Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 07:24 PM EDT

PDB ID	:	6PSG
Title	:	Crystal Structure of Class D Beta-lactamase OXA-48 with Faropenem
Authors	:	Akhtar, A.; Chen, Y.
Deposited on	:	2019-07-12
Resolution	:	2.13 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*
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 (i)) 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	:	FAILED
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)	:	2.35.1

PERCENTILES INFOmissingINFO

1 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8491 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 Class D Carbapenemase OXA-48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			2019	1288	355	369	7			
1	B	246	Total	C	N	O	S	0	0	0
			2012	1286	353	366	7			
1	C	249	Total	C	N	O	S	0	0	0
			2042	1302	360	373	7			
1	D	244	Total	C	N	O	S	0	0	0
			1992	1271	351	363	7			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	initiating methionine	UNP A0A482LRD5
A	4	LYS	-	expression tag	UNP A0A482LRD5
A	5	HIS	-	expression tag	UNP A0A482LRD5
A	6	HIS	-	expression tag	UNP A0A482LRD5
A	7	HIS	-	expression tag	UNP A0A482LRD5
A	8	HIS	-	expression tag	UNP A0A482LRD5
A	9	HIS	-	expression tag	UNP A0A482LRD5
A	10	HIS	-	expression tag	UNP A0A482LRD5
A	11	MET	-	expression tag	UNP A0A482LRD5
A	12	HIS	-	expression tag	UNP A0A482LRD5
A	13	HIS	-	expression tag	UNP A0A482LRD5
A	14	HIS	-	expression tag	UNP A0A482LRD5
A	15	HIS	-	expression tag	UNP A0A482LRD5
A	16	HIS	-	expression tag	UNP A0A482LRD5
A	17	HIS	-	expression tag	UNP A0A482LRD5
A	18	GLU	-	expression tag	UNP A0A482LRD5
A	19	ASN	-	expression tag	UNP A0A482LRD5
A	20	LEU	-	expression tag	UNP A0A482LRD5
A	21	TYR	-	expression tag	UNP A0A482LRD5
A	22	PHE	-	expression tag	UNP A0A482LRD5
A	23	GLN	-	expression tag	UNP A0A482LRD5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP A0A482LRD5
B	3	MET	-	initiating methionine	UNP A0A482LRD5
B	4	LYS	-	expression tag	UNP A0A482LRD5
B	5	HIS	-	expression tag	UNP A0A482LRD5
B	6	HIS	-	expression tag	UNP A0A482LRD5
B	7	HIS	-	expression tag	UNP A0A482LRD5
B	8	HIS	-	expression tag	UNP A0A482LRD5
B	9	HIS	-	expression tag	UNP A0A482LRD5
B	10	HIS	-	expression tag	UNP A0A482LRD5
B	11	MET	-	expression tag	UNP A0A482LRD5
B	12	HIS	-	expression tag	UNP A0A482LRD5
B	13	HIS	-	expression tag	UNP A0A482LRD5
B	14	HIS	-	expression tag	UNP A0A482LRD5
B	15	HIS	-	expression tag	UNP A0A482LRD5
B	16	HIS	-	expression tag	UNP A0A482LRD5
B	17	HIS	-	expression tag	UNP A0A482LRD5
B	18	GLU	-	expression tag	UNP A0A482LRD5
B	19	ASN	-	expression tag	UNP A0A482LRD5
B	20	LEU	-	expression tag	UNP A0A482LRD5
B	21	TYR	-	expression tag	UNP A0A482LRD5
B	22	PHE	-	expression tag	UNP A0A482LRD5
B	23	GLN	-	expression tag	UNP A0A482LRD5
B	24	GLY	-	expression tag	UNP A0A482LRD5
C	3	MET	-	initiating methionine	UNP A0A482LRD5
C	4	LYS	-	expression tag	UNP A0A482LRD5
C	5	HIS	-	expression tag	UNP A0A482LRD5
C	6	HIS	-	expression tag	UNP A0A482LRD5
C	7	HIS	-	expression tag	UNP A0A482LRD5
C	8	HIS	-	expression tag	UNP A0A482LRD5
C	9	HIS	-	expression tag	UNP A0A482LRD5
C	10	HIS	-	expression tag	UNP A0A482LRD5
C	11	MET	-	expression tag	UNP A0A482LRD5
C	12	HIS	-	expression tag	UNP A0A482LRD5
C	13	HIS	-	expression tag	UNP A0A482LRD5
C	14	HIS	-	expression tag	UNP A0A482LRD5
C	15	HIS	-	expression tag	UNP A0A482LRD5
C	16	HIS	-	expression tag	UNP A0A482LRD5
C	17	HIS	-	expression tag	UNP A0A482LRD5
C	18	GLU	-	expression tag	UNP A0A482LRD5
C	19	ASN	-	expression tag	UNP A0A482LRD5
C	20	LEU	-	expression tag	UNP A0A482LRD5
C	21	TYR	-	expression tag	UNP A0A482LRD5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	PHE	-	expression tag	UNP A0A482LRD5
C	23	GLN	-	expression tag	UNP A0A482LRD5
C	24	GLY	-	expression tag	UNP A0A482LRD5
D	3	MET	-	initiating methionine	UNP A0A482LRD5
D	4	LYS	-	expression tag	UNP A0A482LRD5
D	5	HIS	-	expression tag	UNP A0A482LRD5
D	6	HIS	-	expression tag	UNP A0A482LRD5
D	7	HIS	-	expression tag	UNP A0A482LRD5
D	8	HIS	-	expression tag	UNP A0A482LRD5
D	9	HIS	-	expression tag	UNP A0A482LRD5
D	10	HIS	-	expression tag	UNP A0A482LRD5
D	11	MET	-	expression tag	UNP A0A482LRD5
D	12	HIS	-	expression tag	UNP A0A482LRD5
D	13	HIS	-	expression tag	UNP A0A482LRD5
D	14	HIS	-	expression tag	UNP A0A482LRD5
D	15	HIS	-	expression tag	UNP A0A482LRD5
D	16	HIS	-	expression tag	UNP A0A482LRD5
D	17	HIS	-	expression tag	UNP A0A482LRD5
D	18	GLU	-	expression tag	UNP A0A482LRD5
D	19	ASN	-	expression tag	UNP A0A482LRD5
D	20	LEU	-	expression tag	UNP A0A482LRD5
D	21	TYR	-	expression tag	UNP A0A482LRD5
D	22	PHE	-	expression tag	UNP A0A482LRD5
D	23	GLN	-	expression tag	UNP A0A482LRD5
D	24	GLY	-	expression tag	UNP A0A482LRD5

