



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 11:27 AM EST

PDB ID : 3DWW
Title : Electron crystallographic structure of human microsomal prostaglandin E synthase 1
Authors : Hebert, H.; Jegerschold, C.
Deposited on : 2008-07-23
Resolution : 3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

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>.

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)
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

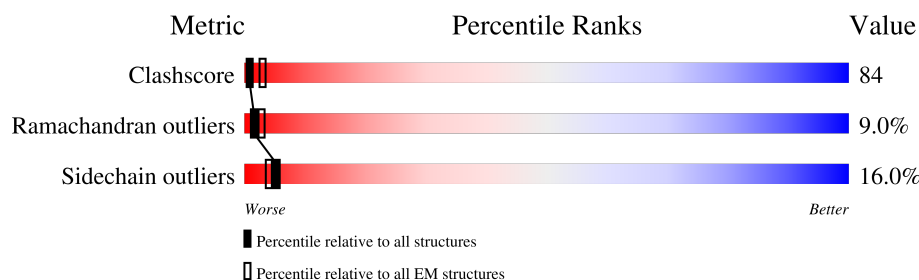
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	158	
1	B	158	
1	C	158	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GSH	A	154	X	-	X	-
2	GSH	B	155	X	-	X	-
2	GSH	C	153	X	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3456 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

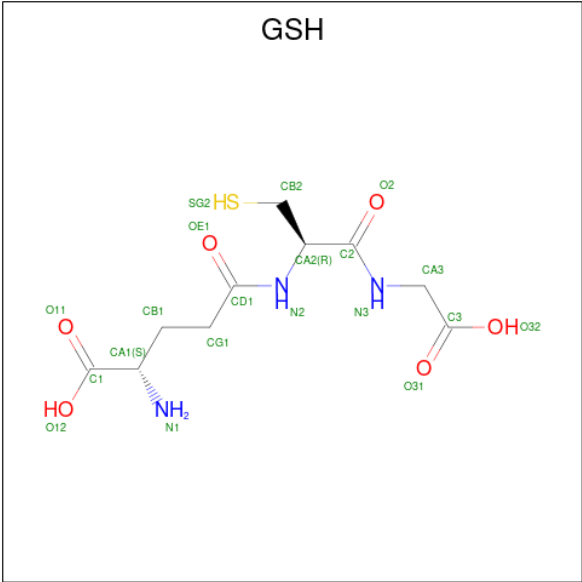
- Molecule 1 is a protein called Prostaglandin E synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	142	Total	C	N	O	S	0	0
			1132	744	198	182	8		
1	B	142	Total	C	N	O	S	0	0
			1132	744	198	182	8		
1	C	142	Total	C	N	O	S	0	0
			1132	744	198	182	8		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP O14684
A	-4	HIS	-	EXPRESSION TAG	UNP O14684
A	-3	HIS	-	EXPRESSION TAG	UNP O14684
A	-2	HIS	-	EXPRESSION TAG	UNP O14684
A	-1	HIS	-	EXPRESSION TAG	UNP O14684
A	0	HIS	-	EXPRESSION TAG	UNP O14684
B	-5	HIS	-	EXPRESSION TAG	UNP O14684
B	-4	HIS	-	EXPRESSION TAG	UNP O14684
B	-3	HIS	-	EXPRESSION TAG	UNP O14684
B	-2	HIS	-	EXPRESSION TAG	UNP O14684
B	-1	HIS	-	EXPRESSION TAG	UNP O14684
B	0	HIS	-	EXPRESSION TAG	UNP O14684
C	-5	HIS	-	EXPRESSION TAG	UNP O14684
C	-4	HIS	-	EXPRESSION TAG	UNP O14684
C	-3	HIS	-	EXPRESSION TAG	UNP O14684
C	-2	HIS	-	EXPRESSION TAG	UNP O14684
C	-1	HIS	-	EXPRESSION TAG	UNP O14684
C	0	HIS	-	EXPRESSION TAG	UNP O14684

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C₁₀H₁₇N₃O₆S).

