

wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 12:39 AM JST

PDB ID : 7EBV

Title : Crystal structure of Aedes aegypti Noppera-bo, glutathione S-transferase ep-

silon 8, in luteolin- and glutathione-bound form

Authors: Inaba, K.; Koiwai, K.; Senda, M.; Senda, T.; Niwa, R.

Deposited on : 2021-03-11

Resolution : 1.50 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
A user guide is available at

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

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

The following versions of software and data (see references (1)) 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 : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

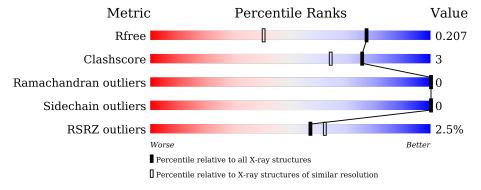
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	A	227	88%	8% •
1	В	227	92%	6% •
1	С	227	88%	7% 5%
1	D	227	91%	7% •



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7838 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Glutathione transferase.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Λ	217	Total	С	N	О	S	0	2	0
1	A	211	1686	1089	286	298	13	U	3	
1	В	221	Total	С	N	О	S	0	2	0
1	Б	221	1712	1107	286	303	16	U	2	
1	С	216	Total	С	N	О	S	0	2	0
1		210	1680	1088	280	298	14	U	2	
1	D	991	Total	С	N	О	S	0	4	0
1	ש	221	1724	1110	291	306	17	U	4	

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP A0A1S4FIB3
A	-5	ASN	-	expression tag	UNP A0A1S4FIB3
A	-4	HIS	-	expression tag	UNP A0A1S4FIB3
A	-3	LYS	-	expression tag	UNP A0A1S4FIB3
A	-2	VAL	-	expression tag	UNP A0A1S4FIB3
A	-1	HIS	_	expression tag	UNP A0A1S4FIB3
A	0	MET	-	expression tag	UNP A0A1S4FIB3
В	-6	MET	-	initiating methionine	UNP A0A1S4FIB3
В	-5	ASN	-	expression tag	UNP A0A1S4FIB3
В	-4	HIS	-	expression tag	UNP A0A1S4FIB3
В	-3	LYS	-	expression tag	UNP A0A1S4FIB3
В	-2	VAL	_	expression tag	UNP A0A1S4FIB3
В	-1	HIS	-	expression tag	UNP A0A1S4FIB3
В	0	MET	_	expression tag	UNP A0A1S4FIB3
С	-6	MET	-	initiating methionine	UNP A0A1S4FIB3
С	-5	ASN	-	expression tag	UNP A0A1S4FIB3
С	-4	HIS	-	expression tag	UNP A0A1S4FIB3
С	-3	LYS	-	expression tag	UNP A0A1S4FIB3
С	-2	VAL	-	expression tag	UNP A0A1S4FIB3
С	-1	HIS		expression tag	UNP A0A1S4FIB3
С	0	MET	_	expression tag	UNP A0A1S4FIB3

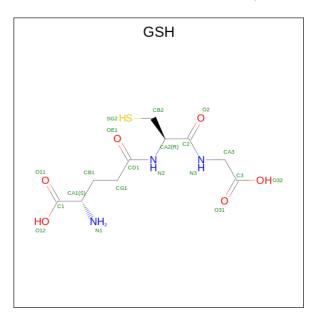
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP A0A1S4FIB3
D	-5	ASN	-	expression tag	UNP A0A1S4FIB3
D	-4	HIS	-	expression tag	UNP A0A1S4FIB3
D	-3	LYS	-	expression tag	UNP A0A1S4FIB3
D	-2	VAL	-	expression tag	UNP A0A1S4FIB3
D	-1	HIS	-	expression tag	UNP A0A1S4FIB3
D	0	MET	-	expression tag	UNP A0A1S4FIB3

