



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 07:32 PM EDT

PDB ID : 4EBL  
Title : BlaC E166A Faropenem Acyl-Intermediate Complex  
Authors : Mire, J.A.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2012-03-23  
Resolution : 2.10 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](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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

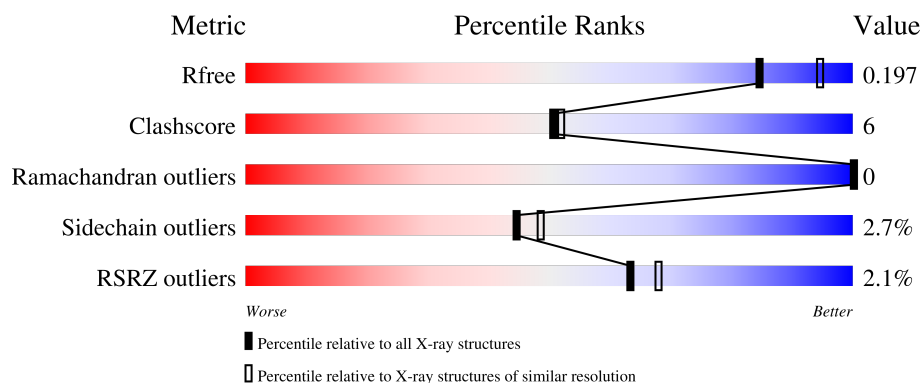
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\leq 5\%$ . 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	265	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	265	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	265	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	265	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </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
2	PO4	C	302	-	X	-	-
3	DGF	B	302	X	-	-	-
3	DGF	C	303	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8380 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			1970	1235	346	383	6			
1	B	265	Total	C	N	O	S	0	0	0
			1948	1224	342	376	6			
1	C	265	Total	C	N	O	S	0	0	0
			1974	1236	349	383	6			
1	D	265	Total	C	N	O	S	0	0	0
			1982	1240	351	385	6			

There are 4 discrepancies between the modelled and reference sequences:

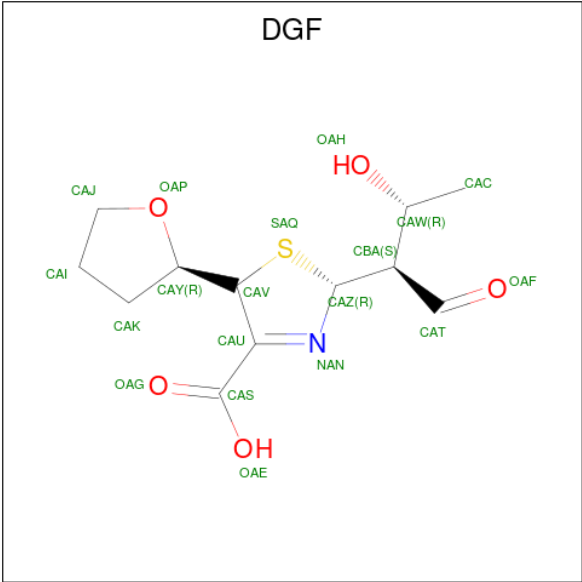
Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ALA	GLU	ENGINEERED MUTATION	UNP P0C5C1
B	166	ALA	GLU	ENGINEERED MUTATION	UNP P0C5C1
C	166	ALA	GLU	ENGINEERED MUTATION	UNP P0C5C1
D	166	ALA	GLU	ENGINEERED MUTATION	UNP P0C5C1

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- 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<sub>12</sub>H<sub>17</sub>NO<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	111	Total	O	0	0
			111	111		
4	C	106	Total	O	0	0
			106	106		
4	D	88	Total	O	0	0
			88	88		

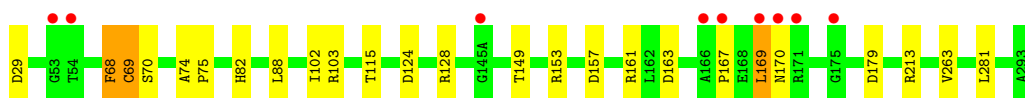
### 3 Residue-property plots [i](#)

