



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 08:08 pm BST

PDB ID : 5ECN  
Title : Crystal Structure of FIN219-FIP1 complex with JA, Leu and ATP  
Authors : Chen, C.Y.; Cheng, Y.S.  
Deposited on : 2015-10-20  
Resolution : 1.72 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The 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

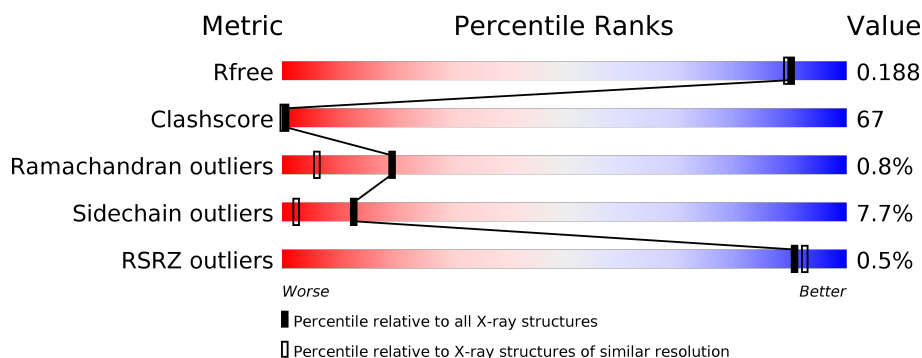
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	575	<div> <div></div> <div>29% 64% 6% .</div> </div>
1	D	575	<div> <div></div> <div>27% 65% 7% .</div> </div>
2	B	223	<div> <div></div> <div>26% 61% 10% .</div> </div>
2	C	223	<div> <div></div> <div>34% 58% . .</div> </div>
2	E	223	<div> <div></div> <div>24% 64% 8% .</div> </div>
2	F	223	<div> <div></div> <div>38% 53% 5% .</div> </div>

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
4	LEU	A	602	-	-	X	-
4	LEU	D	602	-	-	X	-
5	ATP	A	603	-	-	X	-
5	ATP	D	603	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18400 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 Jasmonic acid-amido synthetase JAR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4479	2859	748	850	22			
1	D	569	Total	C	N	O	S	0	0	0
			4479	2859	748	850	22			

- Molecule 2 is a protein called Glutathione S-transferase U20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			
2	C	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			
2	E	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			
2	F	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			

There are 24 discrepancies between the modelled and reference sequences:

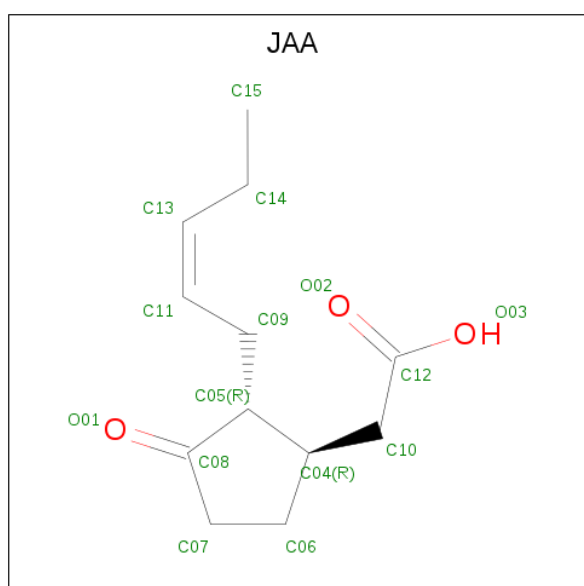
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9
C	-4	HIS	-	expression tag	UNP Q8L7C9
C	-3	HIS	-	expression tag	UNP Q8L7C9
C	-2	HIS	-	expression tag	UNP Q8L7C9
C	-1	HIS	-	expression tag	UNP Q8L7C9
C	0	HIS	-	expression tag	UNP Q8L7C9

*Continued on next page...*

Continued from previous page...

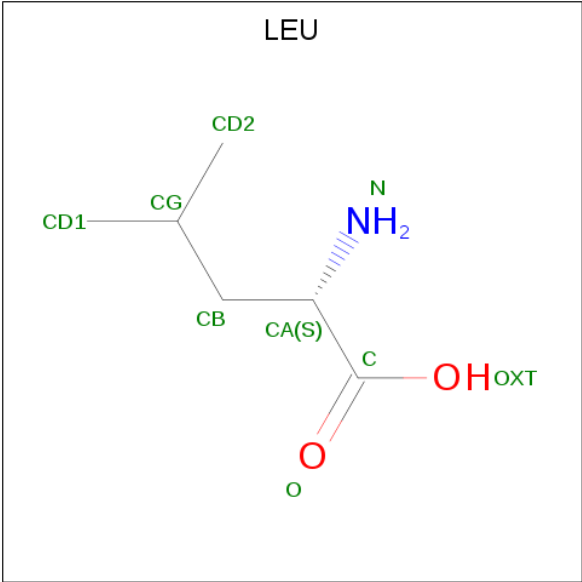
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9
F	-4	HIS	-	expression tag	UNP Q8L7C9
F	-3	HIS	-	expression tag	UNP Q8L7C9
F	-2	HIS	-	expression tag	UNP Q8L7C9
F	-1	HIS	-	expression tag	UNP Q8L7C9
F	0	HIS	-	expression tag	UNP Q8L7C9

- Molecule 3 is {(1R,2R)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetic acid (three-letter code: JAA) (formula: C<sub>12</sub>H<sub>18</sub>O<sub>3</sub>).



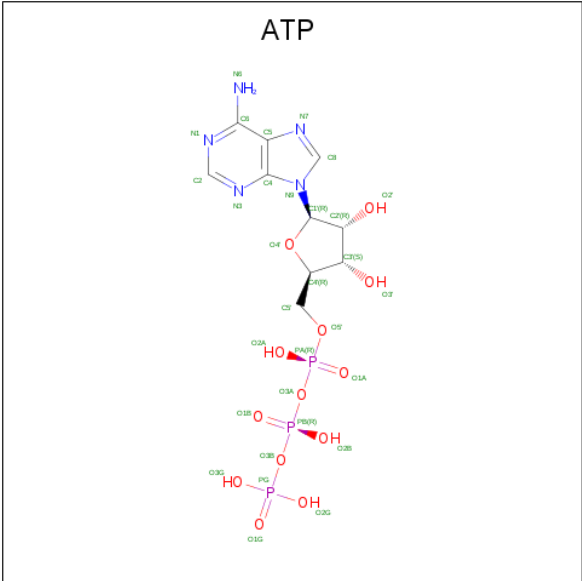
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 4 is LEUCINE (three-letter code: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	6	1	2		
4	D	1	Total	C	N	O	0	0
			9	6	1	2		