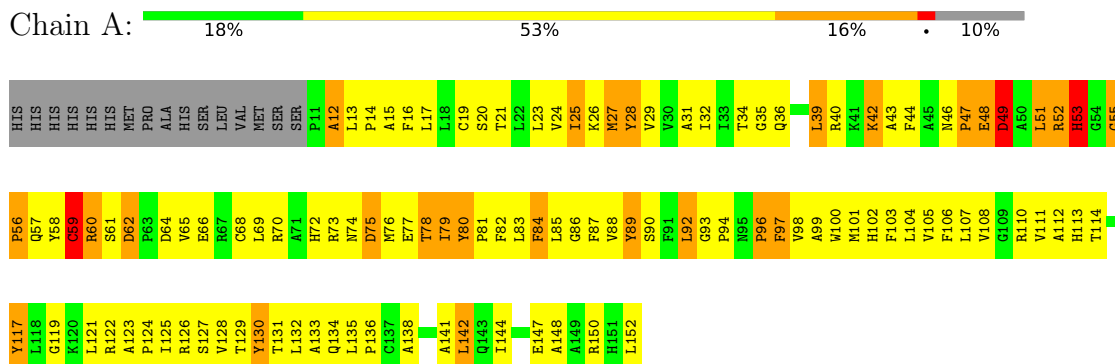


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			20	10	3	6	1	
2	B	1	Total	C	N	O	S	0
			20	10	3	6	1	
2	C	1	Total	C	N	O	S	0
			20	10	3	6	1	

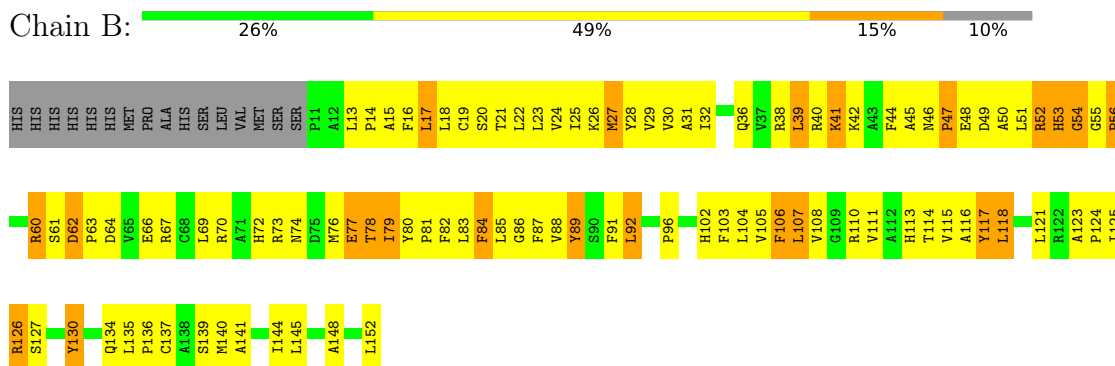
3 Residue-property plots

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.

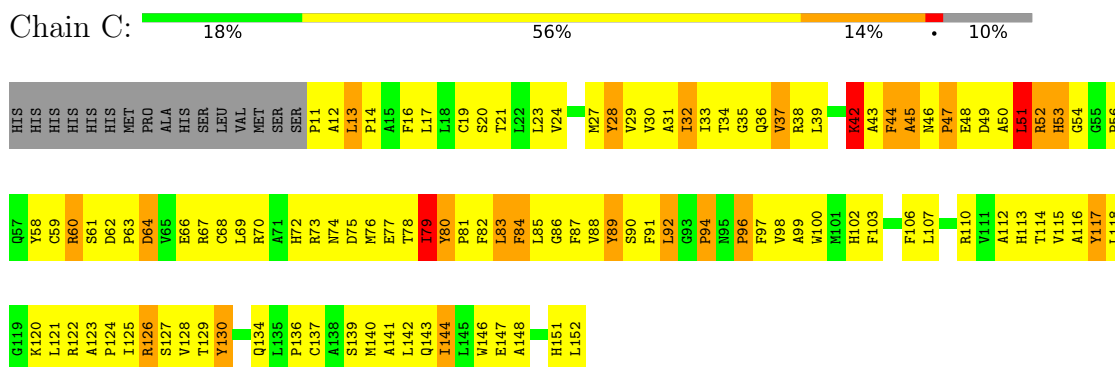
- Molecule 1: Prostaglandin E synthase



- Molecule 1: Prostaglandin E synthase



- Molecule 1: Prostaglandin E synthase



4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.20Å 84.60Å 100.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3456	wwPDB-VP
Average B, all atoms (Å ²)	3.0	wwPDB-VP

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	0.54	0/1165	0.75	0/1585
1	B	0.58	0/1165	0.74	0/1585
1	C	0.54	0/1165	0.78	0/1585
All	All	0.55	0/3495	0.76	0/4755

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	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	ASP	Peptide
1	C	44	PHE	Peptide
1	C	51	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	1132	0	1163	229	0
1	B	1132	0	1163	207	0
1	C	1132	0	1163	252	0
2	A	20	0	15	19	0
2	B	20	0	15	18	0
2	C	20	0	15	19	0
All	All	3456	0	3534	585	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 84.

