



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2017 – 11:16 PM EDT

PDB ID : 1KR3  
Title : Crystal Structure of the Metallo beta-Lactamase from *Bacteroides fragilis* (CfiA) in Complex with the Tricyclic Inhibitor SB-236050.  
Authors : Payne, D.J.; Hueso-Rodriguez, J.A.; Boyd, H.; Concha, N.O.; Janson, C.A.; Gilpin, M.; Bateson, J.H.; Cheever, C.; Nikonovich, N.L.; Pearson, S.; Ritzenhouse, S.; Tew, D.; Dez, E.; Prez, P.; de la Fuente, J.; Rees, M.; Rivera-Sagredo, A.  
Deposited on : unknown  
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

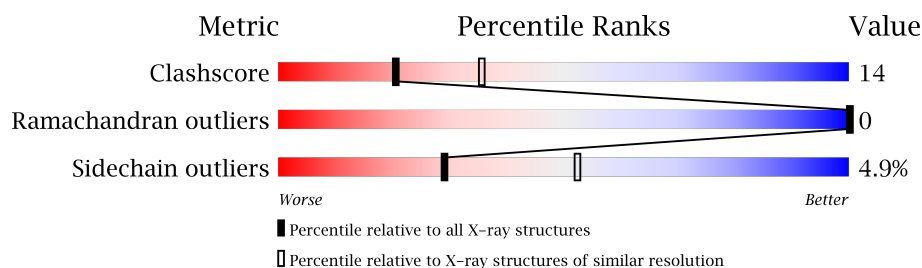
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	232	
1	B	232	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3576 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, type II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	40	0	0
			1742	1104	288	341	9			
1	B	227	Total	C	N	O	S	15	0	0
			1742	1104	288	341	9			

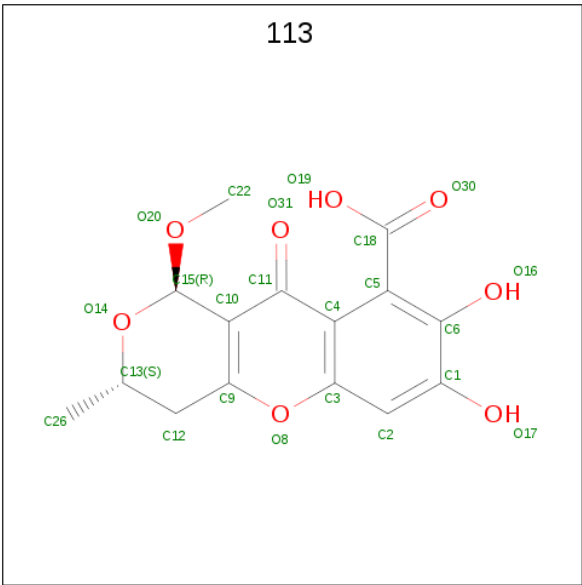
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is 7,8-DIHYDROXY-1-METHOXY-3-METHYL-10-OXO-4,10-DIHYDRO-1H,3H-PYRANO[4,3-B]CHROMENE-9-CARBOXYLIC ACID (three-letter code: 113) (formula: C<sub>15</sub>H<sub>14</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	15	8		
4	B	1	Total	C	O	0	0
			23	15	8		

- Molecule 5 is water.

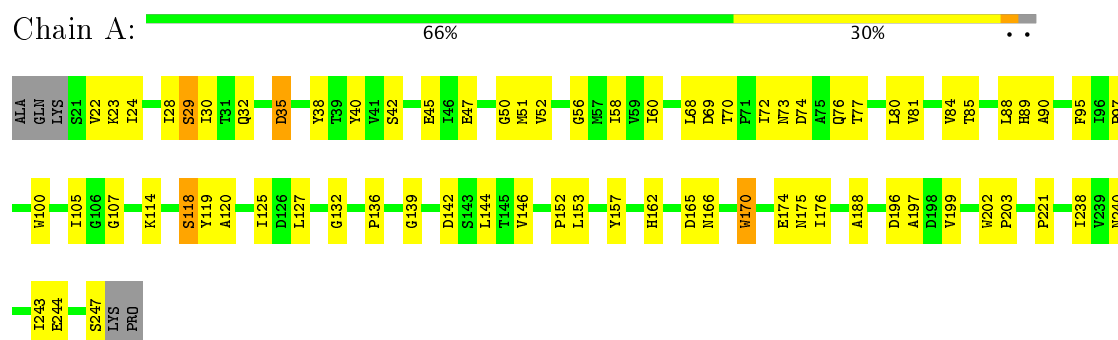
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	B	23	Total	O	0	0
			23	23		