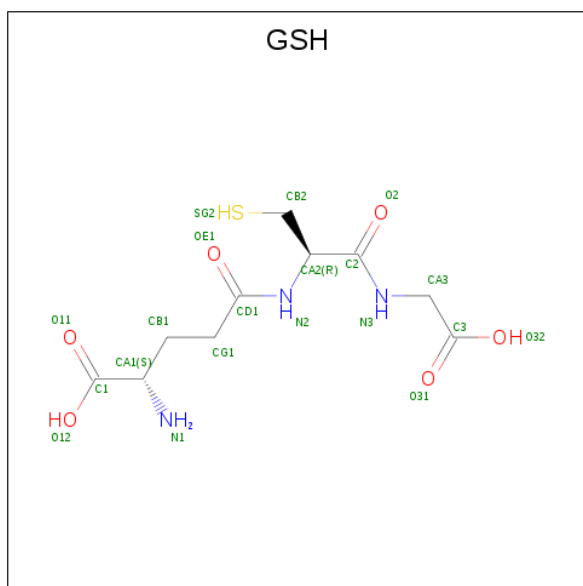
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is GLUTATHIONE (three-letter code: GSH) (formula:  $C_{10}H_{17}N_3O_6S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
6	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
6	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
6	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	545	Total	O	0	0
			545	545		
7	B	306	Total	O	0	0
			306	306		
7	C	270	Total	O	0	0
			270	270		
7	D	528	Total	O	0	0
			528	528		

*Continued on next page...*

*Continued from previous page...*

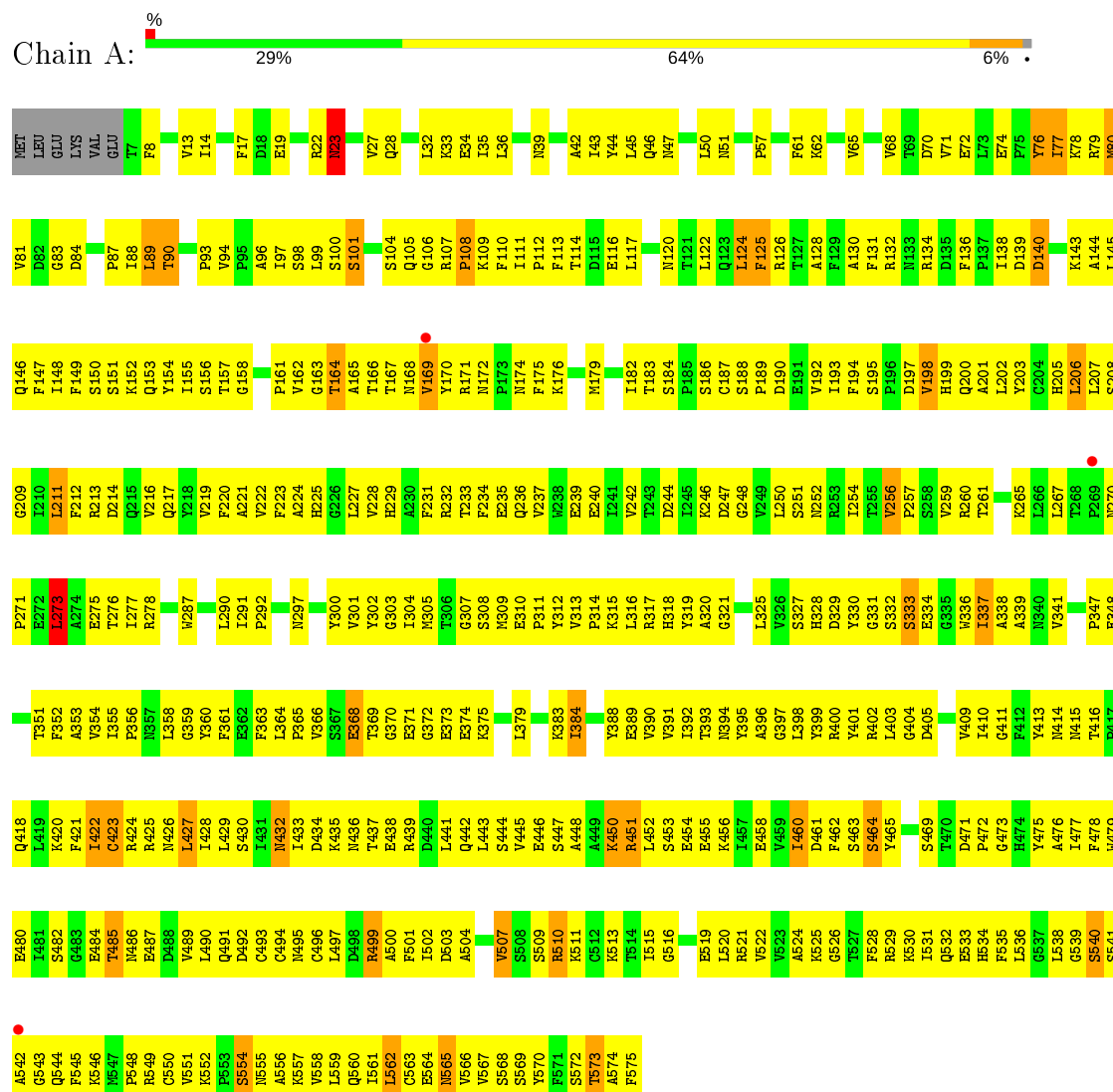
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	320	Total 320	O 320	0	0
7	F	291	Total 291	O 291	0	0



### 3 Residue-property plots

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.

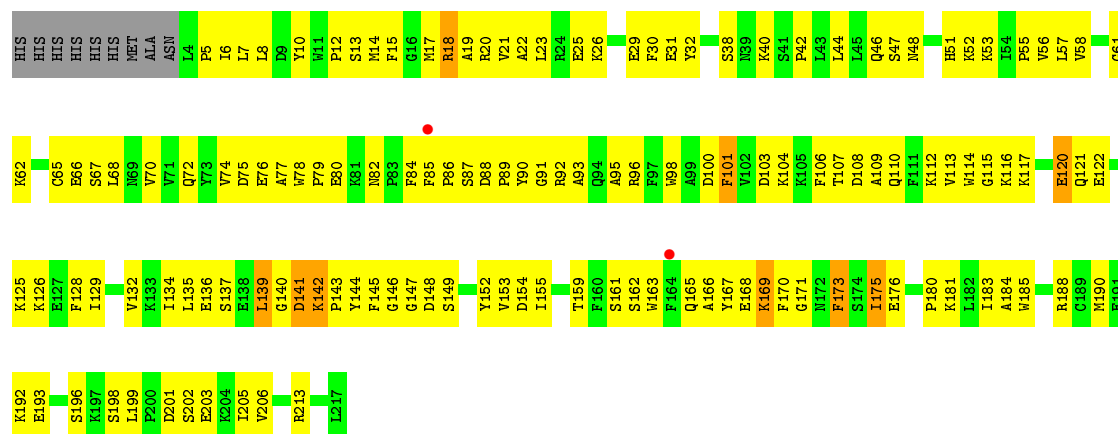
#### • Molecule 1: Jasmonic acid-amido synthetase JAR1



