



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:43 pm BST

PDB ID : 5DUJ  
Title : Crystal structure of ldtMt2 in complex with Faropenem adduct  
Authors : Kumar, P.; Lamichhane, G.  
Deposited on : 2015-09-18  
Resolution : 2.17 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

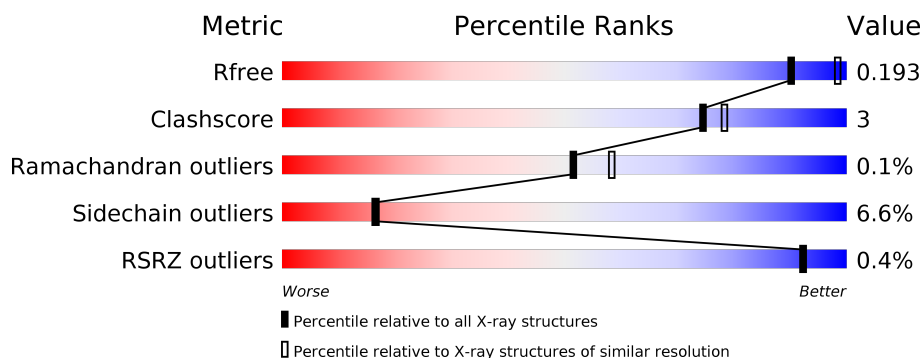
# 1 Overall quality at a glance ⓘ

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)
RSRZ outliers	127900	6738 (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 on 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	370	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>• 5%</div> </div> </div>
1	B	370	<div> <div></div> <div>84%</div> <div>9%</div> <div>• 5%</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
4	DGF	B	502	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5790 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 L,D-transpeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	1	0
			2661	1669	468	516	8			
1	B	350	Total	C	N	O	S	0	0	0
			2642	1657	463	514	8			

There are 6 discrepancies between the modelled and reference sequences:

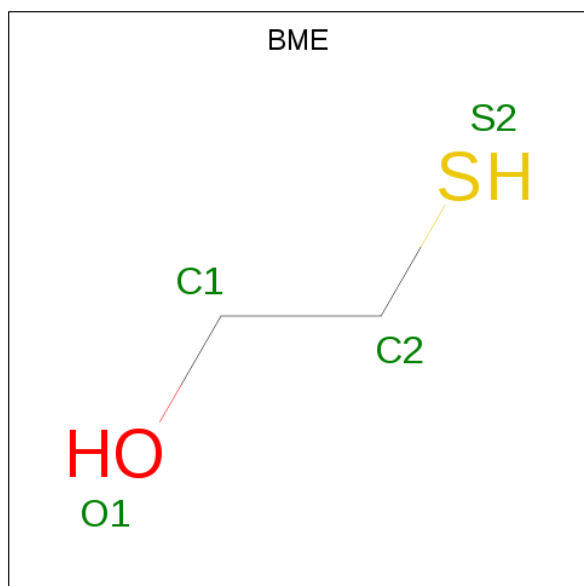
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	expression tag	UNP O53223
A	40	HIS	-	expression tag	UNP O53223
A	41	MET	-	expression tag	UNP O53223
B	39	GLY	-	expression tag	UNP O53223
B	40	HIS	-	expression tag	UNP O53223
B	41	MET	-	expression tag	UNP O53223

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



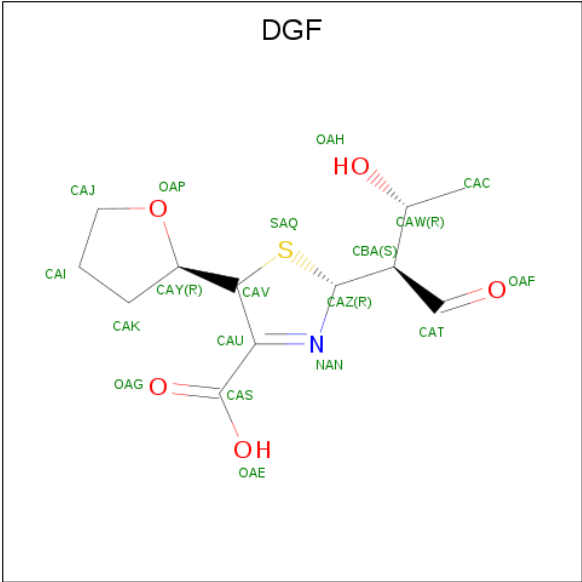
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 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:  $C_{12}H_{17}NO_5S$ ).