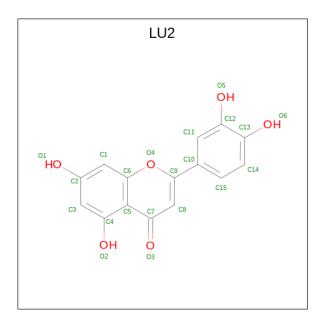
• Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Λ	1	Total	С	N	О	S	0	0
2	A	1	20	10	3	6	1	0	
2	B	1	Total	С	N	О	S	0	0
2	Ъ	1	20	10	3	6	1	0	
2	С	1	Total	С	N	О	S	0	0
2		1	20	10	3	6	1	0	
9	D	1	Total	С	N	О	S	0	1
	ע	1	40	20	6	12	2	0	1

• Molecule 3 is 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-chromen-4-one (three-letter code: LU2) (formula: $C_{15}H_{10}O_6$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Λ	1	Total C O	0	0
)	А	1	21 15 6	0	0
3	В	1	Total C O	0	0
)	Б	1	21 15 6	0	U
3	С	1	Total C O	0	0
)	C	1	21 15 6	0	0
3	D	1	Total C O	0	0
)	D	1	21 15 6	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Ca 4 4	0	0
4	В	1	Total Ca 1 1	0	0
4	С	1	Total Ca 1 1	0	0
4	D	2	Total Ca 2 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	201	Total O 201 201	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	209	Total O 209 209	0	0
5	С	221	Total O 221 221	0	0
5	D	213	Total O 213 213	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glutathione transferase

Chain A:

88%

88%

• Molecule 1: Glutathione transferase

Chain B:

92%

6%

• Molecule 1: Glutathione transferase

Chain C:

88%

• Molecule 1: Glutathione transferase

Chain C:

88%

7%

5%

• Molecule 1: Glutathione transferase

Chain C:

88%

• Molecule 1: Glutathione transferase

Chain D:

91%

• Molecule 1: Glutathione transferase



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	I 41 2 2	Depositor	
Cell constants	151.70Å 151.70Å 146.75Å	Donositon	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	36.69 - 1.50	Depositor	
Resolution (A)	47.97 - 1.50	EDS	
% Data completeness	100.0 (36.69-1.50)	Depositor	
(in resolution range)	$100.0 \ (47.97 - 1.50)$	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	3.26 (at 1.50Å)	Xtriage	
Refinement program	PHENIX 1.19_4092	Depositor	
D.D.	0.186 , 0.208	Depositor	
R, R_{free}	0.185 , 0.207	DCC	
R_{free} test set	6770 reflections (5.00%)	wwPDB-VP	
Wilson B-factor (Å ²)	18.2	Xtriage	
Anisotropy	0.115	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.35\;,52.7$	EDS	
L-test for twinning ²	$< L > = 0.51, < L^2> = 0.34$	Xtriage	
Estimated twinning fraction	0.000 for l,-k,h	Ytriago	
Estimated twinning fraction	0.004 for -h,-l,-k	Xtriage	
F_o, F_c correlation	0.97	EDS	
Total number of atoms	7838	wwPDB-VP	
Average B, all atoms (Å ²)	24.0	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 38.99 % 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 3.3950e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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



¹Intensities estimated from amplitudes.

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: LU2, CA, 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		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.37	0/1723	0.60	0/2346	
1	В	0.35	0/1750	0.59	0/2383	
1	С	0.36	0/1716	0.61	0/2338	
1	D	0.39	0/1762	0.59	0/2399	
All	All	0.37	0/6951	0.60	0/9466	

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1686	0	1628	12	0
1	В	1712	0	1668	8	0
1	С	1680	0	1653	12	0
1	D	1724	0	1671	9	0
2	A	20	0	15	0	0
2	В	20	0	15	0	0
2	С	20	0	15	0	0
2	D	40	0	30	0	0
3	A	21	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	21	0	10	1	0
3	С	21	0	10	1	0
3	D	21	0	10	0	0
4	A	4	0	0	0	0
4	В	1	0	0	0	0
4	С	1	0	0	0	0
4	D	2	0	0	0	0
5	A	201	0	0	2	0
5	В	209	0	0	3	0
5	С	221	0	0	1	0
5	D	213	0	0	2	0
All	All	7838	0	6735	43	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.