#### • Molecule 1: Jasmonic acid-amido synthetase JAR1

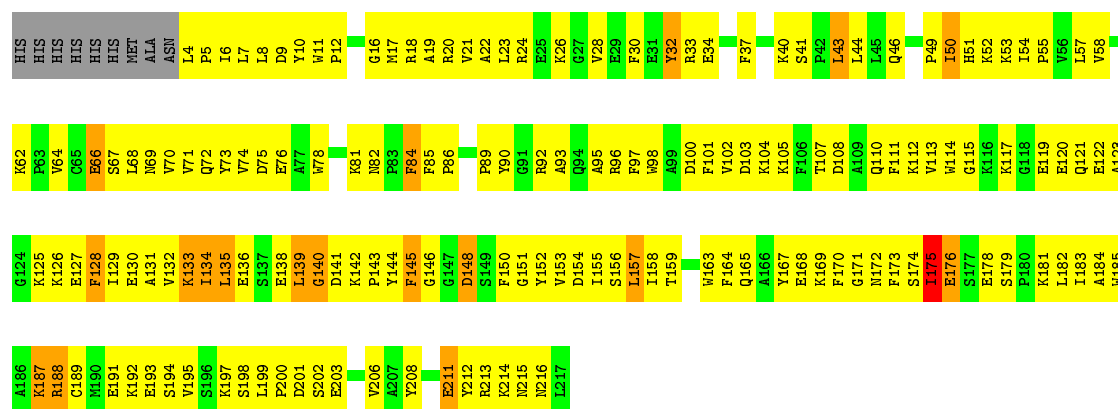






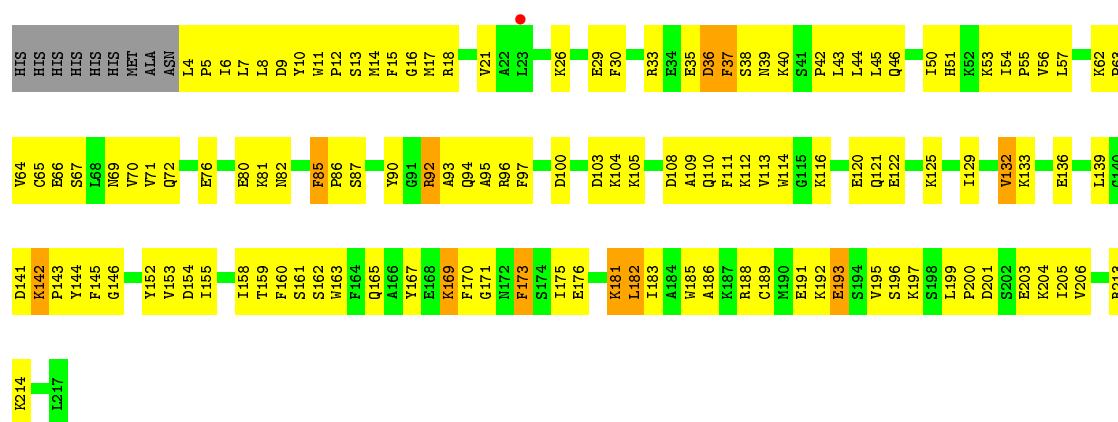
• Molecule 2: Glutathione S-transferase U20

Chain E: 24% 64% 8%



• Molecule 2: Glutathione S-transferase U20

Chain F: 38% 53% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.83Å 53.88Å 196.79Å 92.27° 97.16° 113.60°	Depositor
Resolution (Å)	24.19 – 1.72 24.19 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.19-1.72) 99.2 (24.19-1.72)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.169 , 0.188 0.169 , 0.188	Depositor DCC
$R_{free}$ test set	21071 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	7.0	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.54 , 255.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.068 for k,h,-h-k-l 0.009 for -k,-h,l 0.005 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	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 55.83 % 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 2.9873e-05. 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, ATP, JAA

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	0.55	1/4581 (0.0%)	0.77	3/6219 (0.0%)
1	D	0.65	6/4581 (0.1%)	0.83	4/6219 (0.1%)
2	B	0.61	0/1799	0.86	5/2428 (0.2%)
2	C	0.52	0/1799	0.68	1/2428 (0.0%)
2	E	0.60	0/1799	0.80	2/2428 (0.1%)
2	F	0.51	0/1799	0.64	2/2428 (0.1%)
All	All	0.58	7/16358 (0.0%)	0.78	17/22150 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	4
All	All	0	6

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	570	TYR	CD2-CE2	-9.47	1.25	1.39
1	D	570	TYR	CB-CG	-7.34	1.40	1.51
1	D	570	TYR	CD1-CE1	-7.33	1.28	1.39
1	D	570	TYR	CZ-OH	-7.27	1.25	1.37
1	A	169	VAL	CB-CG2	-7.15	1.37	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	188	ARG	NE-CZ-NH1	-12.69	113.96	120.30
1	D	510	ARG	NE-CZ-NH1	-12.11	114.24	120.30
2	B	188	ARG	NE-CZ-NH2	10.65	125.63	120.30
1	D	510	ARG	NE-CZ-NH2	9.65	125.13	120.30
2	E	188	ARG	NE-CZ-NH1	-7.83	116.39	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ASN	Sidechain
1	A	540	SER	Peptide
1	D	168	ASN	Sidechain
1	D	318	HIS	Sidechain
1	D	427	LEU	Peptide

## 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	4479	0	4434	641	8
1	D	4479	0	4434	721	6
2	B	1748	0	1704	266	0
2	C	1748	0	1704	207	3
2	E	1748	0	1704	284	1
2	F	1748	0	1704	156	3
3	A	15	0	0	2	0
3	D	15	0	0	3	0
4	A	9	0	10	13	0
4	D	9	0	10	8	0
5	A	31	0	7	23	0
5	D	31	0	8	27	0
6	B	20	0	15	3	0
6	C	20	0	15	1	0
6	E	20	0	15	5	0
6	F	20	0	15	3	0
7	A	545	0	0	96	3
7	B	306	0	0	79	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	270	0	0	31	6
7	D	528	0	0	98	5
7	E	320	0	0	96	7
7	F	291	0	0	21	4
All	All	18400	0	15779	2154	32

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 67.