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0
2	C	1	Total 1	Cl 1	0	0

- Molecule 3 is (2R,5R)-2-[(2S,3R)-3-hydroxy-1-oxobutan-2-yl]-5-[(2R)-tetrahydrofuran-2-yl]-2,5-dihydro-1,3-thiazole-4-carboxylic acid (three-letter code: DGF) (formula: $C_{12}H_{17}NO_5S$) (labeled as "Ligand of Interest" by depositor).

DGF
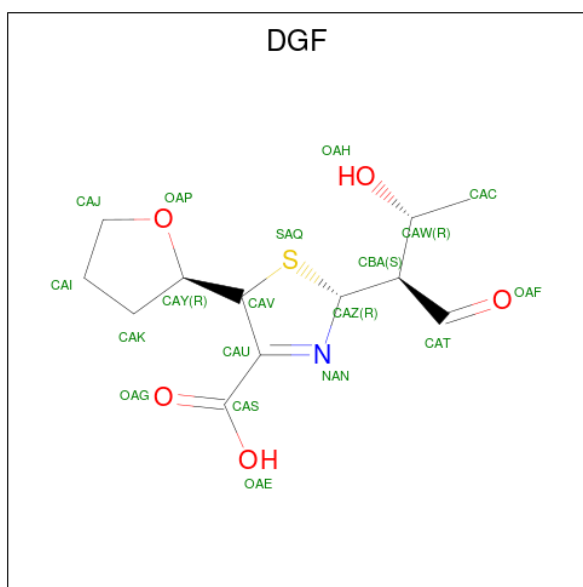
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			19	12	1	5	1		
3	B	1	Total	C	N	O	S	0	0
			19	12	1	5	1		
3	C	1	Total	C	N	O	S	0	0
			19	12	1	5	1		
3	D	1	Total	C	N	O	S	0	0
			19	12	1	5	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total 90	O 90	0	0
5	B	84	Total 84	O 84	0	0
5	C	84	Total 84	O 84	0	0
5	D	84	Total 84	O 84	0	0