The worst 5 of 585 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:16:PHE:CZ	1:A:90:SER:HB2	1.59	1.34
1:A:16:PHE:CE2	1:A:90:SER:HB2	1.64	1.32
1:B:77:GLU:OE1	2:B:155:GSH:HA2	1.33	1.24
1:C:51:LEU:O	1:C:52:ARG:HG2	1.38	1.21
1:B:74:ASN:HA	1:B:110:ARG:HH21	1.06	1.19

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 PDB entries followed by that with respect to all EM entries.

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	140/158 (89%)	100 (71%)	25 (18%)	15 (11%)	0 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	140/158 (89%)	102 (73%)	31 (22%)	7 (5%)	2	19
1	C	140/158 (89%)	99 (71%)	25 (18%)	16 (11%)	0	6
All	All	420/474 (89%)	301 (72%)	81 (19%)	38 (9%)	1	8

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	PRO
1	A	96	PRO
1	B	47	PRO
1	B	56	PRO
1	C	47	PRO

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 PDB entries followed by that with respect to all EM entries.

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	119/134 (89%)	97 (82%)	22 (18%)	1	8
1	B	119/134 (89%)	99 (83%)	20 (17%)	2	12
1	C	119/134 (89%)	104 (87%)	15 (13%)	4	22
All	All	357/402 (89%)	300 (84%)	57 (16%)	5	14

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	41	LYS
1	C	126	ARG
1	B	84	PHE
1	C	117	TYR
1	C	79	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	102	HIS
1	C	151	HIS
1	B	102	HIS
1	B	134	GLN
1	C	36	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	A	154	-	18,19,19	3.18	2 (11%)	23,24,24	1.78	6 (26%)
2	GSH	C	153	-	18,19,19	3.06	2 (11%)	23,24,24	1.47	5 (21%)
2	GSH	B	155	-	18,19,19	3.15	2 (11%)	23,24,24	1.60	8 (34%)

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	A	154	-	1/1/6/8	8/24/24/24	-
2	GSH	C	153	-	1/1/6/8	13/24/24/24	-
2	GSH	B	155	-	1/1/6/8	6/24/24/24	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	155	GSH	OE1-CD1	9.44	1.42	1.23
2	A	154	GSH	O2-C2	9.36	1.42	1.23
2	A	154	GSH	OE1-CD1	9.22	1.42	1.23
2	C	153	GSH	OE1-CD1	9.04	1.41	1.23
2	B	155	GSH	O2-C2	8.99	1.41	1.23

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	GSH	O12-C1-O11	-4.11	114.75	124.09
2	A	154	GSH	CA2-CB2-SG2	-3.12	110.69	114.19
2	A	154	GSH	O32-C3-CA3	3.01	123.18	112.74
2	C	153	GSH	CA2-CB2-SG2	-2.91	110.93	114.19
2	B	155	GSH	O12-C1-O11	-2.90	117.51	124.09

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	154	GSH	CA1
2	B	155	GSH	CA1
2	C	153	GSH	CA1

5 of 27 torsion outliers are listed below:

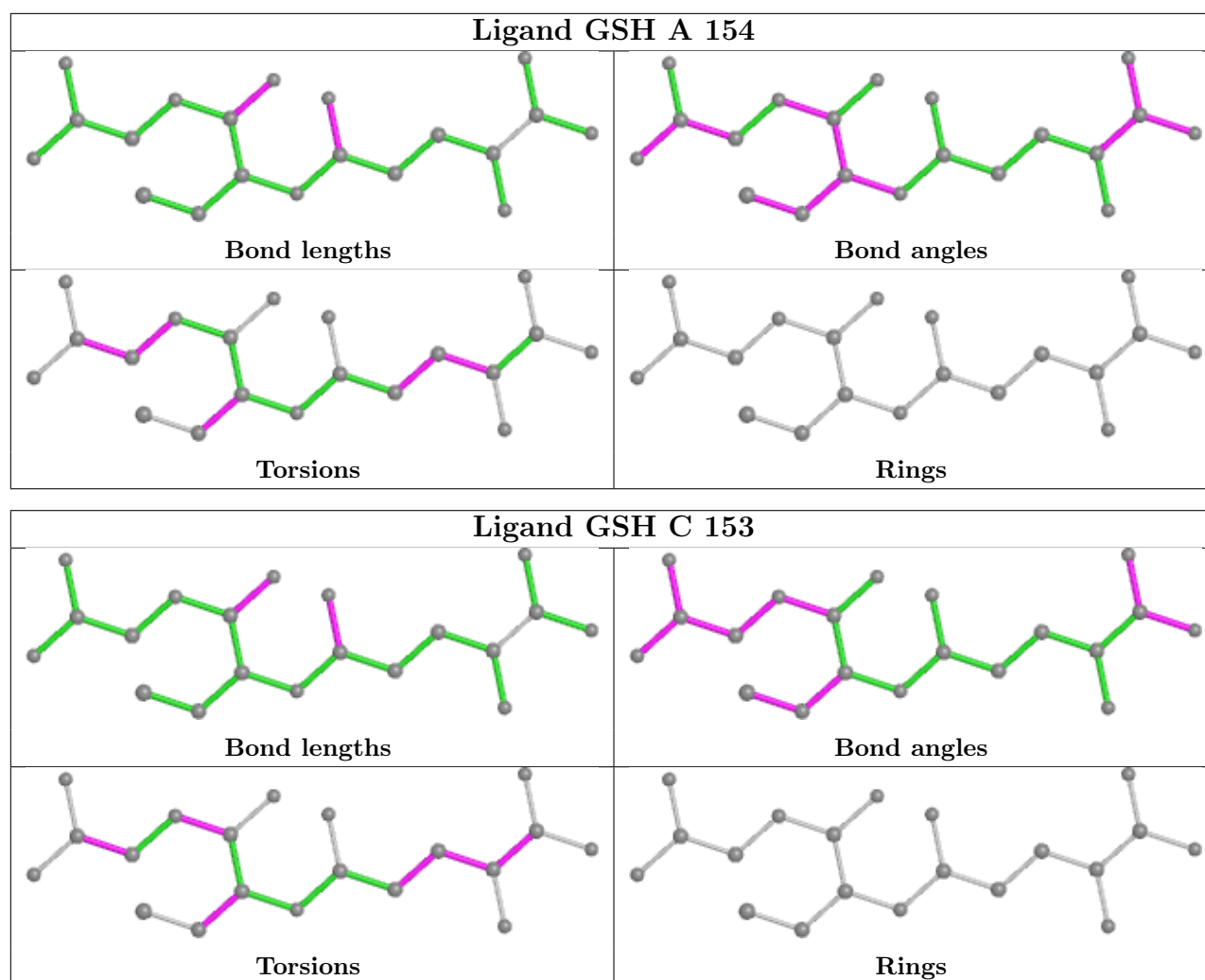
Mol	Chain	Res	Type	Atoms
2	A	154	GSH	N1-CA1-CB1-CG1
2	A	154	GSH	C1-CA1-CB1-CG1
2	A	154	GSH	N2-CA2-CB2-SG2
2	A	154	GSH	C2-CA2-CB2-SG2
2	B	155	GSH	N1-CA1-CB1-CG1

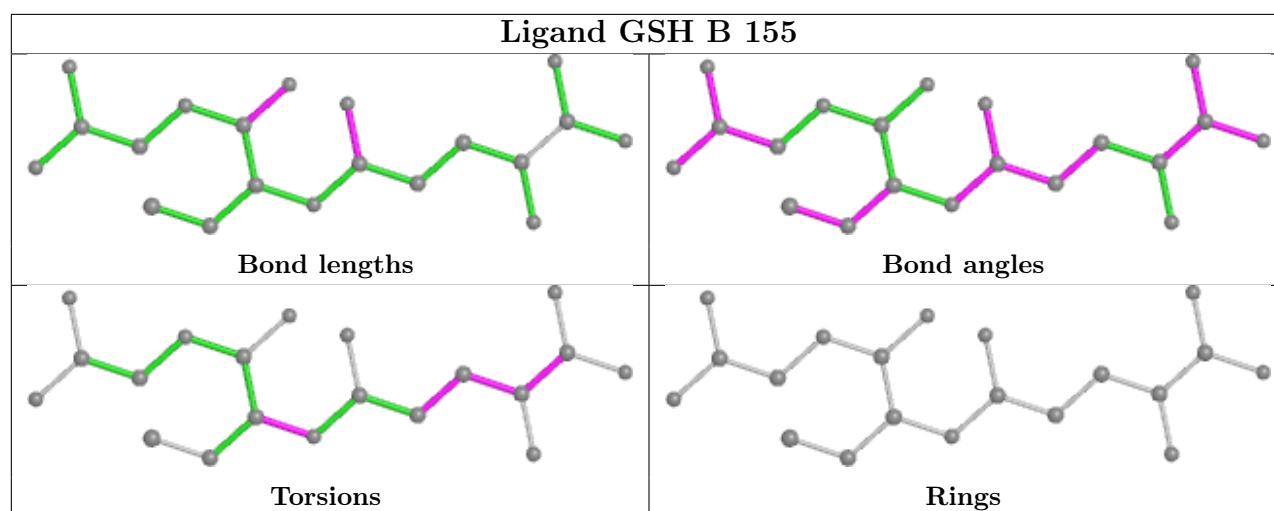
There are no ring outliers.

3 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	154	GSH	19	0
2	C	153	GSH	19	0
2	B	155	GSH	18	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.