The worst 5 of 2154 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:A:499:ARG:O	2:B:188:ARG:NH1	1.69	1.26
2:E:34:GLU:OE2	7:E:401:HOH:O	1.54	1.21
1:A:492:ASP:O	2:B:187:LYS:NZ	1.76	1.17
2:E:127:GLU:OE2	7:E:402:HOH:O	1.61	1.16
1:A:451:ARG:NH1	1:A:493:CYS:SG	2.20	1.15

The worst 5 of 32 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASP:OD2	1:A:475:TYR:OH[1_565]	1.83	0.37
1:A:211:LEU:O	1:A:509:SER:OG[1_565]	1.91	0.29
1:D:211:LEU:O	1:D:509:SER:OG[1_565]	1.92	0.28
1:A:270:ASN:O	1:A:511:LYS:NZ[1_565]	1.96	0.24
1:D:272:GLU:OE2	1:D:495:ASN:O[1_565]	2.01	0.19

## 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	567/575 (99%)	529 (93%)	35 (6%)	3 (0%)	29	13
1	D	567/575 (99%)	535 (94%)	26 (5%)	6 (1%)	14	3
2	B	212/223 (95%)	194 (92%)	14 (7%)	4 (2%)	8	1
2	C	212/223 (95%)	200 (94%)	12 (6%)	0	100	100
2	E	212/223 (95%)	192 (91%)	17 (8%)	3 (1%)	11	2
2	F	212/223 (95%)	202 (95%)	10 (5%)	0	100	100
All	All	1982/2042 (97%)	1852 (93%)	114 (6%)	16 (1%)	19	6

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLU
2	B	140	GLY
1	D	368	GLU
1	D	436	ASN
1	D	544	GLN

### 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	499/505 (99%)	456 (91%)	43 (9%)	10	2
1	D	499/505 (99%)	467 (94%)	32 (6%)	17	4
2	B	187/195 (96%)	168 (90%)	19 (10%)	7	1
2	C	187/195 (96%)	178 (95%)	9 (5%)	25	8
2	E	187/195 (96%)	169 (90%)	18 (10%)	8	1
2	F	187/195 (96%)	173 (92%)	14 (8%)	13	3
All	All	1746/1790 (98%)	1611 (92%)	135 (8%)	13	2

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	204	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	92	HIS
2	F	38	SER
2	C	18	ARG
2	C	169	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	82	ASN
2	C	51	HIS
1	D	560	GLN
1	A	560	GLN
2	B	60	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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
6	GSH	C	301	-	12,19,19	1.63	2 (16%)	15,24,24	2.46	5 (33%)
5	ATP	D	603	-	26,33,33	4.98	13 (50%)	31,52,52	3.30	15 (48%)
6	GSH	F	301	-	12,19,19	1.62	2 (16%)	15,24,24	2.38	11 (73%)
6	GSH	B	301	-	12,19,19	1.86	3 (25%)	15,24,24	2.89	5 (33%)
5	ATP	A	603	-	26,33,33	4.83	16 (61%)	31,52,52	3.34	15 (48%)
3	JAA	D	601	-	12,15,15	5.60	6 (50%)	12,19,19	1.72	3 (25%)
3	JAA	A	601	-	12,15,15	5.56	6 (50%)	12,19,19	2.10	3 (25%)
6	GSH	E	301	-	12,19,19	1.58	4 (33%)	15,24,24	1.36	3 (20%)

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
6	GSH	C	301	-	-	6/18/24/24	-
5	ATP	D	603	-	-	0/18/38/38	0/3/3/3
6	GSH	F	301	-	-	3/18/24/24	-
6	GSH	B	301	-	-	4/18/24/24	-
5	ATP	A	603	-	-	4/18/38/38	0/3/3/3
3	JAA	D	601	-	-	4/7/22/22	0/1/1/1
3	JAA	A	601	-	-	5/7/22/22	0/1/1/1
6	GSH	E	301	-	-	7/18/24/24	-

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	JAA	C05-C08	-12.90	1.30	1.52
3	A	601	JAA	C05-C08	-12.33	1.31	1.52
5	A	603	ATP	C3'-C4'	-12.18	1.21	1.53
5	D	603	ATP	C3'-C4'	-11.87	1.22	1.53
5	D	603	ATP	C4-N3	11.75	1.51	1.35

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	603	ATP	C4-C5-N7	-10.15	98.82	109.40
5	D	603	ATP	C4-C5-N7	-8.66	100.38	109.40
5	A	603	ATP	C5'-C4'-C3'	-8.01	85.16	115.18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	301	GSH	CA2-CB2-SG2	-7.20	106.10	114.19
5	D	603	ATP	PA-O3A-PB	-6.78	109.55	132.83