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: Beta-lactamase



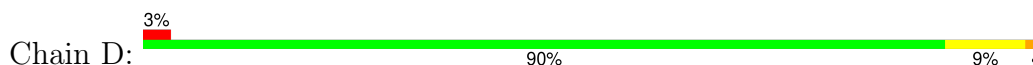
- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.79Å 96.95Å 109.53Å 90.00° 107.95° 90.00°	Depositor
Resolution (Å)	46.86 – 2.10 46.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (46.86-2.10) 98.1 (46.86-2.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.173 , 0.204 0.169 , 0.197	Depositor DCC
$R_{free}$ test set	4474 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, DGF

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	0.72	0/2009	0.81	1/2745 (0.0%)
1	B	0.65	1/1987 (0.1%)	0.72	2/2718 (0.1%)
1	C	0.67	1/2013 (0.0%)	0.74	2/2750 (0.1%)
1	D	0.61	0/2021	0.71	2/2760 (0.1%)
All	All	0.66	2/8030 (0.0%)	0.74	7/10973 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	70	SER	C-N	7.04	1.50	1.34
1	B	70	SER	C-N	6.77	1.49	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	CYS	O-C-N	-7.71	110.36	122.70
1	B	69	CYS	C-N-CA	7.61	140.73	121.70
1	A	153	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	277	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	69	CYS	CA-C-N	5.25	128.76	117.20
1	B	69	CYS	CA-C-N	5.25	128.75	117.20
1	D	222	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1970	0	1929	21	0
1	B	1948	0	1903	34	0
1	C	1974	0	1939	16	0
1	D	1982	0	1948	20	0
2	A	15	0	0	0	0
2	B	5	0	0	1	0
2	C	10	0	0	2	0
2	D	10	0	0	0	0
3	B	19	0	0	2	0
3	C	19	0	0	2	0
4	A	123	0	0	1	0
4	B	111	0	0	5	0
4	C	106	0	0	1	0
4	D	88	0	0	2	0
All	All	8380	0	7719	89	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 6.

