



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2022 – 04:48 pm GMT

PDB ID : 6T48  
Title : Bovine enterovirus F3 in complex with glutathione and a Cysteinylglycine dipeptide  
Authors : Duyvesteyn, H.M.E.; Ren, J.; Walter, T.S.; Fry, E.E.; Stuart, D.I.  
Deposited on : 2019-10-12  
Resolution : 2.17 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
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)	:	2.31.3

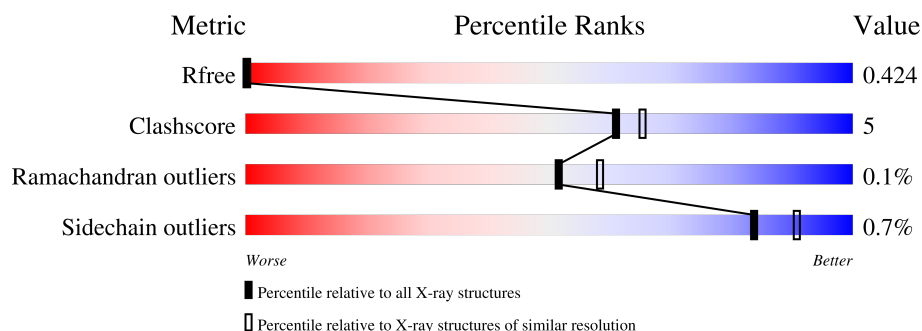
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	275	
2	B	244	
3	C	243	
4	D	71	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 6992 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2102	1320	361	411	10			

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1892	1208	323	356	5			

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	243	Total	C	N	O	S	0	0	0
			1911	1232	310	357	12			

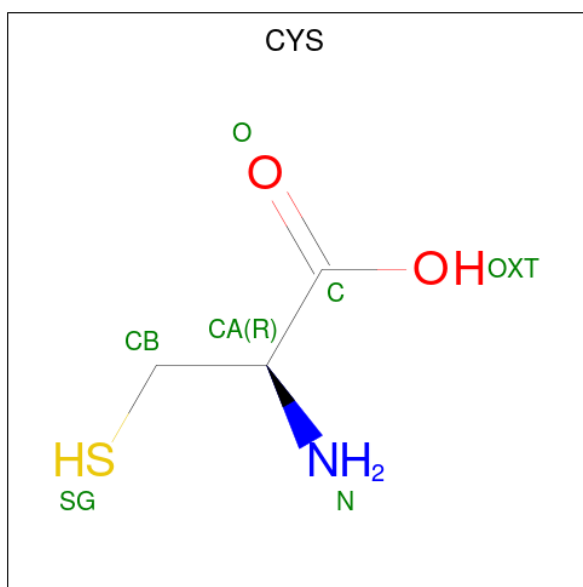
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	102	PHE	LEU	conflict	UNP Q2LKZ0
C	103	THR	HIS	conflict	UNP Q2LKZ0
C	143	ASN	ALA	conflict	UNP Q2LKZ0
C	192	ALA	ARG	conflict	UNP Q2LKZ0
C	211	THR	ASN	conflict	UNP Q2LKZ0
C	212	THR	HIS	conflict	UNP Q2LKZ0

- Molecule 4 is a protein called VP4.

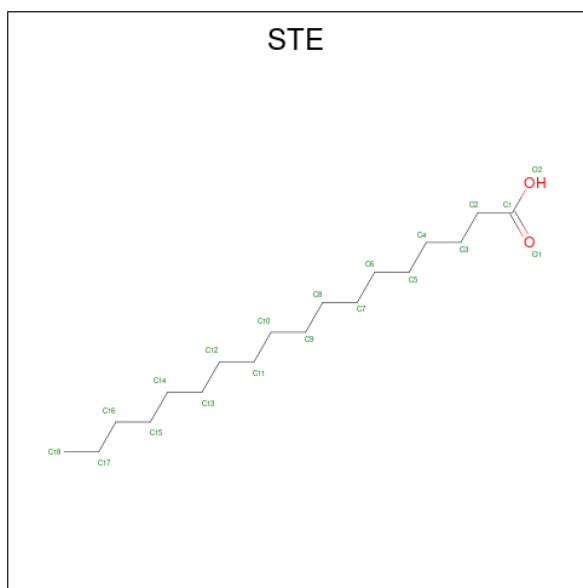
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	48	Total	C	N	O	S	0	0	0
			381	238	65	77	1			

- Molecule 5 is CYSTEINE (three-letter code: CYS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S).