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

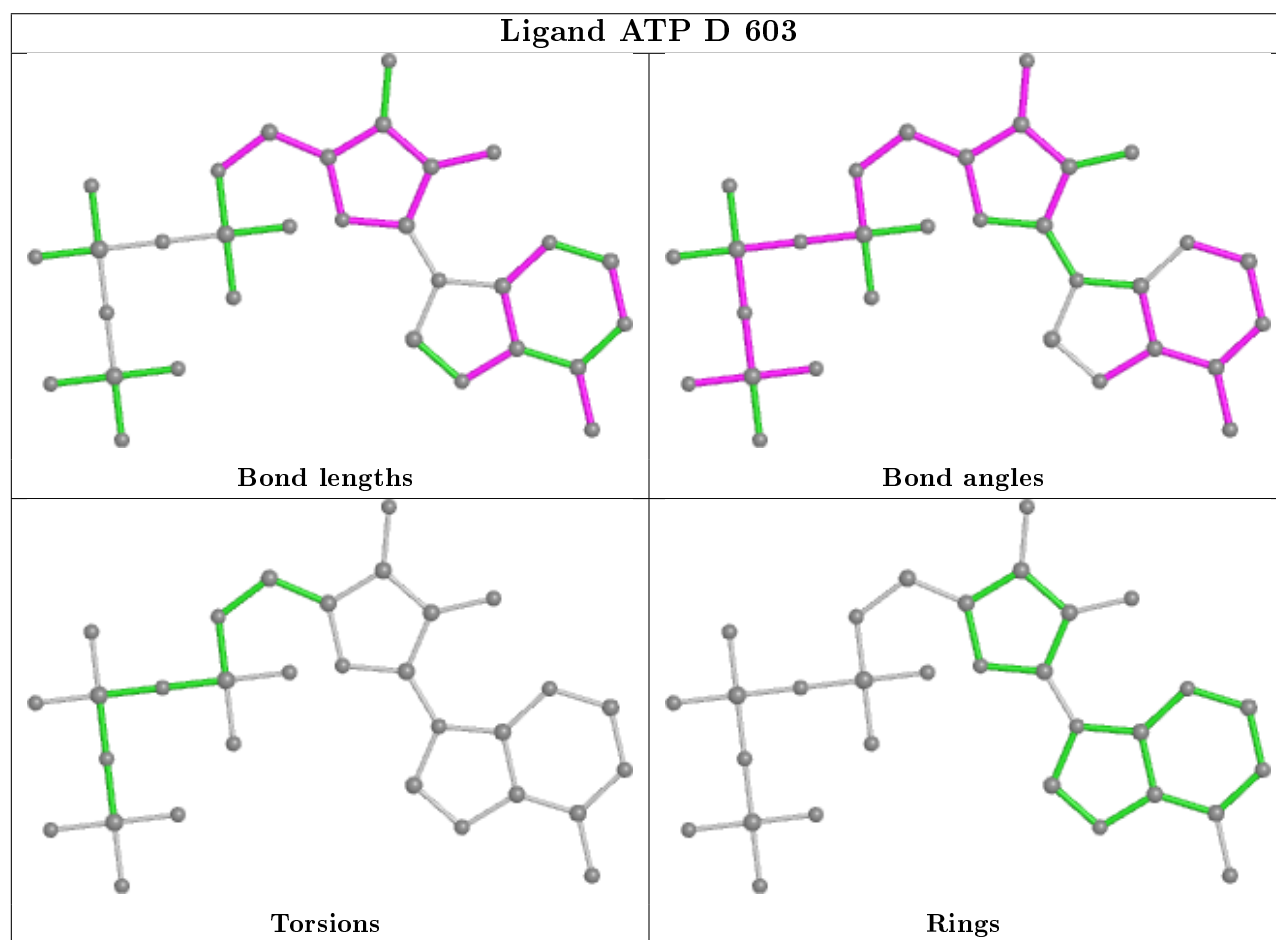
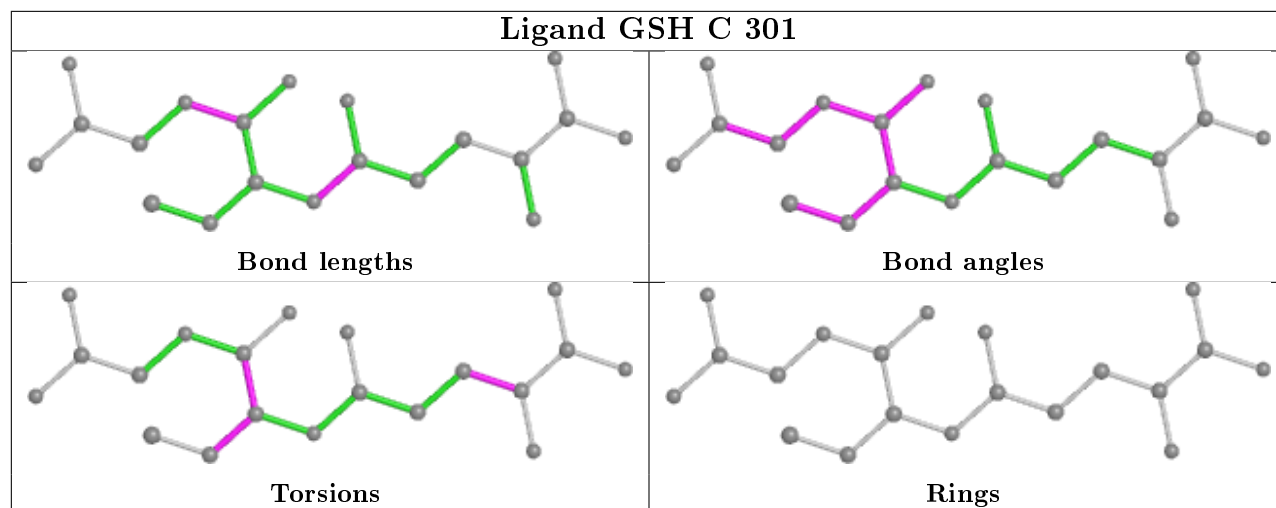
Mol	Chain	Res	Type	Atoms
6	C	301	GSH	N1-CA1-CB1-CG1
6	C	301	GSH	C1-CA1-CB1-CG1
6	C	301	GSH	N2-CA2-CB2-SG2
6	C	301	GSH	C2-CA2-CB2-SG2
6	B	301	GSH	N1-CA1-CB1-CG1

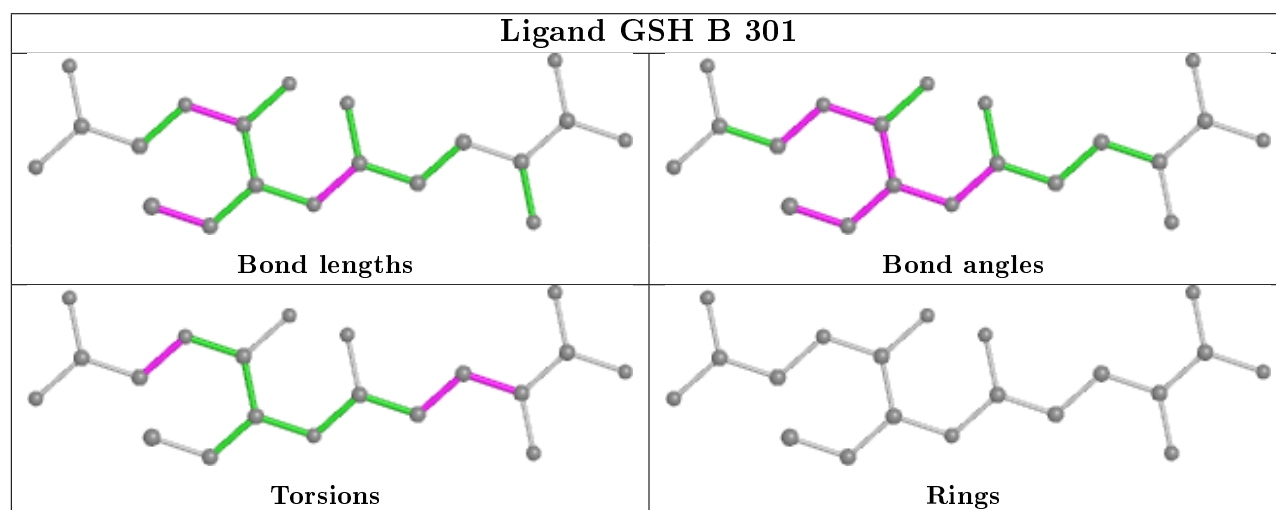
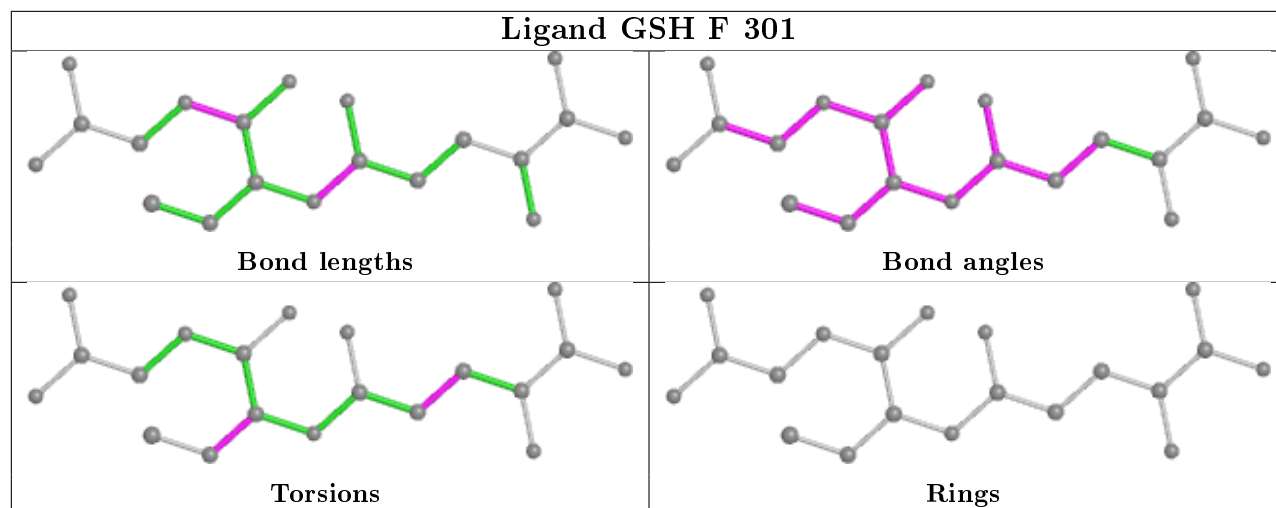
There are no ring outliers.