All (89) 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:B:169:LEU:O	1:B:169:LEU:HD13	1.39	1.21
1:B:169:LEU:HD13	1:B:169:LEU:C	1.76	1.05
1:B:169:LEU:C	1:B:169:LEU:CD1	2.30	1.00
1:D:263:VAL:HG12	1:D:281:LEU:HD22	1.54	0.88
1:D:104:SER:HB3	1:D:167:PRO:HB3	1.54	0.88
1:D:103:ARG:HH11	1:D:103:ARG:HG2	1.41	0.84
3:C:303:DGF:OAE	3:C:303:DGF:CAK	2.30	0.78
1:B:74:ALA:HB3	1:B:75:PRO:CD	2.16	0.76
1:B:169:LEU:HD22	1:B:179:ASP:OD2	1.87	0.73
1:A:263:VAL:HG12	1:A:281:LEU:HD22	1.69	0.72
3:B:302:DGF:OAE	3:B:302:DGF:CAK	2.36	0.72
1:B:169:LEU:HD21	1:B:179:ASP:HB3	1.74	0.70
1:B:169:LEU:HD22	1:B:179:ASP:CG	2.12	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LEU:O	1:B:169:LEU:CD1	2.30	0.69
1:B:169:LEU:CD2	1:B:179:ASP:CG	2.63	0.68
1:B:169:LEU:CD2	1:B:179:ASP:HB3	2.25	0.66
1:B:169:LEU:CD2	1:B:179:ASP:CB	2.74	0.65
1:C:74:ALA:HB3	1:C:75:PRO:CD	2.25	0.65
1:D:220:ARG:HG2	1:D:281:LEU:HD12	1.78	0.65
1:A:263:VAL:CG1	1:A:281:LEU:HD22	2.27	0.65
1:B:169:LEU:CD1	4:B:497:HOH:O	2.45	0.64
1:B:169:LEU:HD11	4:B:497:HOH:O	1.98	0.63
3:B:302:DGF:OAE	3:B:302:DGF:CAY	2.44	0.63
2:C:302:PO4:O3	1:D:171:ARG:NH2	2.30	0.62
1:A:220:ARG:HG2	1:A:281:LEU:HD12	1.81	0.62
3:C:303:DGF:OAE	3:C:303:DGF:CAY	2.44	0.62
1:D:103:ARG:HG2	1:D:103:ARG:NH1	2.15	0.62
1:D:263:VAL:CG1	1:D:281:LEU:HD22	2.27	0.61
1:A:33:ARG:NH1	1:C:290:GLY:O	2.31	0.60
1:B:74:ALA:HB3	1:B:75:PRO:HD3	1.83	0.60
1:C:118:THR:OG1	1:C:121:GLN:HG3	2.01	0.60
1:D:128:ARG:HD2	1:D:213:ARG:O	2.02	0.59
1:A:65:ARG:HD2	1:A:177:GLU:HG2	1.86	0.58
1:A:104:SER:HB2	1:A:167:PRO:HB3	1.86	0.57
1:B:82:HIS:ND1	4:B:502:HOH:O	2.32	0.56
1:B:169:LEU:C	1:B:169:LEU:HD12	2.24	0.56
1:C:220:ARG:HD3	1:C:281:LEU:HD12	1.89	0.54
1:B:169:LEU:HD21	4:B:454:HOH:O	2.08	0.53
1:A:102:ILE:HD11	1:A:113:VAL:CG2	2.38	0.53
1:B:74:ALA:CB	1:B:75:PRO:CD	2.86	0.52
1:B:263:VAL:HG12	1:B:281:LEU:HD22	1.91	0.51
1:B:153:ARG:HD3	1:B:157:ASP:O	2.09	0.51
1:C:74:ALA:HB3	1:C:75:PRO:HD3	1.91	0.51
1:A:65:ARG:CD	1:A:177:GLU:HG2	2.41	0.50
1:D:82:HIS:ND1	4:D:483:HOH:O	2.35	0.49
1:A:105:ILE:HG23	1:B:102:ILE:HG21	1.93	0.49
1:C:124:ASP:OD2	2:C:301:PO4:O1	2.31	0.49
1:A:275:GLU:HB3	1:B:115:THR:HG22	1.94	0.49
1:C:128:ARG:HD2	1:C:213:ARG:O	2.13	0.49
1:A:178:ARG:CB	1:A:178:ARG:HH11	2.26	0.48
1:B:263:VAL:CG1	1:B:281:LEU:HD22	2.42	0.48
4:C:475:HOH:O	1:D:278:GLU:HG3	2.14	0.47
1:B:169:LEU:HD22	1:B:179:ASP:CB	2.42	0.47
1:B:161:ARG:O	1:B:179:ASP:HA	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:SER:CB	1:D:167:PRO:HB3	2.34	0.47
1:B:74:ALA:HB3	1:B:75:PRO:HD2	1.92	0.46
1:A:105:ILE:HG12	1:B:102:ILE:HG13	1.96	0.45
1:D:220:ARG:HE	1:D:278:GLU:HG2	1.81	0.45
1:C:74:ALA:CB	1:C:75:PRO:CD	2.93	0.45
1:C:113:VAL:HG21	1:D:105:ILE:HD11	1.98	0.45
1:A:178:ARG:HH11	1:A:178:ARG:HB2	1.81	0.45
1:B:169:LEU:HD12	1:B:170:ASN:N	2.32	0.44
1:B:124:ASP:OD2	2:B:301:PO4:O4	2.35	0.44
1:A:30:LEU:HD22	1:A:291:VAL:HG21	2.00	0.44
1:C:72:PHE:O	1:C:75:PRO:HG2	2.17	0.44
1:A:275:GLU:HA	1:A:276:PRO:HD3	1.87	0.44
1:D:229:TRP:CE3	1:D:252:SER:HA	2.54	0.43
1:B:103:ARG:O	1:B:167:PRO:HG3	2.18	0.43
1:A:178:ARG:NH1	4:A:522:HOH:O	2.52	0.43
1:B:169:LEU:HD13	4:B:497:HOH:O	2.12	0.43
1:A:104:SER:OG	1:A:105:ILE:N	2.51	0.42
1:A:110:GLN:O	1:A:110:GLN:HG3	2.19	0.42
1:C:263:VAL:HG12	1:C:281:LEU:HD22	2.00	0.42
1:C:74:ALA:HB3	1:C:75:PRO:HD2	2.01	0.42
1:D:103:ARG:HD3	4:D:435:HOH:O	2.19	0.42
1:B:128:ARG:HD2	1:B:213:ARG:O	2.19	0.42
1:D:131:ASP:HB3	1:D:134:ALA:HB3	2.02	0.42
1:A:105:ILE:HG22	1:A:107:PRO:HD3	2.01	0.41
1:D:44:ARG:O	1:D:265:SER:HA	2.20	0.41
1:D:99:SER:HA	1:D:102:ILE:HD12	2.02	0.41
1:A:105:ILE:HG23	1:B:102:ILE:CG2	2.51	0.41
1:C:68:PHE:HB2	1:C:179:ASP:O	2.20	0.41
1:D:172:ASP:OD1	1:D:179:ASP:OD2	2.38	0.41
1:C:122:LEU:HD22	1:C:134:ALA:HA	2.03	0.41
1:C:166:ALA:HA	1:C:167:PRO:HA	1.79	0.41
1:D:104:SER:HB2	1:D:105:ILE:H	1.65	0.41
1:B:68:PHE:O	1:B:69:CYS:HB2	2.22	0.40
1:A:233:ASP:OD2	1:A:246:ASP:OD1	2.38	0.40
1:C:172:ASP:OD2	1:C:179:ASP:OD2	2.40	0.40