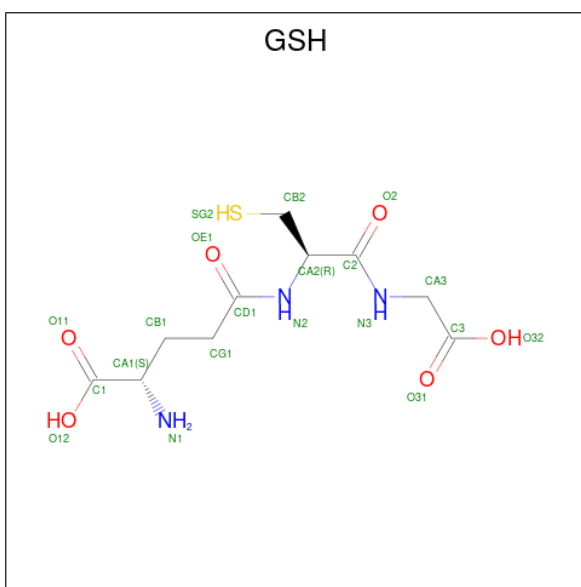
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			6	3	1	1	1		

- Molecule 6 is STEARIC ACID (three-letter code: STE) (formula:  $C_{18}H_{36}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	18	2		

- Molecule 7 is GLUTATHIONE (three-letter code: GSH) (formula:  $C_{10}H_{17}N_3O_6S$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	K	0	0
			2	2		
10	B	1	Total	K	0	0
			1	1		
10	C	1	Total	K	0	0
			1	1		

- Molecule 11 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	2	Total	Cl	0	0
			2	2		

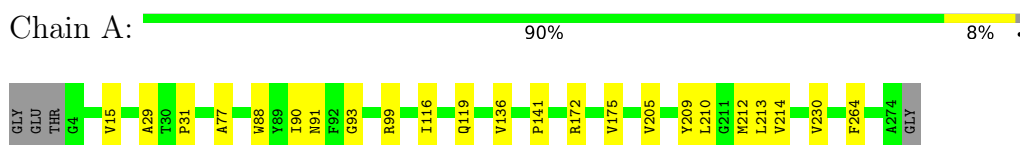
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	215	Total	O	0	0
			215	215		
13	B	196	Total	O	0	0
			196	196		
13	C	173	Total	O	0	0
			173	173		
13	D	28	Total	O	0	0
			28	28		

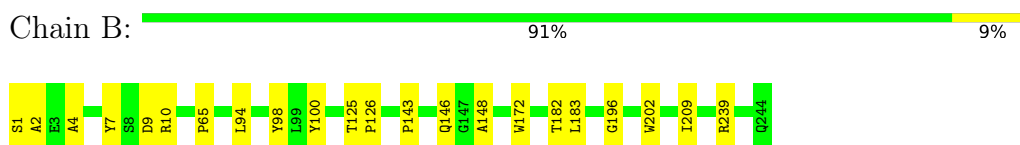
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