The worst 5 of 43 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:C:11:ILE:HD11	1:C:38:LEU:HD12	1.57	0.86	
1:A:113:GLU:HG2	1:A:168[B]:CYS:SG	2.22	0.79	
1:A:109:LEU:HG	1:A:168[B]:CYS:SG	2.30	0.72	
1:B:200:GLN:NE2	5:B:401:HOH:O	2.25	0.69	
1:D:113:GLU:OE2	1:D:117[A]:MET:HG3	1.98	0.64	

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	216/227 (95%)	211 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	voured Allowed		Percentiles	
1	В	221/227 (97%)	216 (98%)	5 (2%)	0	100	100
1	С	214/227 (94%)	207 (97%)	7 (3%)	0	100	100
1	D	223/227 (98%)	217 (97%)	6 (3%)	0	100	100
All	All	874/908 (96%)	851 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percen	ntiles
1	A	172/206 (84%)	172 (100%)	0	100	100
1	В	178/206~(86%)	178 (100%)	0	100	100
1	С	177/206 (86%)	177 (100%)	0	100	100
1	D	179/206 (87%)	179 (100%)	0	100	100
All	All	706/824~(86%)	706 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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, 8 are monoatomic - leaving 9 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	Peg	Res Link		ond leng	$\overline{ ext{gths}}$	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GSH	A	301	-	18,19,19	0.69	0	23,24,24	0.83	0
3	LU2	A	302	-	23,23,23	2.33	4 (17%)	34,34,34	1.38	4 (11%)
2	GSH	D	301[B]	-	18,19,19	0.71	0	23,24,24	0.72	0
2	GSH	С	301	-	18,19,19	0.67	0	23,24,24	0.77	0
3	LU2	D	302	-	23,23,23	2.05	5 (21%)	34,34,34	1.70	9 (26%)
2	GSH	D	301[A]	-	18,19,19	0.72	0	23,24,24	0.79	0
3	LU2	С	302	-	23,23,23	2.29	6 (26%)	34,34,34	1.31	4 (11%)
2	GSH	В	301	-	18,19,19	0.73	0	23,24,24	0.74	0
3	LU2	В	302	-	23,23,23	2.13	5 (21%)	34,34,34	1.35	5 (14%)

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	301	-	=	1/24/24/24	-
3	LU2	A	302	-	-	0/4/4/4	0/3/3/3
2	GSH	D	301[B]	-	-	1/24/24/24	-
2	GSH	С	301	-	-	1/24/24/24	-
3	LU2	D	302	-	-	0/4/4/4	0/3/3/3
2	GSH	D	301[A]	-	=	1/24/24/24	-
3	LU2	С	302	-	-	0/4/4/4	0/3/3/3
2	GSH	В	301	-	=	1/24/24/24	-
3	LU2	В	302	-	-	0/4/4/4	0/3/3/3



The worst	5	of	20	bond	length	outliers	are	listed	below:
110 110100	$\overline{}$	01		OIIG	10115011	Cattions	COL C	IID CCC	CIC III.

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
3	A	302	LU2	O4-C6	7.59	1.50	1.38
3	С	302	LU2	O4-C6	7.42	1.50	1.38
3	В	302	LU2	O4-C6	6.72	1.48	1.38
3	D	302	LU2	O4-C6	6.29	1.48	1.38
3	A	302	LU2	O4-C9	4.43	1.43	1.36

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	A	302	LU2	O4-C9-C10	5.15	119.70	111.92
3	С	302	LU2	O4-C9-C10	4.22	118.29	111.92
3	В	302	LU2	C9-C8-C7	-3.79	118.17	122.25
3	D	302	LU2	C10-C11-C12	-3.62	117.02	120.09
3	D	302	LU2	C15-C10-C11	3.54	123.43	119.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301[B]	GSH	N2-CA2-CB2-SG2
2	A	301	GSH	C3-CA3-N3-C2
2	D	301[A]	GSH	O12-C1-CA1-N1
2	В	301	GSH	C3-CA3-N3-C2
2	С	301	GSH	C3-CA3-N3-C2

There are no ring outliers.