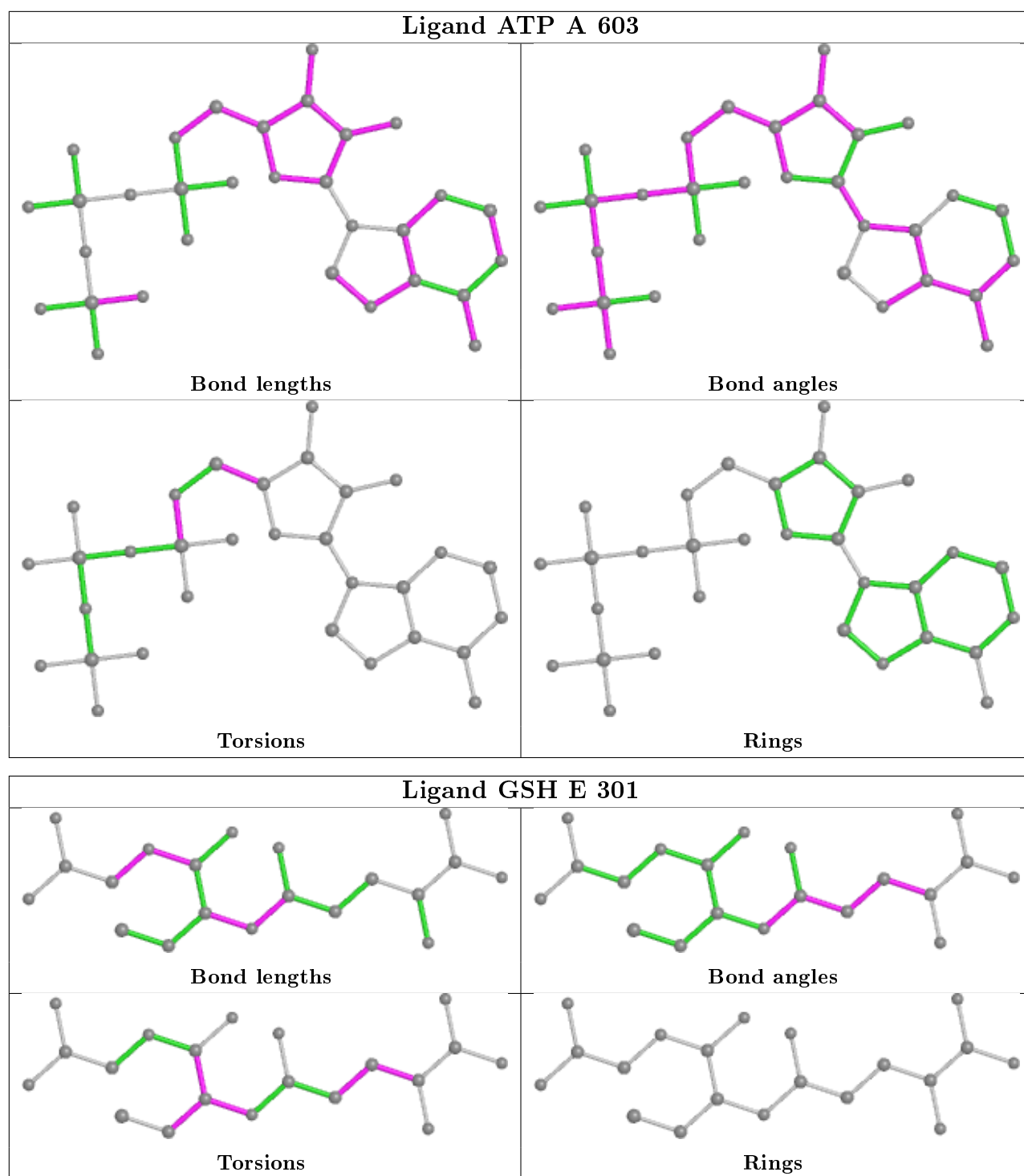
8 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	301	GSH	1	0
5	D	603	ATP	27	0
6	F	301	GSH	3	0
6	B	301	GSH	3	0
5	A	603	ATP	23	0
3	D	601	JAA	3	0
3	A	601	JAA	2	0
6	E	301	GSH	5	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 ⓘ

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, 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	569/575 (98%)	0.10	3 (0%) 91 92	3, 8, 8, 10	0
1	D	569/575 (98%)	0.10	3 (0%) 91 92	3, 8, 9, 16	0
2	B	214/223 (95%)	-0.12	0 100 100	2, 3, 7, 11	0
2	C	214/223 (95%)	-0.01	2 (0%) 84 87	7, 8, 8, 9	0
2	E	214/223 (95%)	-0.15	0 100 100	2, 3, 7, 11	0
2	F	214/223 (95%)	0.03	1 (0%) 91 92	7, 8, 8, 9	0
All	All	1994/2042 (97%)	0.03	9 (0%) 91 92	2, 8, 8, 16	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	PRO	3.1
1	A	542	ALA	2.6
1	A	169	VAL	2.6
1	D	510	ARG	2.2
2	F	23	LEU	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands