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.55Å 106.67Å 96.26Å 90.00° 104.19° 90.00°	Depositor
Resolution (Å)	35.12 – 2.13	Depositor
% Data completeness (in resolution range)	98.0 (35.12-2.13)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.171 , 0.220	Depositor
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.243	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8491	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

3 Model quality (i)

3.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DGF, CL, GOL

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	0.43	0/2070	0.55	0/2801
1	B	0.42	0/2063	0.55	0/2790
1	C	0.47	0/2094	0.56	0/2832
1	D	0.41	0/2042	0.54	0/2761
All	All	0.43	0/8269	0.55	0/11184

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

3.2 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	2019	0	1962	11	0
1	B	2012	0	1963	9	0
1	C	2042	0	1986	11	0
1	D	1992	0	1943	11	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	19	0	0	0	0
3	B	19	0	0	0	0
3	C	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	19	0	0	0	0
4	C	6	0	8	0	0
5	A	90	0	0	1	0
5	B	84	0	0	0	0
5	C	84	0	0	0	0
5	D	84	0	0	0	0
All	All	8491	0	7862	42	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 (42) 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:D:23:GLN:HG3	1:D:53:GLN:HE21	1.62	0.64
1:C:28:ASN:OD1	1:C:30:SER:HB3	2.01	0.61
1:C:139:LEU:HD12	1:C:149:ILE:HD11	1.87	0.56
1:C:31:TRP:HB2	1:C:57:ASN:HB3	1.88	0.55
1:B:31:TRP:HB2	1:B:57:ASN:HB3	1.90	0.54
1:D:23:GLN:HB2	1:D:53:GLN:HG2	1.90	0.53
1:A:28:ASN:OD1	1:A:30:SER:HB3	2.09	0.53
1:B:136:SER:OG	1:B:149:ILE:HG12	2.09	0.53
1:C:230:ASP:N	1:C:230:ASP:OD1	2.42	0.52
1:D:255:LYS:O	1:D:259:LYS:HG3	2.09	0.52
1:C:69:ALA:HB2	1:C:212:SER:HB2	1.93	0.50
1:C:220:GLY:O	1:C:238:ASN:HA	2.12	0.50
1:D:29:LYS:HE3	1:D:32:ASN:OD1	2.11	0.50
1:C:49:GLU:OE1	1:C:174:ARG:NH2	2.46	0.49
1:A:134:ARG:HA	1:A:137:LYS:HE3	1.95	0.49
1:B:125:GLU:O	1:B:129:GLN:HG3	2.13	0.48
1:D:148:ASP:H	1:D:162:ILE:HD12	1.79	0.48
1:A:214:ARG:O	1:A:215:ILE:HD13	2.15	0.47
1:D:140:HIS:HA	1:D:147:GLU:HG2	1.96	0.47
1:A:230:ASP:N	1:A:230:ASP:OD1	2.45	0.46
1:D:133:ALA:O	1:D:137:LYS:HE2	2.14	0.46
1:B:65:ALA:HB1	1:B:163:ARG:HB3	1.96	0.46
1:D:31:TRP:HB2	1:D:57:ASN:HB3	1.97	0.45
1:B:48:ASN:HB2	1:B:233:TRP:CH2	2.52	0.45
1:D:133:ALA:O	1:D:137:LYS:HG2	2.17	0.45
1:B:205:ILE:HG12	1:B:226:VAL:HG22	1.99	0.44
1:C:124:GLN:HB3	1:C:154:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASN:ND2	1:A:230:ASP:O	2.45	0.44
1:A:177:TYR:CZ	1:A:232:VAL:HG21	2.54	0.43
1:C:102:ILE:HD12	1:C:105:TRP:CZ2	2.53	0.43
1:A:128:ARG:NH2	5:A:404:HOH:O	2.51	0.43
1:D:177:TYR:CZ	1:D:232:VAL:HG21	2.54	0.42
1:A:34:HIS:NE2	1:A:260:GLN:OE1	2.47	0.42
1:B:220:GLY:O	1:B:238:ASN:HA	2.18	0.42
1:C:170:ILE:HD13	1:C:234:PHE:HB3	2.00	0.42
1:A:204:ILE:HB	1:A:227:GLU:HB2	2.02	0.41
1:B:261:GLU:HB2	1:B:263:ILE:HD12	2.03	0.41
1:B:45:VAL:O	1:B:235:PHE:HA	2.21	0.41
1:A:94:LYS:NZ	1:A:94:LYS:HB3	2.35	0.41
1:C:204:ILE:HB	1:C:227:GLU:HB2	2.03	0.41
1:A:157:TRP:HA	1:A:162:ILE:CG2	2.52	0.40
1:D:45:VAL:O	1:D:235:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