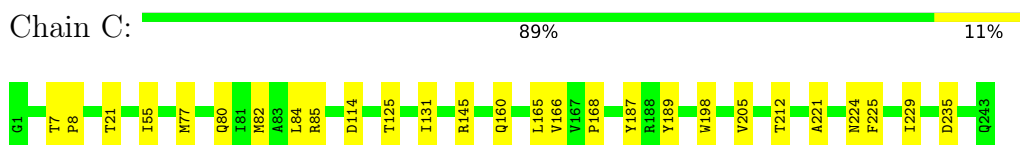
#### • Molecule 1: VP1



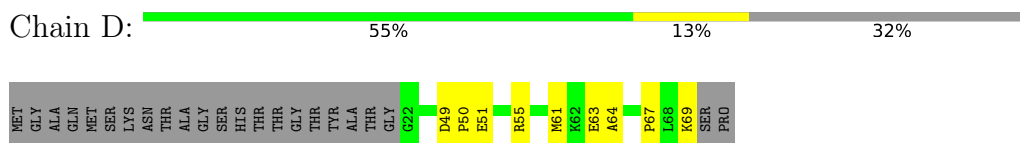
#### • Molecule 2: VP2



#### • Molecule 3: VP3



#### • Molecule 4: VP4





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	344.00Å 349.40Å 352.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.17 110.32 – 2.17	Depositor EDS
% Data completeness (in resolution range)	82.6 (19.98-2.17) 76.9 (110.32-2.17)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.200 , 0.203 0.424 , 0.424	Depositor DCC
$R_{free}$ test set	45615 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.3	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 6.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for l,-k,h 0.000 for -k,-h,-l 0.009 for k,-l,-h 0.009 for -l,h,-k	Xtriage
$F_o, F_c$ correlation	0.39	EDS
Total number of atoms	6992	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, K, GOL, CL, STE, 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	0.31	0/2150	0.63	0/2928
2	B	0.31	0/1947	0.62	0/2671
3	C	0.33	0/1964	0.67	0/2681
4	D	0.34	0/389	0.57	0/528
All	All	0.32	0/6450	0.63	0/8808

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2102	0	2035	19	0
2	B	1892	0	1830	16	0
3	C	1911	0	1876	20	0
4	D	381	0	358	9	0
5	A	6	0	4	1	0
6	A	20	0	35	3	0
7	A	20	0	15	0	0
8	A	10	0	0	0	0
8	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	10	0	0	0	0
9	A	12	0	16	0	0
10	A	2	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
11	C	5	0	2	1	0
12	C	2	0	0	0	0
13	A	215	0	0	1	0
13	B	196	0	0	1	0
13	C	173	0	0	2	0
13	D	28	0	0	0	0
All	All	6992	0	6171	57	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 5.

The worst 5 of 57 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)
3:C:145:ARG:HH11	3:C:145:ARG:HG3	1.43	0.82
4:D:49:ASP:OD1	4:D:51:GLU:HG2	1.91	0.71
5:A:301:CYS:HB2	3:C:235:ASP:O	2.01	0.61
1:A:212:MET:CE	1:A:214:VAL:HB	2.31	0.60
3:C:145:ARG:HH11	3:C:145:ARG:CG	2.17	0.57

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	269/275 (98%)	257 (96%)	12 (4%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	242/244 (99%)	232 (96%)	10 (4%)	0	100	100
3	C	241/243 (99%)	234 (97%)	6 (2%)	1 (0%)	34	35
4	D	46/71 (65%)	44 (96%)	2 (4%)	0	100	100
All	All	798/833 (96%)	767 (96%)	30 (4%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	229	ILE