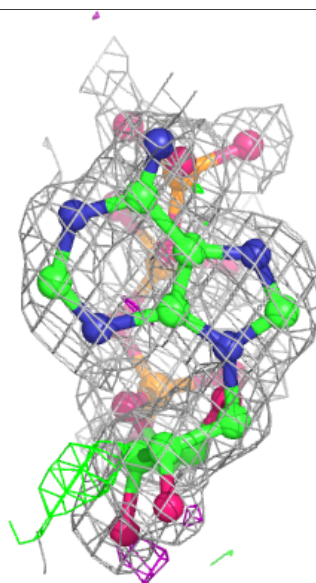
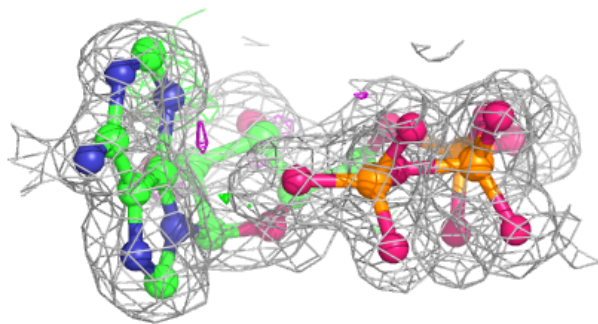
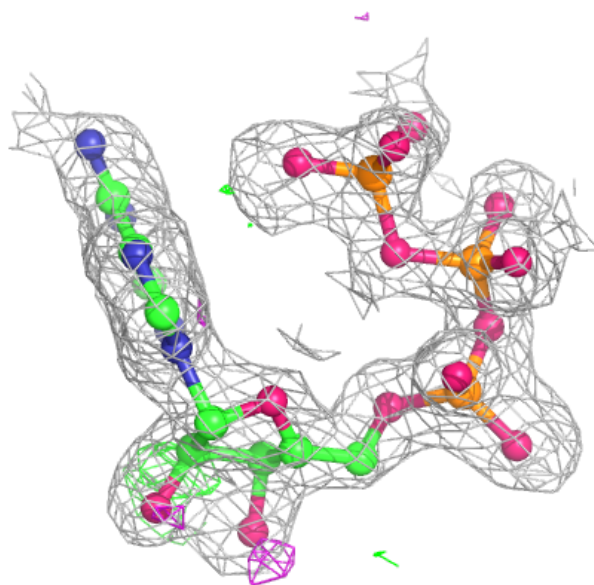
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	LEU	A	602	9/9	0.81	0.16	12,12,12,12	0
3	JAA	A	601	15/15	0.89	0.13	8,8,9,11	0
4	LEU	D	602	9/9	0.89	0.14	12,12,12,12	0
5	ATP	D	603	31/31	0.94	0.12	9,11,12,13	0
6	GSH	B	301	20/20	0.94	0.12	10,11,13,13	0
6	GSH	C	301	20/20	0.94	0.13	10,11,13,13	0
6	GSH	E	301	20/20	0.94	0.10	10,11,13,13	0
5	ATP	A	603	31/31	0.95	0.09	9,10,12,13	0
6	GSH	F	301	20/20	0.96	0.12	10,12,13,13	0
3	JAA	D	601	15/15	0.96	0.09	7,9,9,9	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.

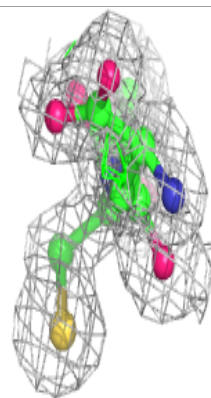
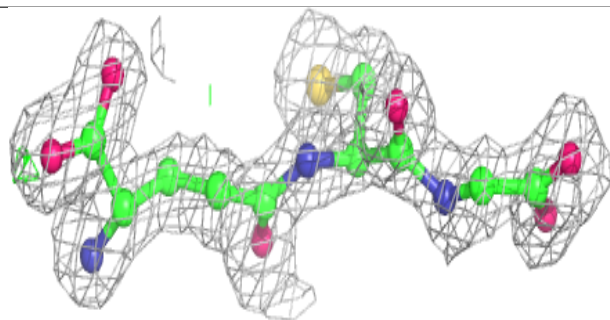
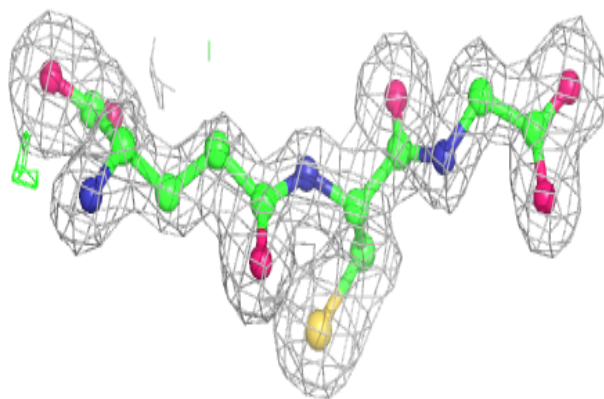
**Electron density around ATP D 603:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

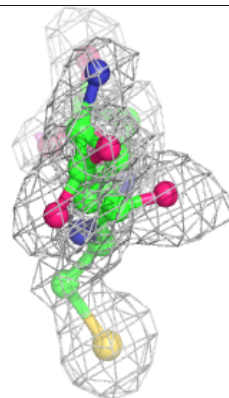
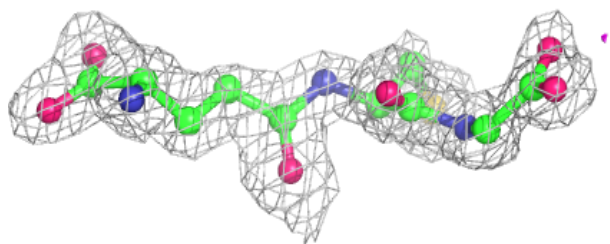
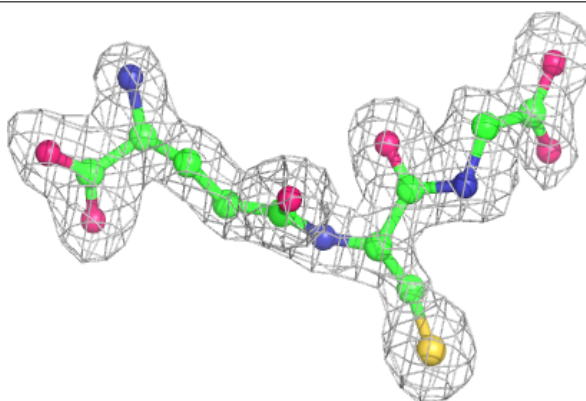