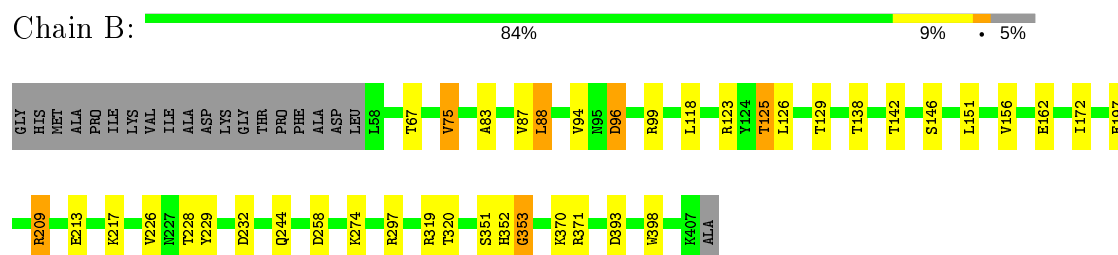
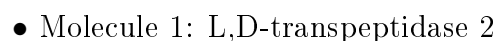
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	232	Total	O	0	0
			232	232		
5	B	230	Total	O	0	0
			230	230		



- Molecule 1: L,D-transpeptidase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.05Å 93.93Å 75.22Å 90.00° 92.72° 90.00°	Depositor
Resolution (Å)	50.00 – 2.17 37.57 – 2.17	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-2.17) 95.4 (37.57-2.17)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.22 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.180 , 0.234 0.191 , 0.193	Depositor DCC
$R_{free}$ test set	2113 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.078 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5790	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: DGF, SO4, BME

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	0.84	0/2727	1.11	14/3733 (0.4%)
1	B	0.86	2/2708 (0.1%)	1.08	17/3708 (0.5%)
All	All	0.85	2/5435 (0.0%)	1.10	31/7441 (0.4%)

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	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	GLU	CG-CD	8.74	1.65	1.51
1	B	353	GLY	N-CA	-7.72	1.34	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ARG	NE-CZ-NH2	-24.53	108.03	120.30
1	A	209	ARG	NE-CZ-NH1	19.32	129.96	120.30
1	B	209	ARG	NE-CZ-NH2	-17.97	111.31	120.30
1	B	209	ARG	NE-CZ-NH1	14.80	127.70	120.30
1	B	232	ASP	CB-CG-OD1	9.87	127.19	118.30
1	A	209	ARG	CD-NE-CZ	9.84	137.38	123.60
1	A	297	ARG	NE-CZ-NH1	8.49	124.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ASP	CB-CG-OD1	7.94	125.44	118.30
1	A	319	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	352	HIS	CA-C-N	7.51	131.22	116.20
1	A	267	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	209	ARG	CD-NE-CZ	6.97	133.35	123.60
1	B	371	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	371	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	99	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	352	HIS	O-C-N	-6.44	112.25	123.20
1	B	99	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	319	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	75	VAL	CB-CA-C	5.72	122.27	111.40
1	A	241	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	162	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	B	319	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	352	HIS	N-CA-C	5.61	126.14	111.00
1	A	232	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	297	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	258	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	162	GLU	CA-CB-CG	5.27	124.99	113.40
1	B	232	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	99	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	96	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	139	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	ARG	Sidechain
1	B	209	ARG	Sidechain