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 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	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	B	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	C	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	D	263/265 (99%)	257 (98%)	6 (2%)	0	100	100
All	All	1052/1060 (99%)	1034 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	197/201 (98%)	192 (98%)	5 (2%)	47	52
1	B	193/201 (96%)	187 (97%)	6 (3%)	40	43
1	C	199/201 (99%)	196 (98%)	3 (2%)	65	71
1	D	200/201 (100%)	193 (96%)	7 (4%)	36	38
All	All	789/804 (98%)	768 (97%)	21 (3%)	44	48

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	93	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	165	GLU
1	A	178	ARG
1	A	233	ASP
1	B	29	ASP
1	B	68	PHE
1	B	88	LEU
1	B	149	THR
1	B	163	ASP
1	B	169	LEU
1	C	29	ASP
1	C	68	PHE
1	C	88	LEU
1	D	88	LEU
1	D	99	SER
1	D	100	ASP
1	D	103	ARG
1	D	104	SER
1	D	233	ASP
1	D	277	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	111	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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
2	PO4	B	301	-	4,4,4	0.77	0	6,6,6	0.52	0
3	DGF	B	302	1	14,20,20	3.41	2 (14%)	14,28,28	1.63	3 (21%)
2	PO4	C	302	-	4,4,4	3.06	4 (100%)	6,6,6	0.46	0
2	PO4	C	301	-	4,4,4	0.86	0	6,6,6	0.48	0
2	PO4	D	301	-	4,4,4	1.04	0	6,6,6	0.43	0
2	PO4	A	302	-	4,4,4	0.90	0	6,6,6	0.57	0
2	PO4	D	302	-	4,4,4	0.94	0	6,6,6	0.68	0
2	PO4	A	301	-	4,4,4	1.84	2 (50%)	6,6,6	0.66	0
2	PO4	A	303	-	4,4,4	0.77	0	6,6,6	0.60	0
3	DGF	C	303	1	14,20,20	3.38	3 (21%)	14,28,28	1.64	3 (21%)