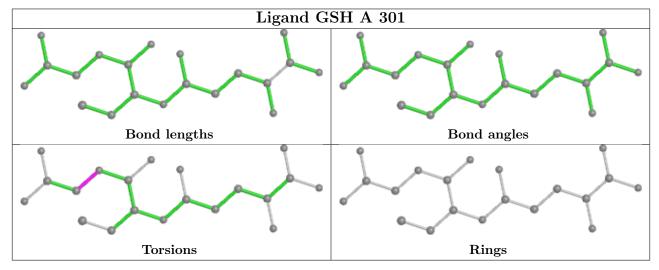
3 monomers are involved in 3 short contacts:

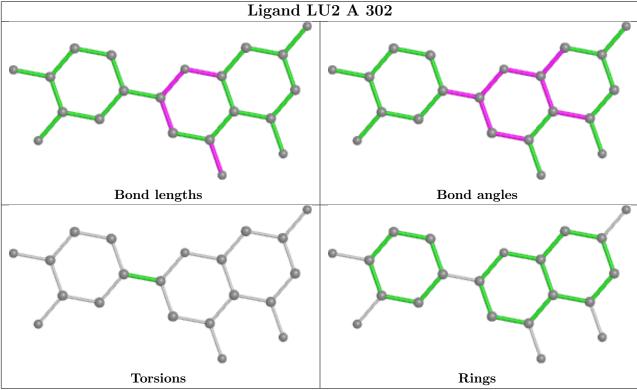
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	LU2	1	0
3	С	302	LU2	1	0
3	В	302	LU2	1	0

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

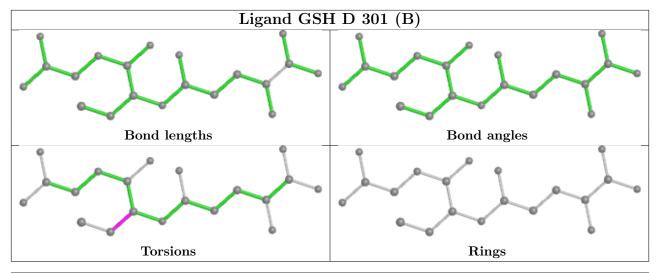


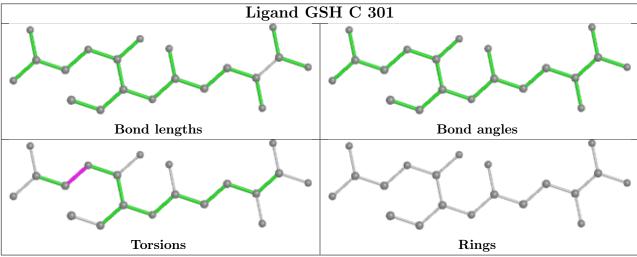
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