## 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	2661	0	2566	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2642	0	2543	13	0
2	A	5	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	1	0
4	A	6	0	0	1	0
4	B	6	0	0	0	0
5	A	232	0	0	6	0
5	B	230	0	0	2	0
All	All	5790	0	5121	33	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 (33) 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:83:ALA:HB2	1:B:88:LEU:HD13	1.44	0.99
1:A:83:ALA:HB2	1:A:88:LEU:HD13	1.53	0.90
1:B:351:SER:OG	1:B:353:GLY:HA2	1.82	0.79
1:A:101:VAL:O	1:A:102:ALA:HB3	1.85	0.75
1:A:75:VAL:HG22	1:A:118:LEU:HB2	1.74	0.70
1:B:125:THR:HG23	5:B:726:HOH:O	1.94	0.68
1:A:215:PHE:CZ	1:A:374:ILE:HD13	2.35	0.62
1:B:75:VAL:HG22	1:B:118:LEU:HB2	1.86	0.56
1:A:101:VAL:O	1:A:102:ALA:CB	2.46	0.56
1:B:75:VAL:CG1	1:B:229:TYR:CE2	2.89	0.56
1:B:125:THR:CG2	5:B:726:HOH:O	2.53	0.56
1:A:125:THR:CG2	5:A:722:HOH:O	2.54	0.55
1:A:125:THR:HG23	5:A:722:HOH:O	2.07	0.54
1:B:75:VAL:HG13	1:B:229:TYR:CE2	2.42	0.54
1:A:75:VAL:HG13	1:A:229:TYR:CE2	2.43	0.53
1:A:297:ARG:HD3	5:A:684:HOH:O	2.08	0.51
1:A:102:ALA:HA	5:A:735:HOH:O	2.11	0.51
1:A:313:ASN:ND2	5:A:605:HOH:O	2.43	0.49
1:B:83:ALA:HB2	1:B:88:LEU:CD1	2.31	0.47
1:B:156:VAL:HG12	1:B:172:ILE:HD13	1.96	0.47
1:B:75:VAL:HG13	1:B:229:TYR:HE2	1.81	0.46
1:B:156:VAL:HG11	1:B:226:VAL:HG21	1.97	0.46
1:A:129:THR:HB	1:A:138:THR:HB	1.98	0.45
1:A:129:THR:HG22	1:A:138:THR:HB	1.98	0.45
1:A:125:THR:HB	1:A:142:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:O	1:A:116:GLU:OE2	2.35	0.45
1:B:351:SER:HB2	3:B:501:BME:H21	1.99	0.45
1:A:353:GLY:HA3	4:A:503:DGF:CAC	2.48	0.44
1:B:213:GLU:HG3	1:B:398:TRP:CG	2.53	0.43
1:A:227:ASN:ND2	5:A:612:HOH:O	2.50	0.43
1:A:172:ILE:HG13	1:A:188:ILE:HD13	2.01	0.41
1:A:129:THR:CG2	1:A:138:THR:HB	2.51	0.41
1:A:274:LYS:HG3	1:A:364:TRP:CE2	2.56	0.40

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	350/370 (95%)	340 (97%)	9 (3%)	1 (0%)	41	43
1	B	348/370 (94%)	342 (98%)	6 (2%)	0	100	100
All	All	698/740 (94%)	682 (98%)	15 (2%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA

### 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	Percentiles	
1	A	283/295 (96%)	268 (95%)	15 (5%)	22	25
1	B	281/295 (95%)	259 (92%)	22 (8%)	12	11
All	All	564/590 (96%)	527 (93%)	37 (7%)	16	16

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	88	LEU
1	A	125	THR
1	A	126	LEU
1	A	129	THR
1	A	138	THR
1	A	146	SER
1	A	151	LEU
1	A	172	ILE
1	A	203	LEU
1	A	244	GLN
1	A	274	LYS
1	A	297	ARG
1	A	320	THR
1	A	393	ASP
1	B	67	THR
1	B	75	VAL
1	B	87	VAL
1	B	88	LEU
1	B	94	VAL
1	B	96	ASP
1	B	123	ARG
1	B	125	THR
1	B	126	LEU
1	B	129	THR
1	B	138	THR
1	B	142	THR
1	B	146	SER
1	B	151	LEU
1	B	197	GLU
1	B	217	LYS
1	B	228	THR
1	B	244	GLN
1	B	274	LYS
1	B	320	THR

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Mol	Chain	Res	Type
1	B	370	LYS
1	B	393	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	140	GLN
1	A	144	GLN
1	A	150	HIS
1	A	227	ASN
1	A	313	ASN
1	A	356	ASN
1	B	227	ASN
1	B	244	GLN
1	B	313	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