3.3 Torsion angles ⓘ

3.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

3.3.2 Protein sidechains ⓘ

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

3.3.3 RNA ⓘ

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

3.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

3.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#|Z| > 2$
3	DGF	D	301	1	15,20,20	0.95	0	11,28,28	0.77	0
3	DGF	B	301	1	15,20,20	0.89	1 (6%)	11,28,28	1.10	2 (18%)
3	DGF	C	302	1	15,20,20	0.78	0	11,28,28	0.99	0
3	DGF	A	302	1	15,20,20	0.87	0	11,28,28	0.91	0
4	GOL	C	303	-	5,5,5	0.75	0	5,5,5	1.02	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
3	DGF	D	301	1	-	2/12/37/37	0/2/2/2
3	DGF	B	301	1	-	2/12/37/37	0/2/2/2
3	DGF	C	302	1	-	2/12/37/37	0/2/2/2
3	DGF	A	302	1	-	2/12/37/37	0/2/2/2
4	GOL	C	303	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	DGF	CBA-CAW	-2.03	1.51	1.54

All (2) bond angle outliers are listed below:

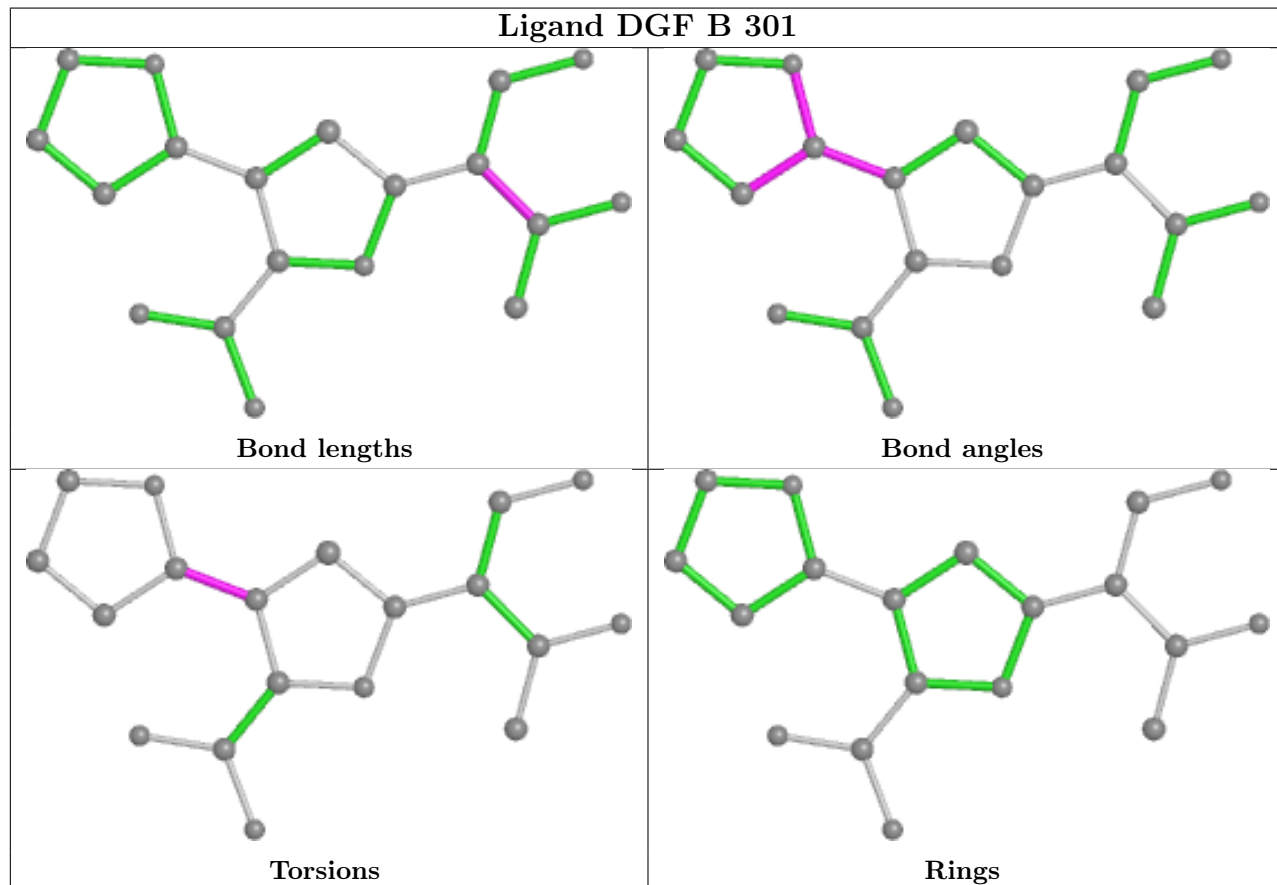| Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	DGF	CAK-CAY-CAV	-2.07	111.71	114.33
3	B	301	DGF	OAP-CAY-CAV	2.01	113.45	109.26