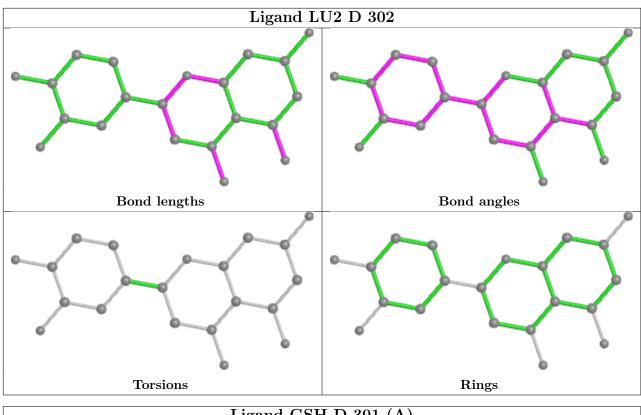


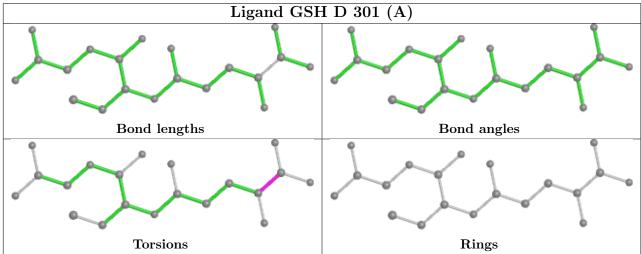




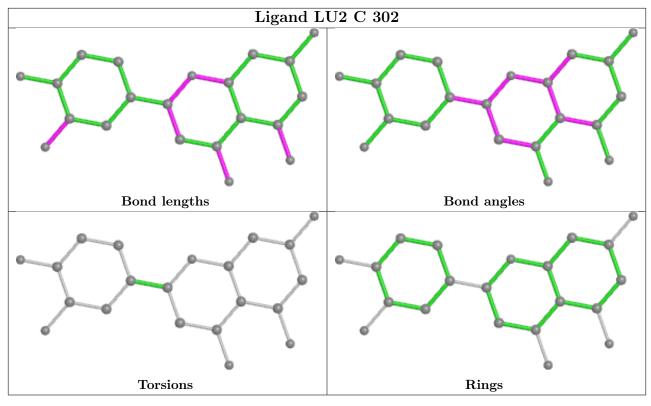


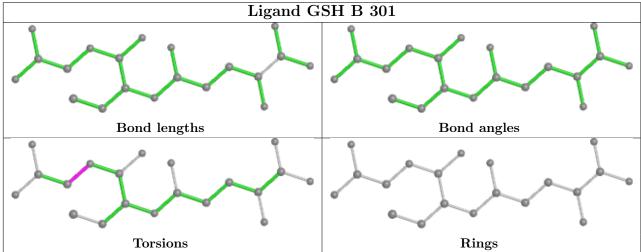




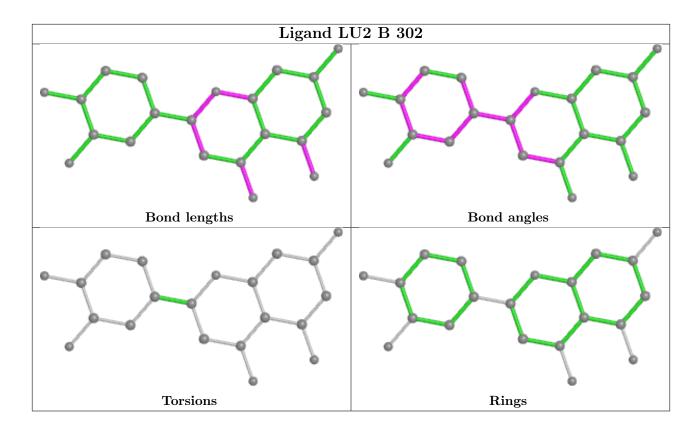












5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	$217/227 \ (95\%)$	-0.04	7 (3%) 47 52	13, 23, 51, 62	0
1	В	221/227 (97%)	-0.02	8 (3%) 42 47	14, 21, 48, 68	0
1	С	$216/227 \ (95\%)$	-0.08	6 (2%) 53 57	13, 21, 41, 51	0
1	D	221/227 (97%)	-0.14	1 (0%) 91 93	13, 21, 42, 57	0
All	All	875/908 (96%)	-0.07	22 (2%) 57 62	13, 21, 45, 68	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	126	VAL	4.4
1	В	127	THR	4.4
1	С	126	VAL	3.8
1	D	-2	VAL	3.6
1	В	121	ILE	3.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