5 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
4	DGF	A	503	1	5,5,20	3.15	2 (40%)	5,5,28	3.88	3 (60%)
4	DGF	B	502	1	5,5,20	1.97	2 (40%)	5,5,28	4.55	4 (80%)
3	BME	B	501	-	3,3,3	0.11	0	1,2,2	1.59	0
2	SO4	A	501	-	4,4,4	0.44	0	6,6,6	0.75	0
3	BME	A	502	-	3,3,3	0.44	0	1,2,2	0.16	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
4	DGF	A	503	1	-	0/3/3/37	-
4	DGF	B	502	1	-	1/3/3/37	-
3	BME	B	501	-	-	0/1/1/1	-
3	BME	A	502	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	DGF	CBA-CAW	5.71	1.60	1.53
4	A	503	DGF	CBA-CAT	3.79	1.59	1.49
4	B	502	DGF	CBA-CAW	3.45	1.57	1.53
4	B	502	DGF	CBA-CAT	2.58	1.56	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	DGF	CAW-CBA-CAT	7.00	125.04	113.33
4	B	502	DGF	CAW-CBA-CAT	6.79	124.70	113.33
4	B	502	DGF	OAF-CAT-CBA	-6.57	106.29	125.43
4	A	503	DGF	OAF-CAT-CBA	-3.45	115.37	125.43
4	A	503	DGF	OAH-CAW-CBA	3.18	120.54	110.42
4	B	502	DGF	OAH-CAW-CBA	3.12	120.38	110.42
4	B	502	DGF	OAH-CAW-CAC	-2.04	100.55	109.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	502	DGF	OAF-CAT-CBA-CAW

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Mol	Chain	Res	Type	Atoms
3	A	502	BME	O1-C1-C2-S2