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	B	302	1	1/1/7/8	0/12/37/37	0/2/2/2
3	DGF	C	303	1	1/1/7/8	1/12/37/37	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	DGF	CAS-CAU	-8.78	1.33	1.48
3	C	303	DGF	CAS-CAU	-8.74	1.33	1.48
3	B	302	DGF	CAU-NAN	8.64	1.35	1.28
3	C	303	DGF	CAU-NAN	8.47	1.34	1.28
2	C	302	PO4	P-O1	4.69	1.61	1.50
2	A	301	PO4	P-O2	-2.48	1.47	1.54
2	C	302	PO4	P-O3	2.36	1.61	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	PO4	P-O2	2.35	1.61	1.54
2	A	301	PO4	P-O3	-2.25	1.48	1.54
2	C	302	PO4	P-O4	-2.13	1.48	1.54
3	C	303	DGF	CBA-CAT	2.04	1.53	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	DGF	CAK-CAY-CAV	-3.86	109.22	114.00
3	B	302	DGF	CAK-CAY-CAV	-3.78	109.31	114.00
3	B	302	DGF	CAJ-OAP-CAY	-2.64	104.21	108.37
3	C	303	DGF	CAJ-OAP-CAY	-2.54	104.36	108.37
3	B	302	DGF	OAE-CAS-CAU	2.43	120.38	115.73
3	C	303	DGF	OAE-CAS-CAU	2.37	120.28	115.73

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	302	DGF	CAV
3	C	303	DGF	CAV

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	303	DGF	CAC-CAW-CBA-CAT

There are no ring outliers.

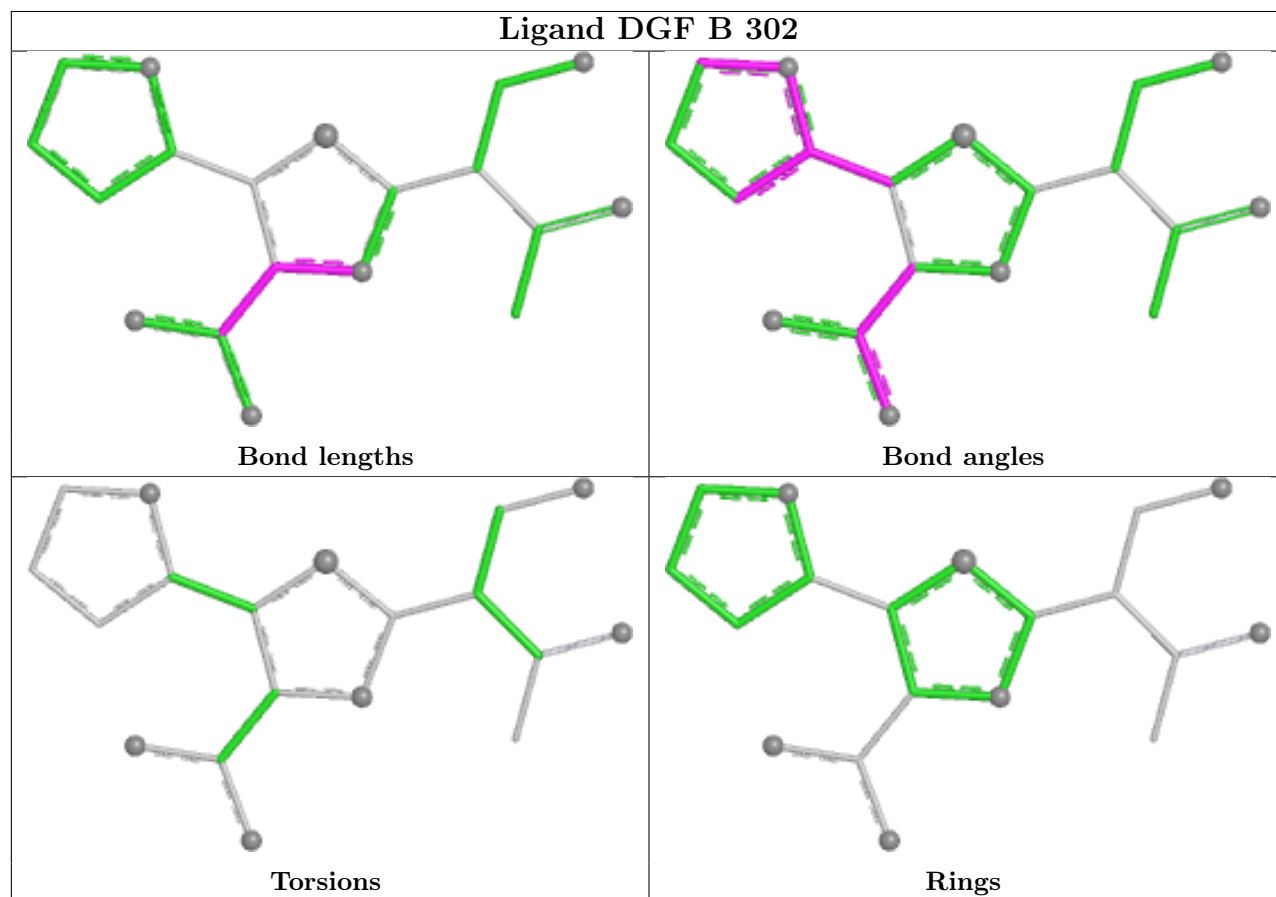
5 monomers are involved in 7 short contacts:

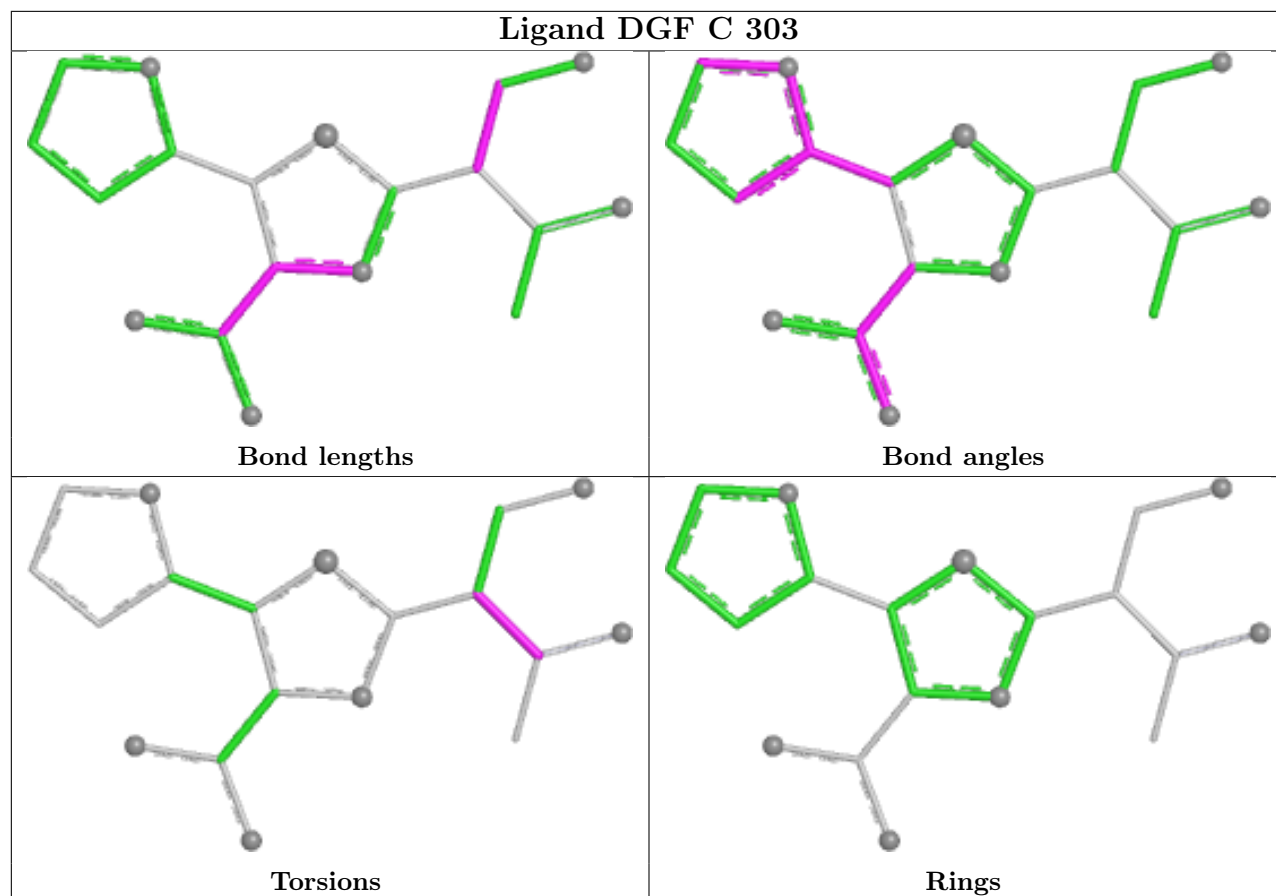
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	PO4	1	0
3	B	302	DGF	2	0
2	C	302	PO4	1	0
2	C	301	PO4	1	0
3	C	303	DGF	2	0