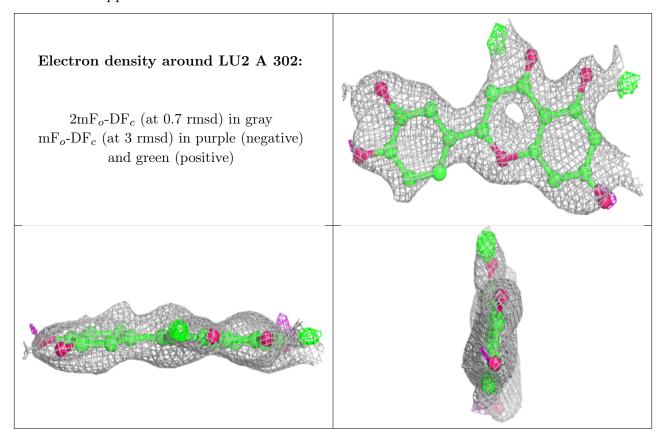
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.



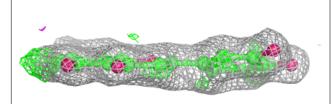
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$ extbf{B-factors}(extbf{A}^2)$	Q<0.9
4	CA	A	304	1/1	0.57	0.23	68,68,68,68	0
3	LU2	A	302	21/21	0.80	0.23	33,40,45,48	0
3	LU2	С	302	21/21	0.81	0.17	28,37,43,48	0
3	LU2	D	302	21/21	0.83	0.14	20,24,28,39	21
3	LU2	В	302	21/21	0.86	0.13	27,32,40,42	0
4	CA	В	303	1/1	0.93	0.08	24,24,24,24	1
2	GSH	D	301[A]	20/20	0.96	0.09	12,15,24,26	20
2	GSH	D	301[B]	20/20	0.96	0.09	13,15,22,24	20
2	GSH	A	301	20/20	0.96	0.08	14,17,29,35	0
4	CA	A	306	1/1	0.96	0.06	26,26,26,26	1
2	GSH	В	301	20/20	0.96	0.06	14,17,28,32	0
4	CA	С	303	1/1	0.96	0.06	22,22,22,22	1
2	GSH	С	301	20/20	0.97	0.06	13,18,27,34	0
4	CA	A	305	1/1	0.98	0.04	24,24,24,24	1
4	CA	D	303	1/1	0.98	0.07	20,20,20,20	1
4	CA	D	304	1/1	0.98	0.06	21,21,21,21	1
4	CA	A	303	1/1	0.99	0.07	18,18,18,18	1

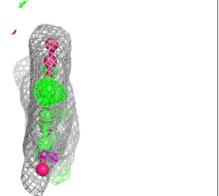
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



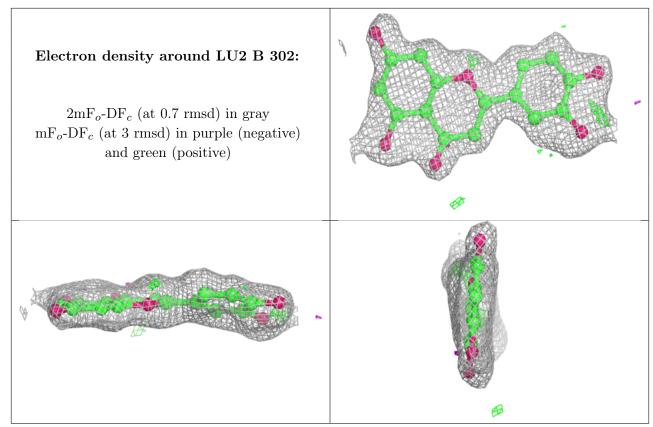


Electron density around LU2 C 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive) Electron density around LU2 D 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)















6.5 Other polymers (i)

There are no such residues in this entry.