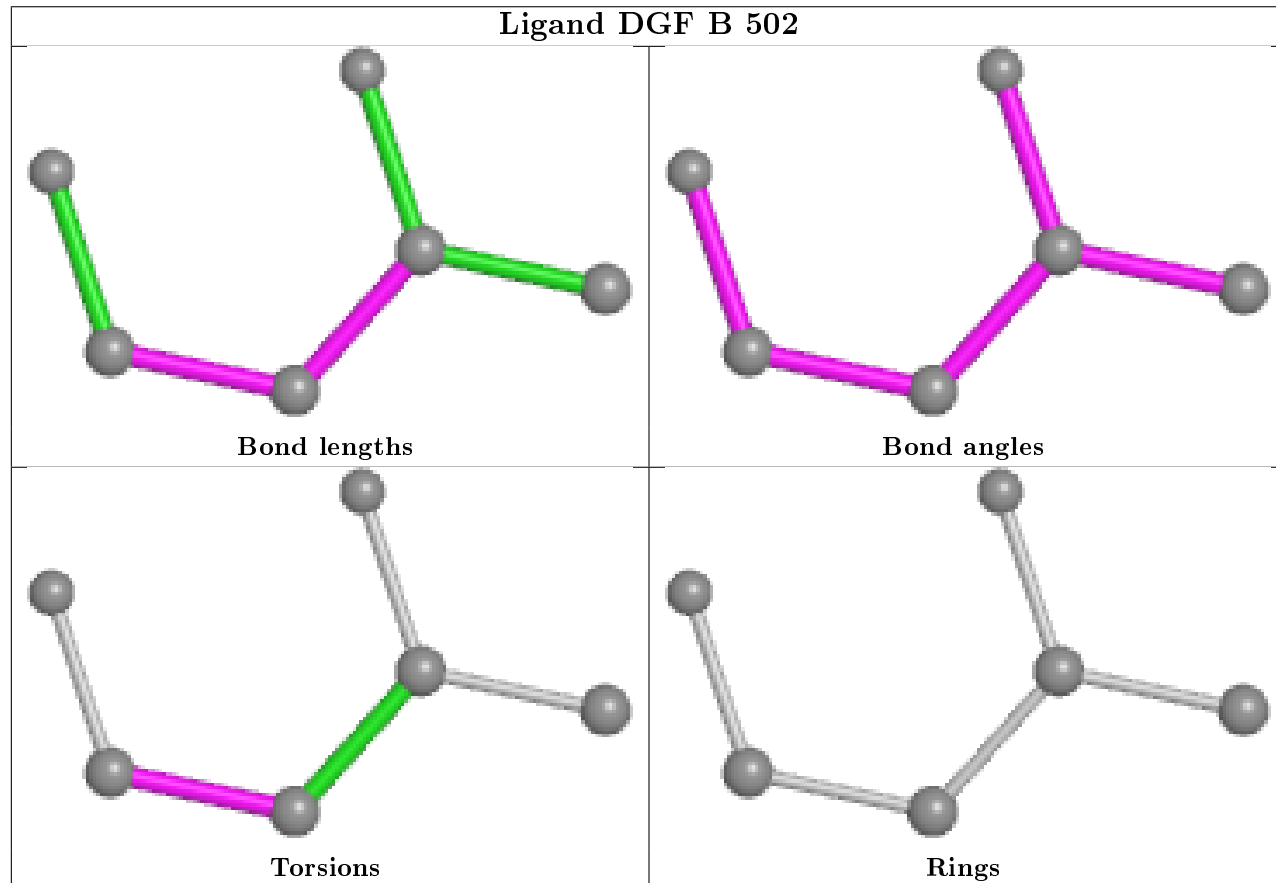
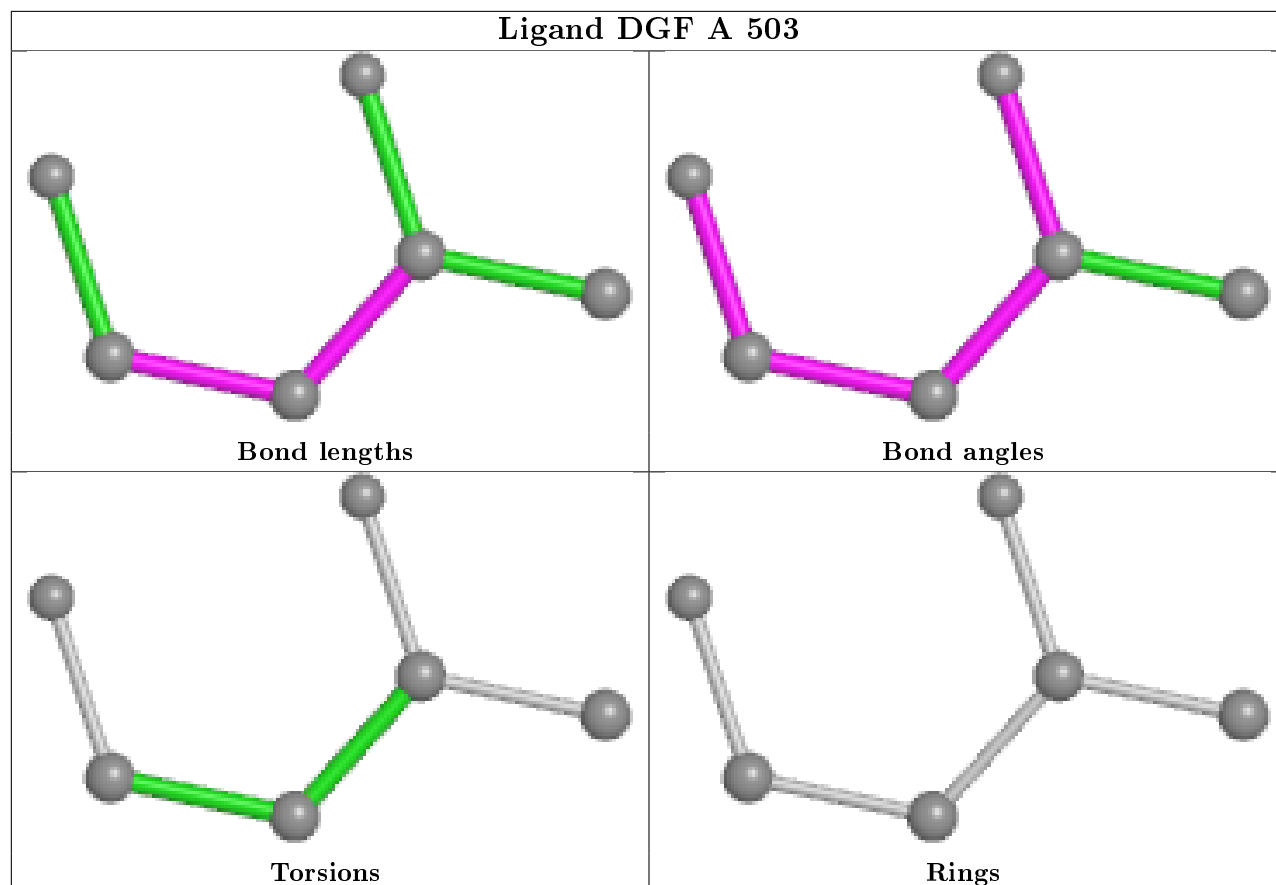
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	DGF	1	0
3	B	501	BME	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 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<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	351/370 (94%)	-0.30	3 (0%) 84 84	15, 25, 40, 75	0
1	B	350/370 (94%)	-0.36	0 100 100	17, 25, 39, 59	0
All	All	701/740 (94%)	-0.33	3 (0%) 92 92	15, 25, 39, 75	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	LEU	3.2
1	A	133	LEU	3.1
1	A	58	LEU	2.7