### 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	230/232 (99%)	229 (100%)	1 (0%)	91	95
2	B	200/200 (100%)	197 (98%)	3 (2%)	65	76
3	C	211/211 (100%)	210 (100%)	1 (0%)	88	94
4	D	42/59 (71%)	42 (100%)	0	100	100
All	All	683/702 (97%)	678 (99%)	5 (1%)	84	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
2	B	9	ASP
2	B	98	TYR
2	B	100	TYR
3	C	114	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	146	GLN
2	B	151	GLN
2	B	244	GLN
4	D	42	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z  > 2$
8	SO4	A	304	-	4,4,4	0.26	0	6,6,6	0.06	0
8	SO4	B	301	-	4,4,4	0.26	0	6,6,6	0.05	0
11	GLY	C	301	-	4,4,4	0.99	0	3,4,4	0.89	0
8	SO4	C	303	-	4,4,4	0.26	0	6,6,6	0.04	0
9	GOL	A	307	-	5,5,5	0.14	0	5,5,5	0.30	0
8	SO4	A	305	-	4,4,4	0.60	0	6,6,6	0.09	0
5	CYS	A	301	-	4,5,6	0.62	0	1,5,7	0.67	0
6	STE	A	302	-	19,19,19	0.91	1 (5%)	19,19,19	0.66	0
9	GOL	A	306	-	5,5,5	0.26	0	5,5,5	0.27	0
7	GSH	A	303	-	18,19,19	0.98	2 (11%)	23,24,24	0.91	0
8	SO4	C	302	-	4,4,4	0.26	0	6,6,6	0.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	GLY	C	301	-	-	0/2/2/2	-
9	GOL	A	307	-	-	0/4/4/4	-
5	CYS	A	301	-	-	0/1/4/6	-
6	STE	A	302	-	-	9/17/17/17	-
9	GOL	A	306	-	-	0/4/4/4	-
7	GSH	A	303	-	-	9/24/24/24	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	302	STE	O2-C1	-3.08	1.20	1.30
7	A	303	GSH	CG1-CD1	2.43	1.56	1.51
7	A	303	GSH	O32-C3	-2.16	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	303	GSH	O11-C1-CA1-N1
7	A	303	GSH	N2-CA2-CB2-SG2
7	A	303	GSH	C2-CA2-CB2-SG2
7	A	303	GSH	O12-C1-CA1-N1
7	A	303	GSH	O31-C3-CA3-N3

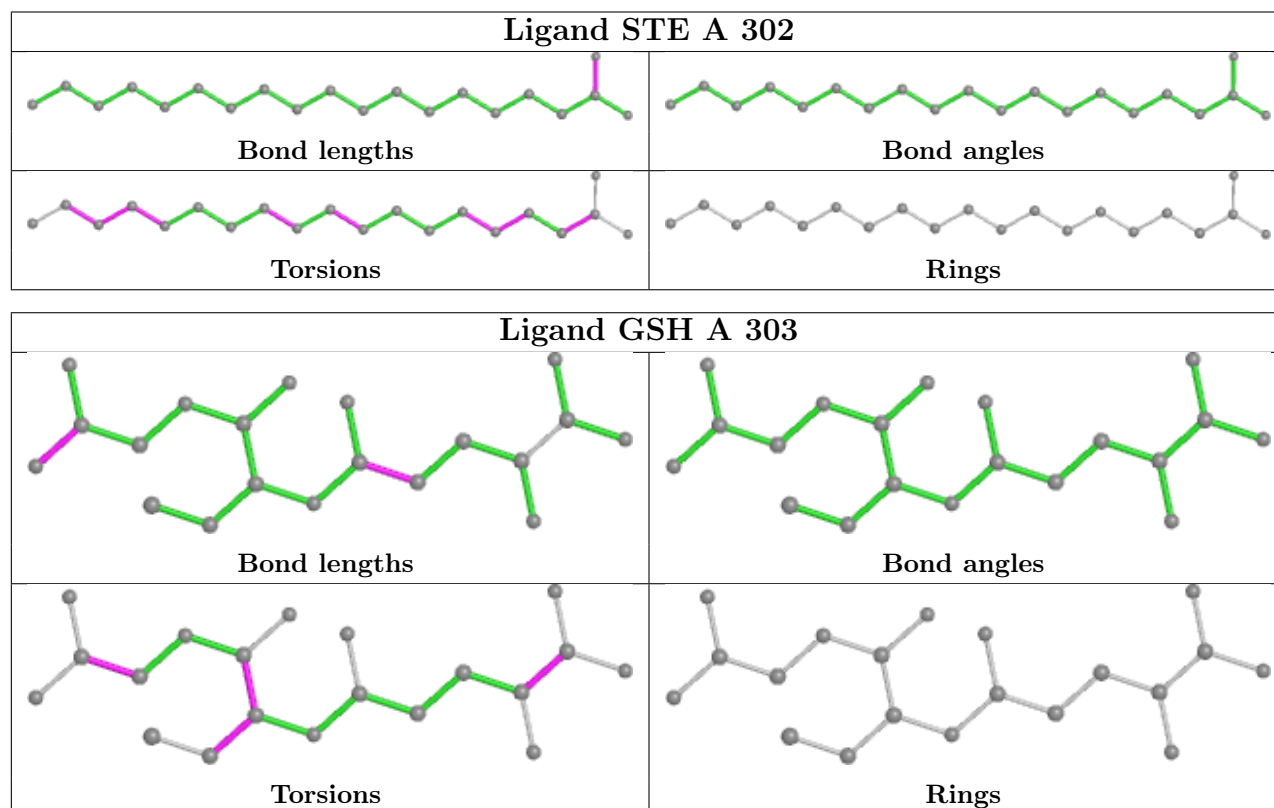
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	301	GLY	1	0
5	A	301	CYS	1	0
6	A	302	STE	3	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