### 3 Residue-property plots

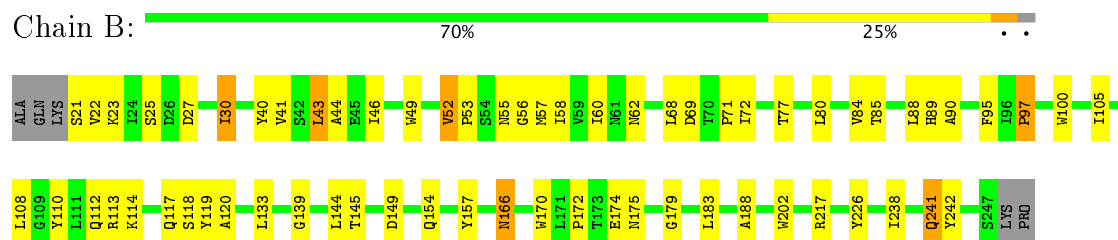
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

- Molecule 1: beta-Lactamase, type II



- Molecule 1: beta-Lactamase, type II



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.80 Å   44.20 Å   58.50 Å 92.80°   95.30°   98.00°	Depositor
Resolution (Å)	29.07 – 2.50	Depositor
% Data completeness (in resolution range)	73.7 (29.07-2.50)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNX 2000.1	Depositor
R, $R_{free}$	0.152 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 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: NA, ZN, 113

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	0.69	1/1782 (0.1%)	0.88	0/2430
1	B	0.73	0/1782	0.90	1/2430 (0.0%)
All	All	0.71	1/3564 (0.0%)	0.89	1/4860 (0.0%)

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	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	TRP	CB-CG	5.28	1.59	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	LEU	CA-CB-CG	5.25	127.38	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	157	TYR	Sidechain
1	B	242	TYR	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	1742	0	1699	51	0
1	B	1742	0	1699	45	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	23	0	13	0	0
4	B	23	0	13	0	0
5	A	17	0	0	0	0
5	B	23	0	0	0	0
All	All	3576	0	3424	95	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 14.