There are no chirality outliers.
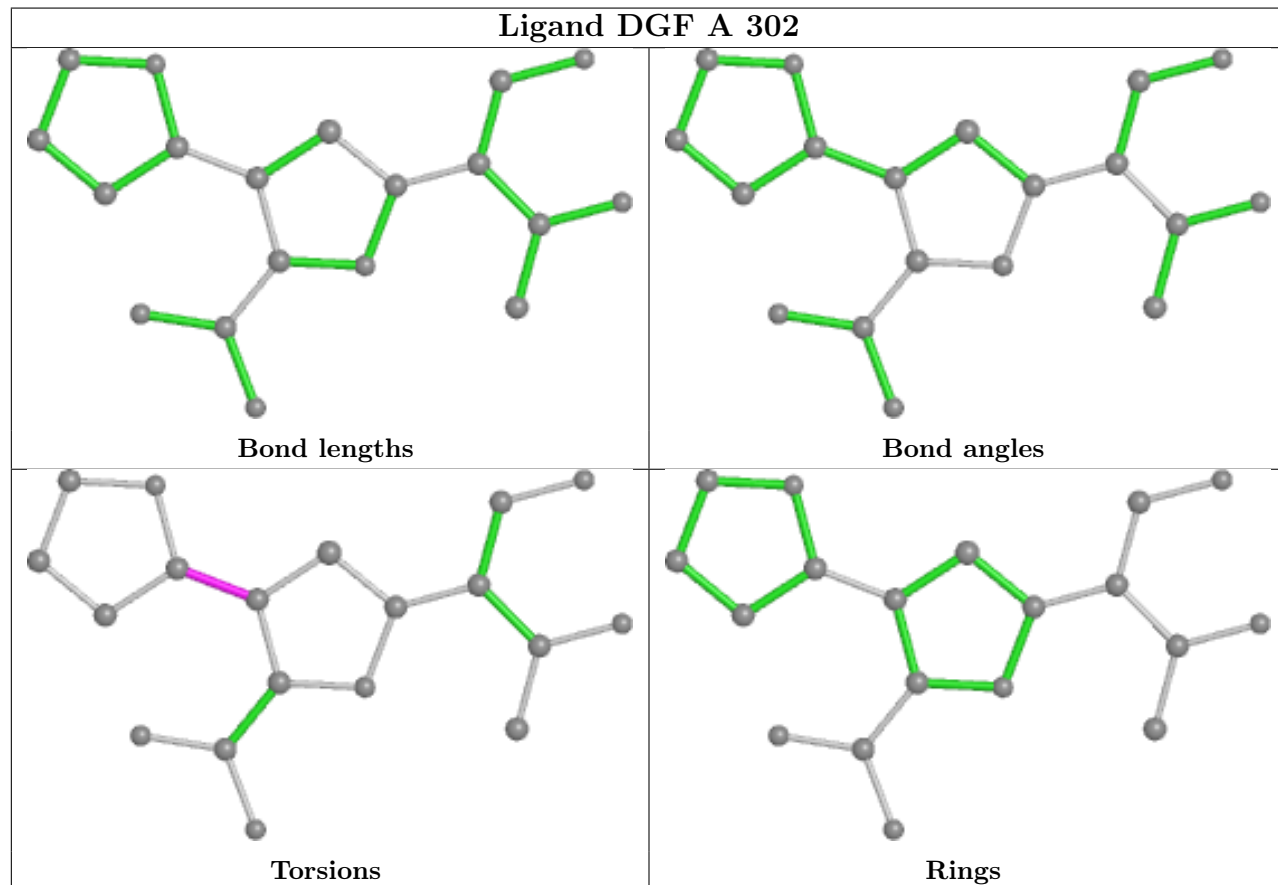
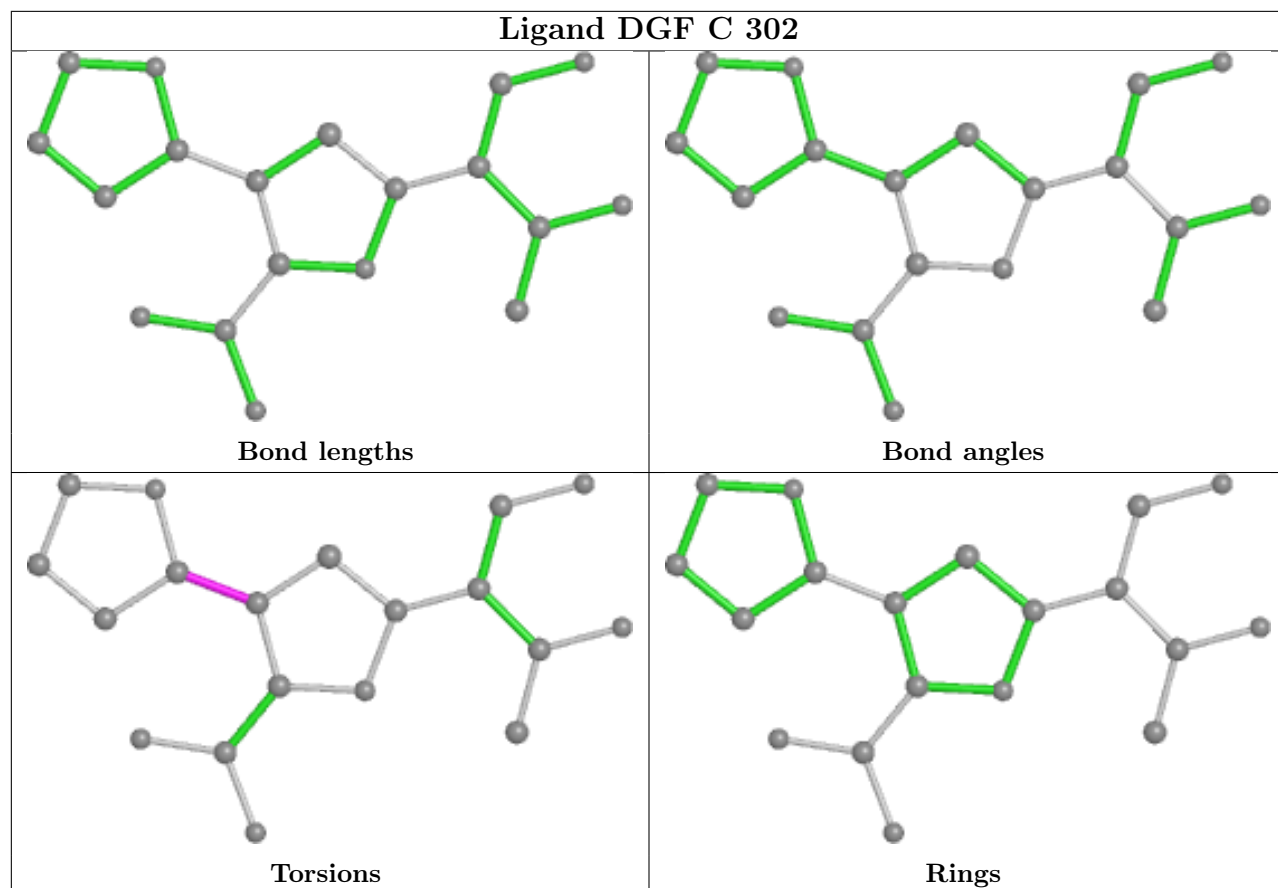All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	DGF	CAU-CAV-CAY-CAK
3	A	302	DGF	CAU-CAV-CAY-OAP
3	B	301	DGF	CAU-CAV-CAY-CAK
3	B	301	DGF	CAU-CAV-CAY-OAP
3	C	302	DGF	CAU-CAV-CAY-CAK
3	C	302	DGF	CAU-CAV-CAY-OAP
3	D	301	DGF	CAU-CAV-CAY-CAK
3	D	301	DGF	CAU-CAV-CAY-OAP
4	C	303	GOL	O1-C1-C2-O2
4	C	303	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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.