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 ⓘ

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	265/265 (100%)	-0.30	2 (0%) 86 88	17, 26, 47, 78	0
1	B	265/265 (100%)	-0.18	9 (3%) 45 51	18, 29, 61, 93	0
1	C	265/265 (100%)	-0.33	2 (0%) 86 88	17, 29, 56, 70	0
1	D	265/265 (100%)	-0.20	9 (3%) 45 51	21, 33, 57, 84	0
All	All	1060/1060 (100%)	-0.25	22 (2%) 63 68	17, 30, 56, 93	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	ALA	5.3
1	B	169	LEU	4.2
1	B	167	PRO	3.9
1	B	53	GLY	3.6
1	D	114	GLN	3.5
1	D	94	LEU	3.4
1	A	29	ASP	3.2
1	B	145(A)	GLY	3.2
1	D	100	ASP	2.9
1	B	175	GLY	2.9
1	D	98	THR	2.8
1	B	170	ASN	2.8
1	D	103	ARG	2.8
1	B	54	THR	2.7
1	D	101	ASP	2.6
1	C	170	ASN	2.6
1	B	171	ARG	2.4
1	D	99	SER	2.4
1	A	100	ASP	2.4
1	C	54	THR	2.3
1	D	96	THR	2.2
1	D	115	THR	2.2

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

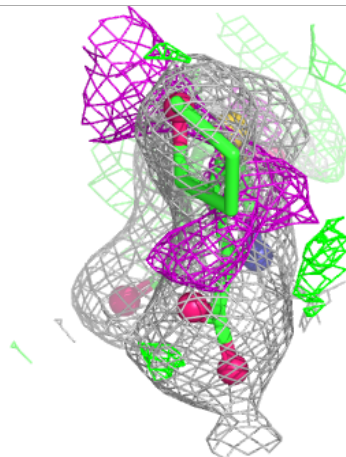
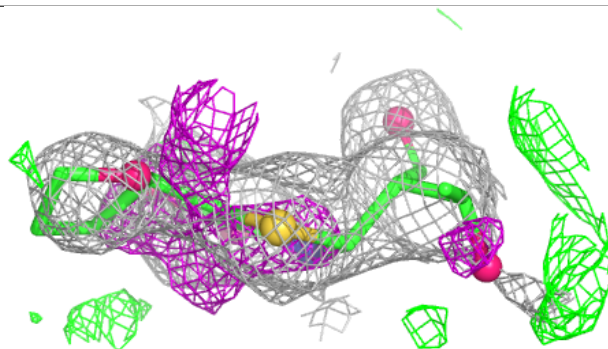
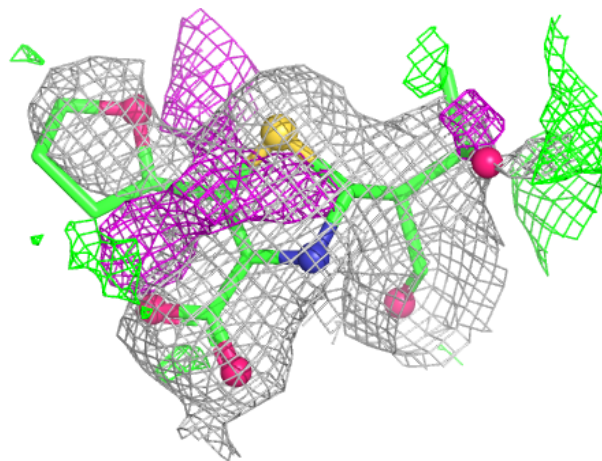
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	PO4	C	302	5/5	0.88	0.17	105,113,113,116	0
3	DGF	C	303	19/19	0.88	0.20	25,50,67,67	0
3	DGF	B	302	19/19	0.89	0.18	39,52,69,70	0
2	PO4	D	302	5/5	0.93	0.17	73,74,75,77	0
2	PO4	B	301	5/5	0.95	0.14	57,59,60,61	0
2	PO4	A	303	5/5	0.96	0.12	65,67,68,69	0
2	PO4	A	302	5/5	0.97	0.15	65,65,66,66	0
2	PO4	C	301	5/5	0.98	0.09	58,59,60,62	0
2	PO4	D	301	5/5	0.99	0.10	38,38,43,43	0
2	PO4	A	301	5/5	0.99	0.14	25,27,33,34	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.