### 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 carbohydrates 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<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.

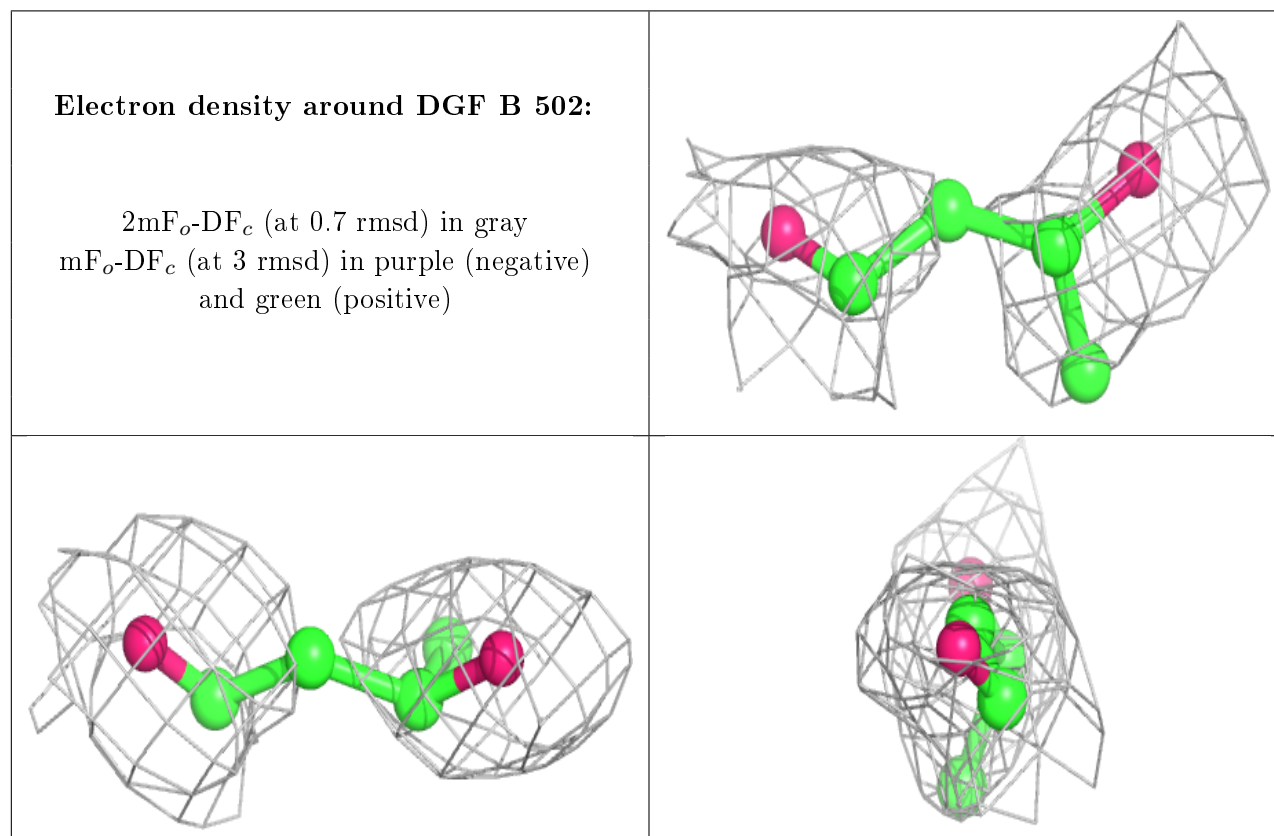
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	DGF	B	502	6/19	0.80	0.21	45,47,50,51	0
4	DGF	A	503	6/19	0.86	0.20	35,43,45,49	0

