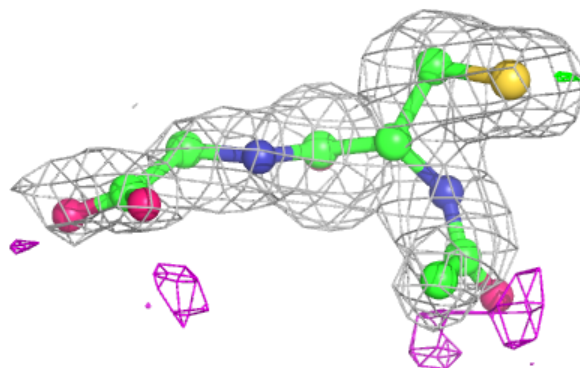
**Electron density around GSH D 301:**

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

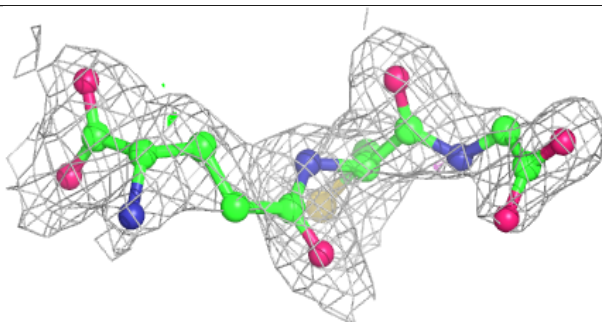
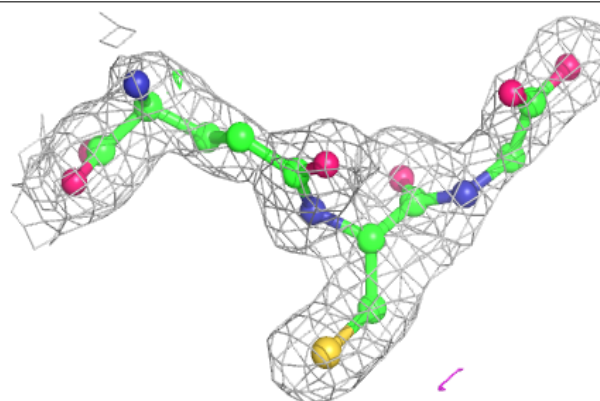


**Electron density around GSH L 301:**

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

**Electron density around GSH B 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.