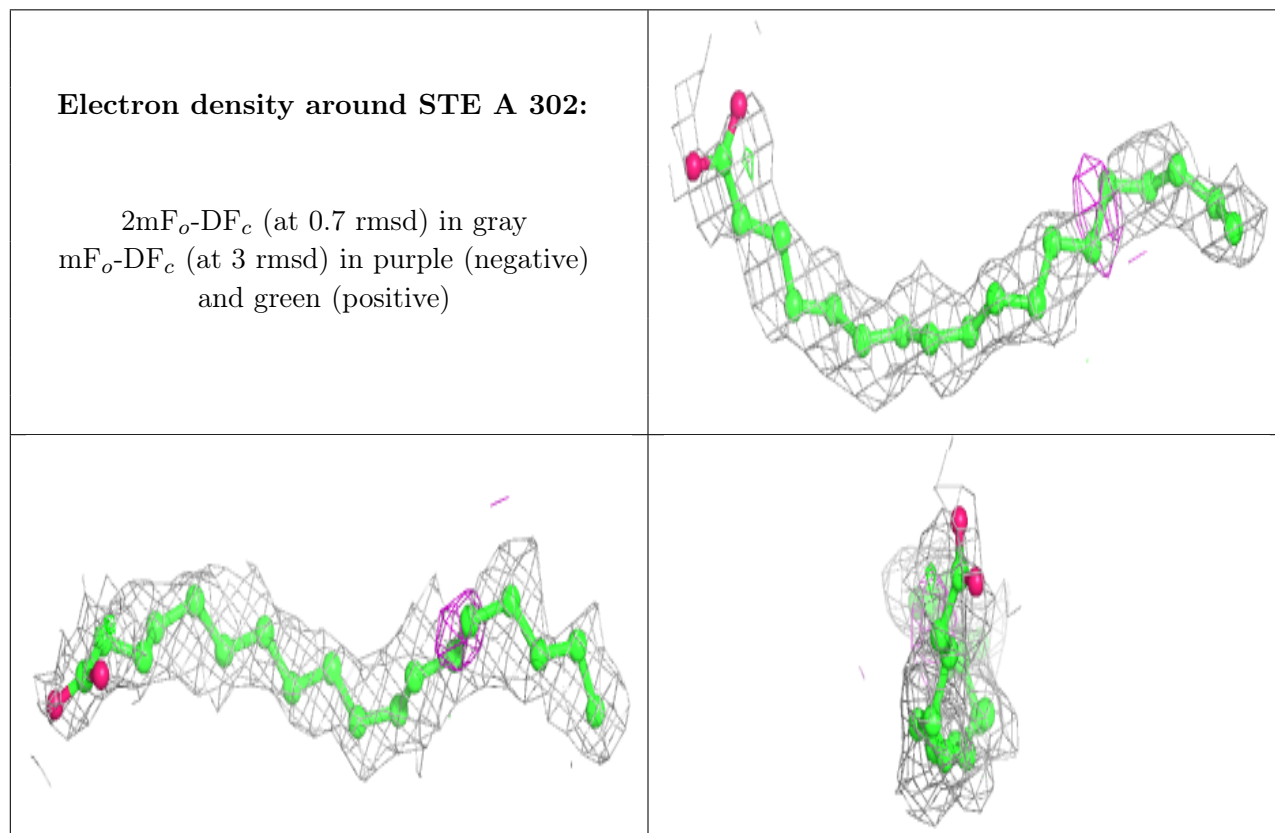
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