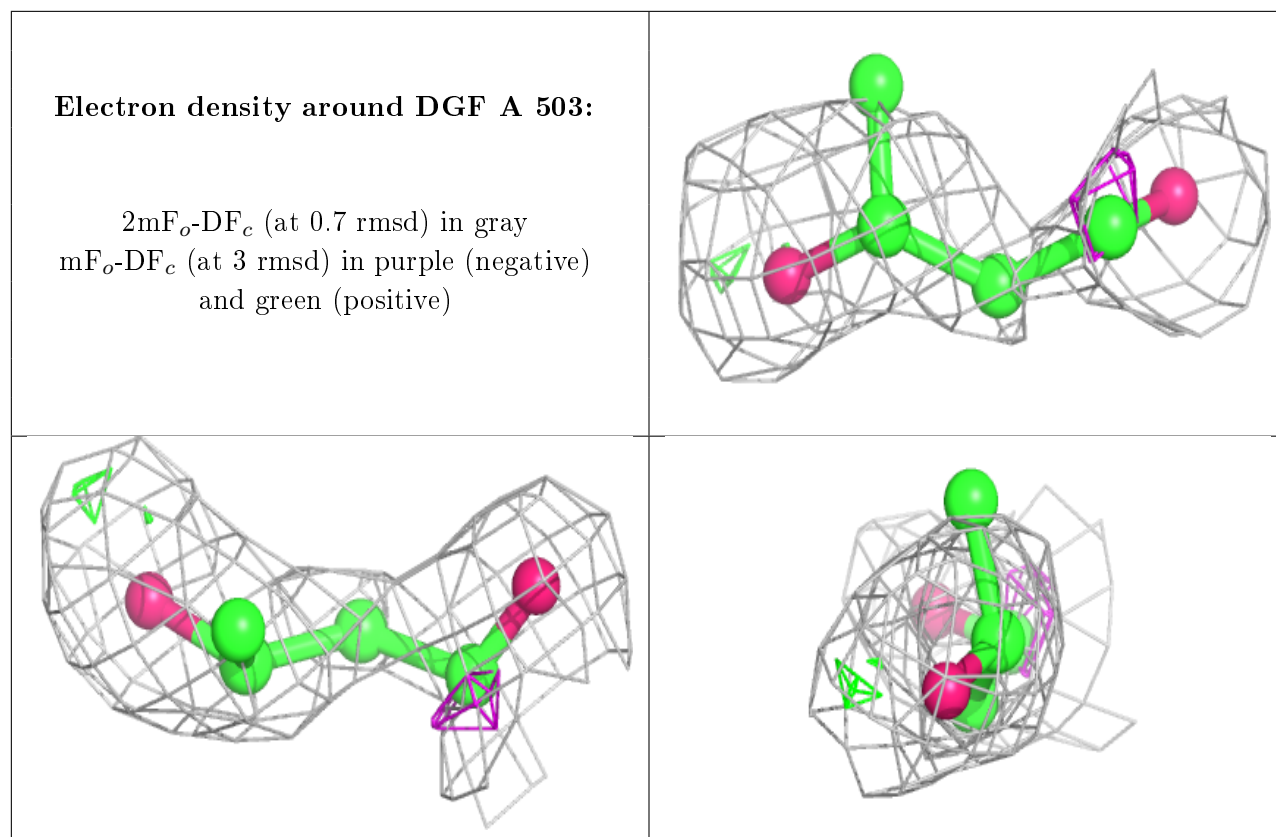
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BME	A	502	4/4	0.86	0.14	66,66,69,70	0
3	BME	B	501	4/4	0.96	0.08	60,61,61,66	0
2	SO4	A	501	5/5	0.98	0.11	45,47,56,57	1

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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.