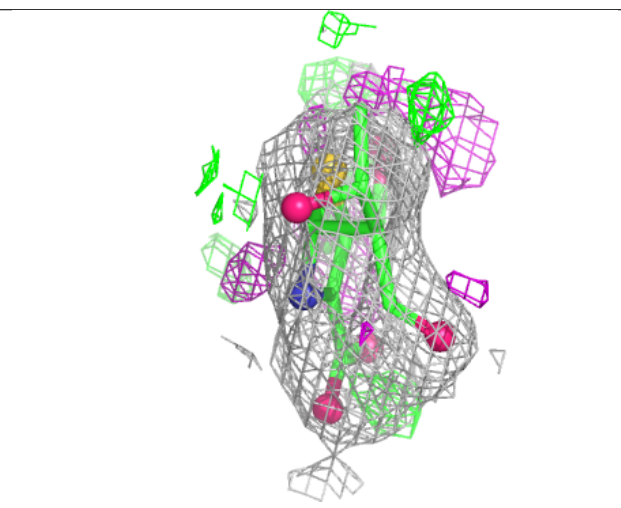
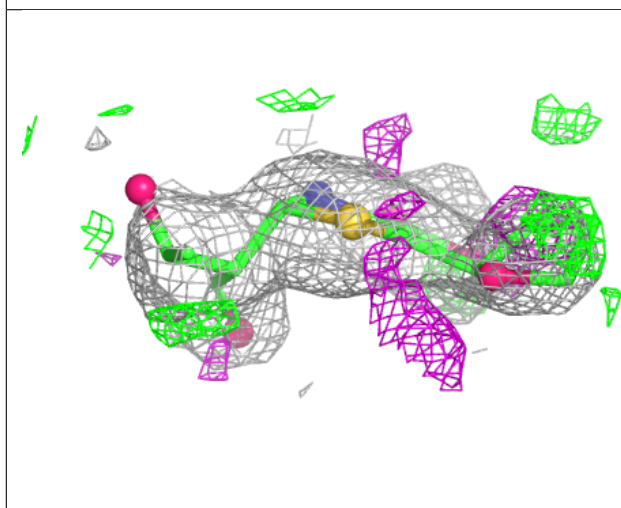
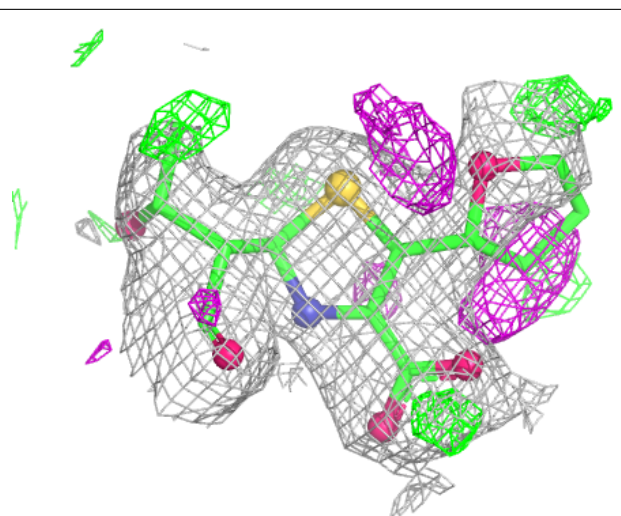
**Electron density around DGF C 303:**

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



**Electron density around DGF B 302:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.