All (95) 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:100:TRP:O	1:B:105:ILE:HD11	1.85	0.77
1:A:152:PRO:O	1:A:153:LEU:HD23	1.89	0.73
1:B:84:VAL:HG13	1:B:88:LEU:HD12	1.70	0.73
1:B:60:ILE:HD11	1:B:88:LEU:HD13	1.72	0.72
1:B:179:GLY:HA3	1:B:183:LEU:HD12	1.72	0.71
1:A:70:THR:HG23	1:A:95:PHE:CE2	2.25	0.71
1:B:46:ILE:HD12	1:B:52:VAL:HG21	1.71	0.70
1:B:44:ALA:HB1	1:B:72:ILE:HD11	1.73	0.69
1:A:45:GLU:OE1	1:A:51:MET:HG2	1.93	0.69
1:A:68:LEU:O	1:A:69:ASP:HB2	1.94	0.66
1:B:40:TYR:CE2	1:B:56:GLY:HA3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:VAL:HG12	1:B:30:ILE:HG22	1.79	0.65
1:B:154:GLN:NE2	1:B:170:TRP:HD1	1.93	0.64
1:A:85:THR:O	1:A:89:HIS:HA	1.98	0.63
1:B:57:MET:HE2	1:B:68:LEU:HD12	1.81	0.63
1:B:40:TYR:CZ	1:B:56:GLY:HA3	2.33	0.63
1:A:170:TRP:CH2	1:A:175:ASN:HA	2.35	0.62
1:B:46:ILE:HD12	1:B:52:VAL:CG2	2.29	0.62
1:A:35:ASP:N	1:A:35:ASP:OD2	2.33	0.61
1:A:24:ILE:HD11	1:A:28:ILE:CG2	2.32	0.60
1:B:44:ALA:CB	1:B:72:ILE:HD11	2.32	0.60
1:B:71:PRO:HD2	1:B:77:THR:OG1	2.01	0.60
1:B:241:GLN:HG2	1:B:241:GLN:O	2.01	0.59
1:B:21:SER:HA	1:B:30:ILE:O	2.02	0.59
1:A:162:HIS:O	1:A:197:ALA:HA	2.02	0.59
1:A:85:THR:HG22	1:A:90:ALA:O	2.03	0.59
1:A:24:ILE:HD11	1:A:28:ILE:HG22	1.85	0.58
1:A:120:ALA:O	1:A:139:GLY:HA2	2.03	0.58
1:A:152:PRO:C	1:A:153:LEU:HD23	2.24	0.57
1:B:170:TRP:CH2	1:B:175:ASN:HA	2.41	0.56
1:A:58:ILE:HD11	1:A:80:LEU:HD11	1.89	0.55
1:A:85:THR:HA	1:A:90:ALA:H	1.71	0.55
1:A:95:PHE:CZ	1:A:97:PRO:HB3	2.42	0.55
1:A:42:SER:HB2	1:A:76:GLN:OE1	2.07	0.54
1:A:100:TRP:CD1	1:A:127:LEU:HD13	2.43	0.54
1:B:202:TRP:O	1:B:202:TRP:HD1	1.92	0.53
1:B:85:THR:O	1:B:89:HIS:HA	2.09	0.53
1:B:62:ASN:HB2	1:B:149:ASP:OD2	2.11	0.51
1:B:188:ALA:O	1:B:238:ILE:HD11	2.10	0.51
1:A:29:SER:O	1:A:30:ILE:HD12	2.10	0.51
1:A:77:THR:O	1:A:81:VAL:HG23	2.10	0.51
1:A:72:ILE:HD12	1:A:73:ASN:N	2.24	0.51
1:A:132:GLY:O	1:B:217:ARG:HD2	2.11	0.50
1:A:174:GLU:O	1:A:176:ILE:HG13	2.12	0.49
1:A:50:GLY:O	1:A:52:VAL:HG13	2.12	0.49
1:B:68:LEU:O	1:B:69:ASP:HB2	2.13	0.49
1:B:154:GLN:NE2	1:B:172:PRO:HG3	2.27	0.48
1:A:243:ILE:O	1:A:247:SER:HB2	2.14	0.48
1:B:226:TYR:CD1	1:B:226:TYR:C	2.87	0.48
1:B:110:TYR:CZ	1:B:114:LYS:HD2	2.48	0.48
1:A:188:ALA:O	1:A:238:ILE:HD11	2.13	0.47
1:A:40:TYR:CE2	1:A:56:GLY:HA3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:O	1:B:118:SER:HA	2.14	0.46
1:B:117:GLN:HA	1:B:117:GLN:OE1	2.15	0.46
1:B:154:GLN:HE21	1:B:170:TRP:HD1	1.63	0.46
1:B:60:ILE:HD11	1:B:88:LEU:HB3	1.98	0.45
1:A:85:THR:CG2	1:A:90:ALA:O	2.64	0.45
1:A:22:VAL:HG12	1:A:23:LYS:N	2.32	0.44
1:A:202:TRP:HB3	1:A:203:PRO:HD3	1.99	0.44
1:B:120:ALA:O	1:B:139:GLY:HA2	2.16	0.44
1:A:100:TRP:HZ2	1:A:196:ASP:OD1	2.01	0.44
1:B:144:LEU:HG	1:B:145:THR:N	2.31	0.44
1:B:22:VAL:HG22	1:B:23:LYS:N	2.31	0.44
1:B:43:LEU:HD22	1:B:53:PRO:HB3	2.00	0.44
1:A:114:LYS:HE2	1:A:114:LYS:HB3	1.72	0.44
1:B:110:TYR:OH	1:B:114:LYS:HD2	2.18	0.44
1:B:174:GLU:O	1:B:175:ASN:HB2	2.18	0.43
1:B:49:TRP:HB3	1:B:52:VAL:HG11	2.00	0.43
1:A:125:ILE:HD12	1:A:139:GLY:HA3	1.99	0.43
1:B:85:THR:HG22	1:B:90:ALA:O	2.19	0.43
1:A:119:TYR:HD2	1:A:144:LEU:HD21	1.82	0.43
1:B:80:LEU:O	1:B:84:VAL:HG23	2.19	0.43
1:A:24:ILE:CD1	1:A:30:ILE:HD13	2.48	0.43
1:A:24:ILE:HD11	1:A:28:ILE:HG21	2.01	0.43
1:A:80:LEU:O	1:A:84:VAL:HG23	2.18	0.42
1:B:57:MET:CE	1:B:68:LEU:HD12	2.48	0.42
1:A:74:ASP:OD1	1:A:107:GLY:HA2	2.19	0.42
1:B:41:VAL:HG13	1:B:55:ASN:OD1	2.19	0.42
1:A:24:ILE:HD13	1:A:30:ILE:HD13	2.02	0.42
1:B:166:ASN:HD22	1:B:166:ASN:C	2.23	0.41
1:A:32:GLN:NE2	1:A:38:TYR:CZ	2.88	0.41
1:A:118:SER:HB2	1:A:136:PRO:HB3	2.03	0.41
1:A:97:PRO:HD2	1:A:119:TYR:O	2.20	0.41
1:A:97:PRO:HB3	1:A:105:ILE:HG22	2.02	0.41
1:A:144:LEU:HG	1:A:146:VAL:CG2	2.51	0.41
1:A:72:ILE:CD1	1:A:73:ASN:HD22	2.34	0.41
1:B:97:PRO:HD2	1:B:119:TYR:O	2.20	0.41
1:A:22:VAL:CG1	1:A:23:LYS:N	2.83	0.41
1:A:40:TYR:CZ	1:A:56:GLY:HA3	2.56	0.41
1:A:60:ILE:HD12	1:A:88:LEU:HB3	2.03	0.41
1:A:119:TYR:CD2	1:A:144:LEU:HD21	2.55	0.41
1:B:23:LYS:HG2	1:B:25:SER:O	2.21	0.41
1:A:72:ILE:CD1	1:A:73:ASN:ND2	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TRP:HD1	1:A:165:ASP:OD2	2.03	0.40
1:B:108:LEU:O	1:B:112:GLN:HG3	2.22	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	225/232 (97%)	203 (90%)	22 (10%)	0	100	100
1	B	225/232 (97%)	212 (94%)	13 (6%)	0	100	100
All	All	450/464 (97%)	415 (92%)	35 (8%)	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	Percentiles	
1	A	193/197 (98%)	183 (95%)	10 (5%)	27	49
1	B	193/197 (98%)	184 (95%)	9 (5%)	30	54
All	All	386/394 (98%)	367 (95%)	19 (5%)	29	52