**Electron density around GSH B 301:**

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

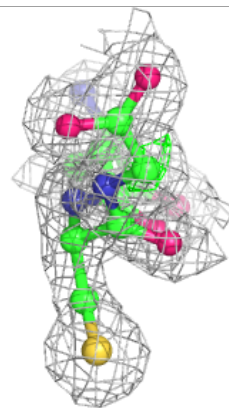
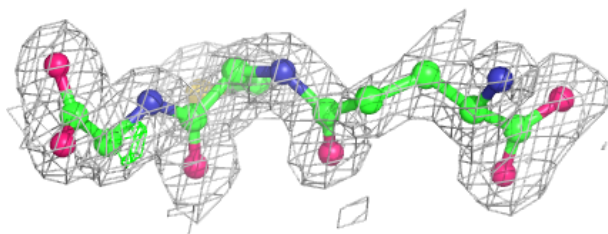
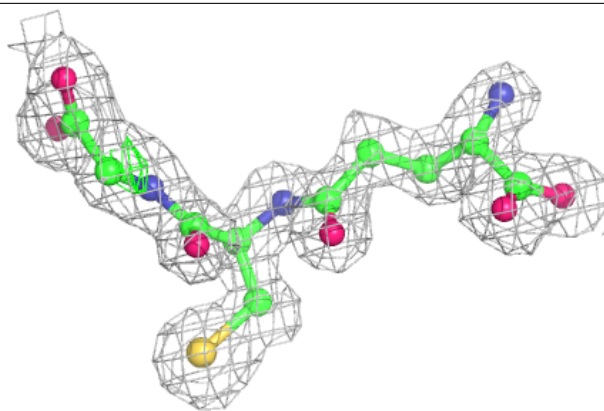
**Electron density around GSH C 301:**

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



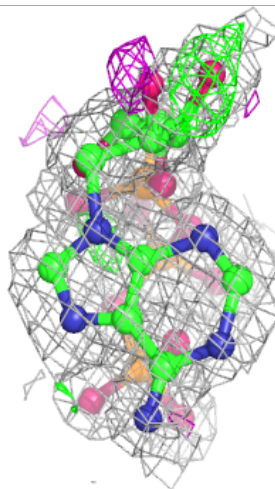
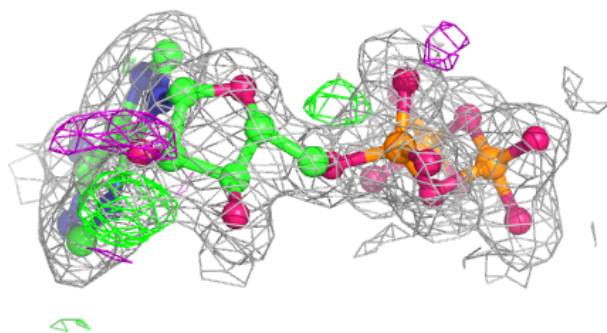
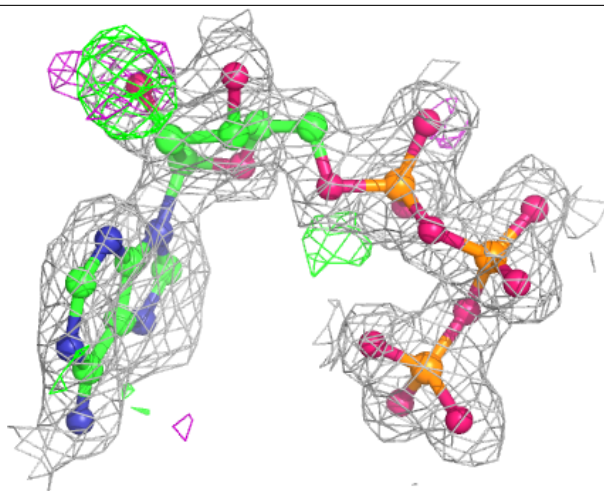
**Electron density around GSH E 301:**

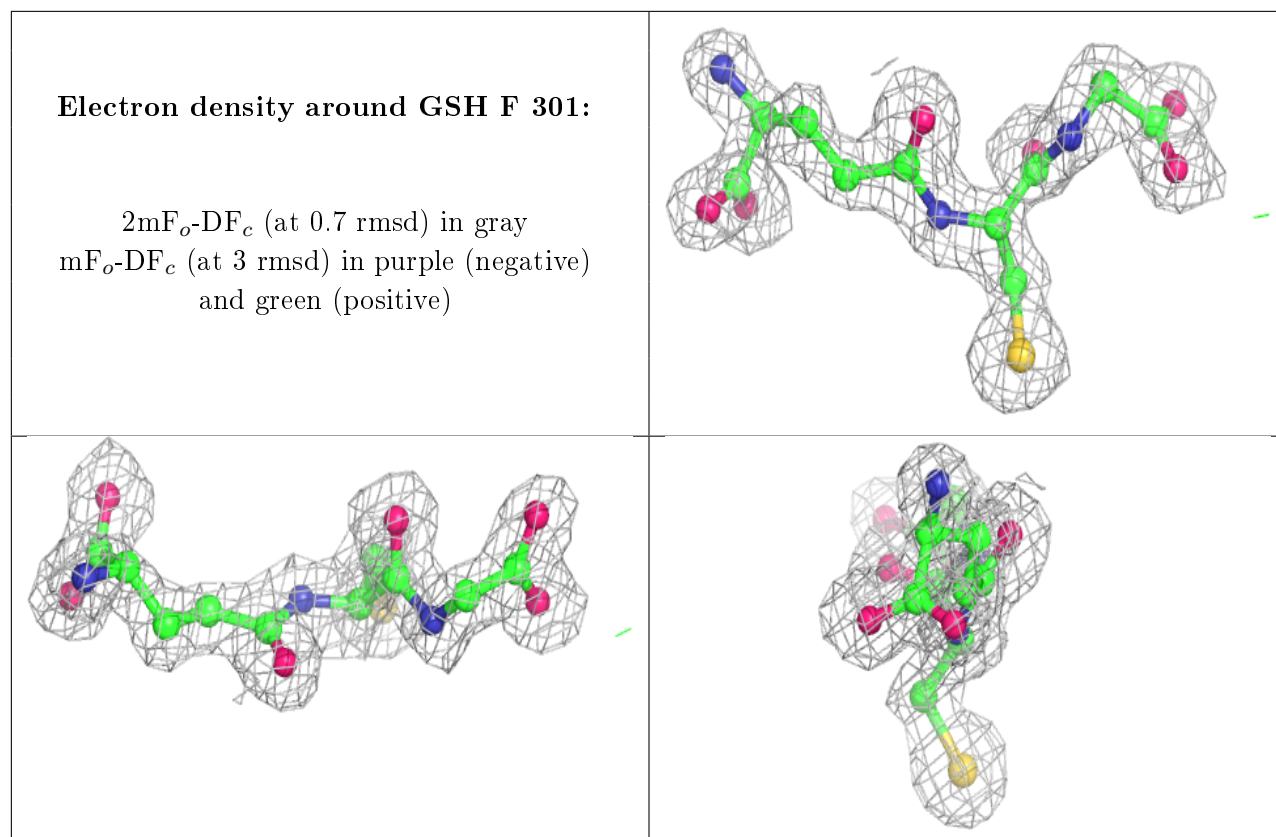
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ATP A 603:**

$2mF_o-DF_c$  (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.