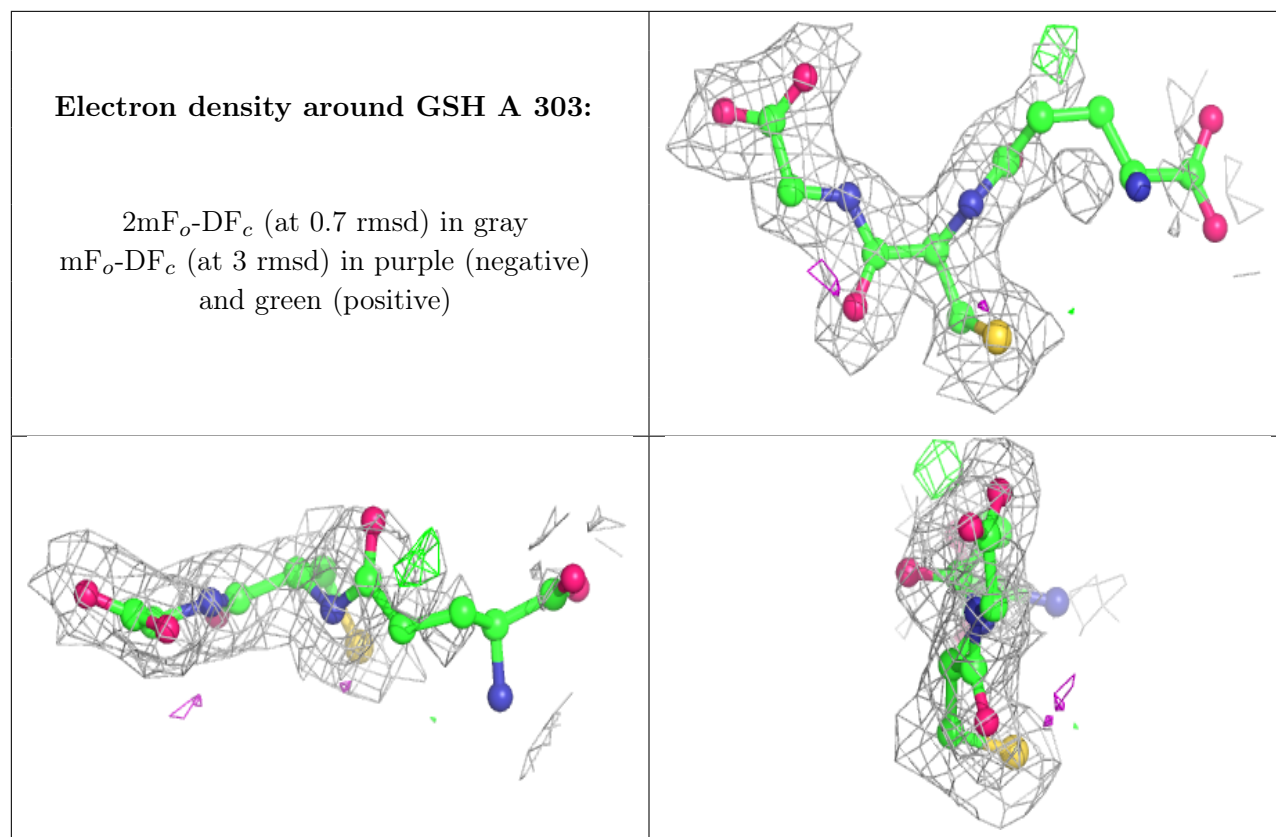
### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.







## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.