Ligand DGF D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand DGF B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand DGF C 302

Bond lengths

Bond angles

Torsions

Rings

Ligand DGF A 302

Bond lengths

Bond angles

Torsions

Rings
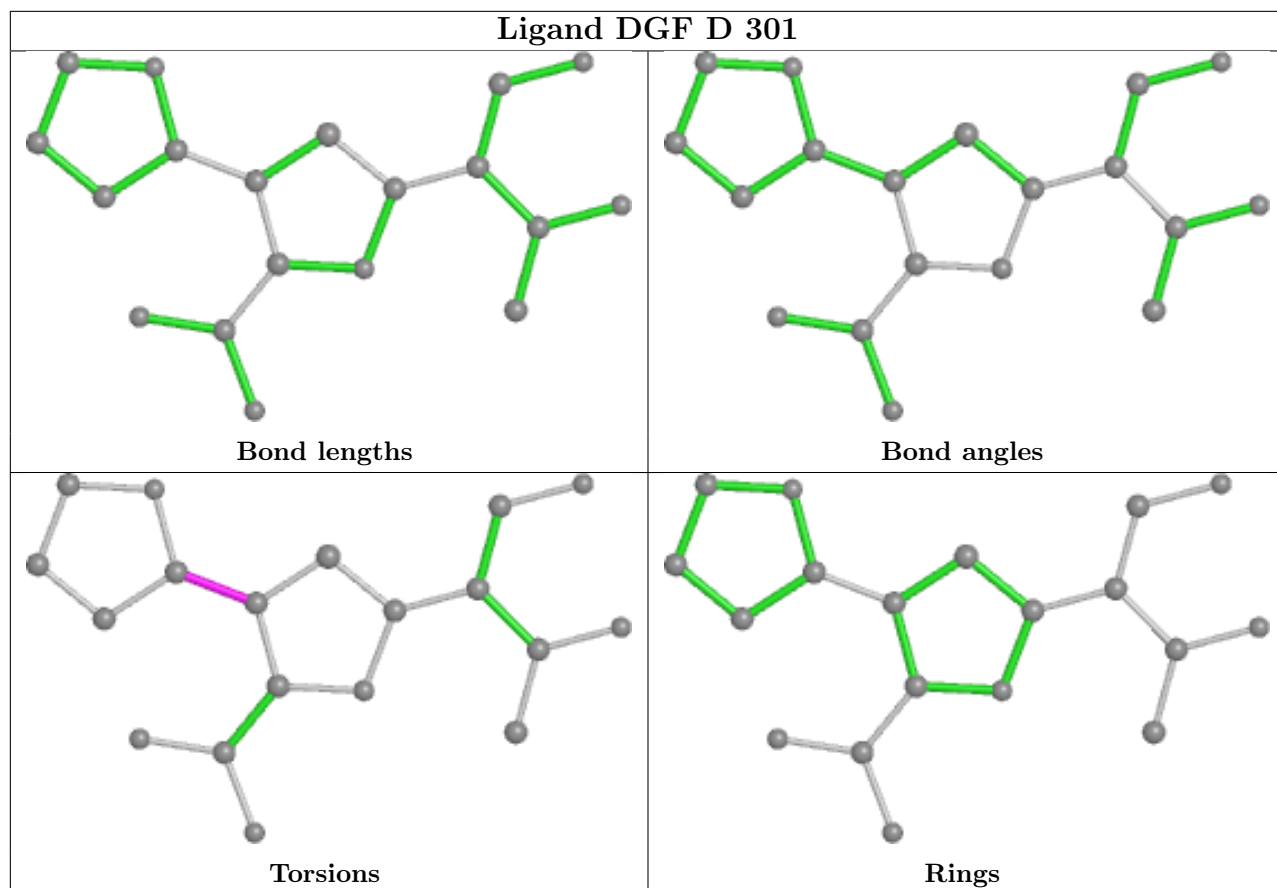
3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4   Fit of model and data ⓘ

4.1   Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

4.2   Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

4.3   Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

4.4   Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

4.5   Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.