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	35	ASP
1	A	47	GLU
1	A	118	SER
1	A	142	ASP
1	A	166	ASN
1	A	199	VAL
1	A	221	PRO
1	A	240	ASN
1	A	244	GLU
1	B	27	ASP
1	B	30	ILE
1	B	43	LEU
1	B	52	VAL
1	B	58	ILE
1	B	97	PRO
1	B	113	ARG
1	B	166	ASN
1	B	241	GLN

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	32	GLN
1	A	82	ASN
1	A	154	GLN
1	A	186	ASN
1	A	240	ASN
1	A	241	GLN
1	B	98	ASN
1	B	154	GLN
1	B	240	ASN
1	B	241	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z  > 2$
4	113	A	602	2	21,25,25	1.93	6 (28%)	22,38,38	1.81	6 (27%)
4	113	B	601	2	21,25,25	1.99	6 (28%)	22,38,38	1.51	5 (22%)

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	113	A	602	2	-	0/2/18/18	0/3/3/3
4	113	B	601	2	-	0/2/18/18	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	113	C10-C9	-2.66	1.36	1.39
4	B	601	113	C10-C9	-2.65	1.36	1.39
4	B	601	113	O8-C9	2.40	1.38	1.35
4	A	602	113	O8-C9	2.66	1.38	1.35
4	A	602	113	C2-C1	2.80	1.40	1.37
4	B	601	113	C2-C1	2.87	1.40	1.37
4	A	602	113	C5-C6	3.12	1.42	1.38
4	B	601	113	C11-C10	3.27	1.50	1.41
4	A	602	113	C11-C10	3.53	1.51	1.41
4	B	601	113	C5-C6	3.63	1.42	1.38
4	A	602	113	C11-C4	4.54	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	113	C11-C4	4.93	1.48	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	113	C1-C2-C3	-3.27	118.55	121.41
4	A	602	113	C2-C3-C4	-2.82	119.92	123.05
4	B	601	113	C1-C2-C3	-2.44	119.28	121.41
4	A	602	113	C10-C11-C4	-2.28	117.48	122.29
4	B	601	113	C10-C11-C4	-2.23	117.58	122.29
4	B	601	113	C2-C3-C4	-2.13	120.69	123.05
4	A	602	113	O8-C3-C2	2.92	119.53	116.11
4	B	601	113	C15-O14-C13	2.93	120.48	112.90
4	A	602	113	C15-O14-C13	3.16	121.08	112.90
4	A	602	113	C22-O20-C15	3.38	121.07	113.71
4	B	601	113	C22-O20-C15	3.42	121.15	113.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.