Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2023 – 09:56 pm GMT

PDB ID	:	7PSE
Title	:	Crystal Structure of a Class D Carbapenemase_K73ALY Complexed with Oxacillin
Authors	:	Zhou, Q.; He, Y.; Jin, Y.
Deposited on	:	2021-09-23
Resolution	:	2.32 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 ⓘ 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:

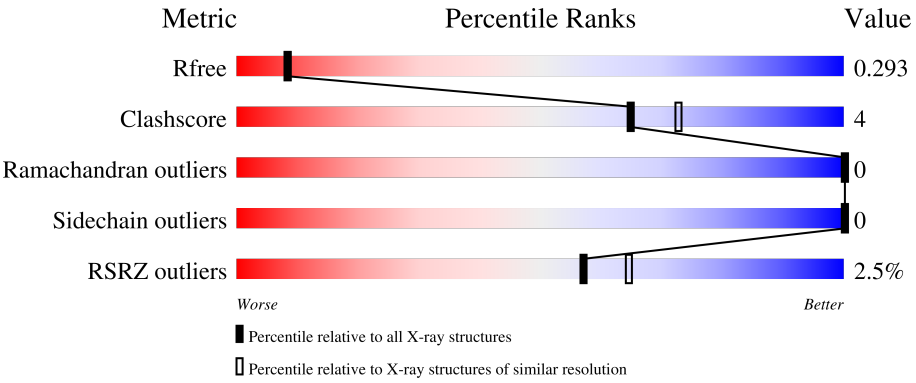
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	AAA	260	2% 83% 10% 7%
1	BBB	260	3% 79% 14% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8055 atoms, of which 3956 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	AAA	241	Total	C	H	N	O	S	45	0	0
			3911	1259	1936	347	362	7			
1	BBB	242	Total	C	H	N	O	S	45	0	0
			3925	1263	1942	349	364	7			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	6	MET	-	initiating methionine	UNP A0A482LRD5
AAA	7	HIS	-	expression tag	UNP A0A482LRD5
AAA	8	HIS	-	expression tag	UNP A0A482LRD5
AAA	9	HIS	-	expression tag	UNP A0A482LRD5
AAA	10	HIS	-	expression tag	UNP A0A482LRD5
AAA	11	HIS	-	expression tag	UNP A0A482LRD5
AAA	12	HIS	-	expression tag	UNP A0A482LRD5
AAA	13	SER	-	expression tag	UNP A0A482LRD5
AAA	14	ALA	-	expression tag	UNP A0A482LRD5
AAA	15	GLY	-	expression tag	UNP A0A482LRD5
AAA	16	GLU	-	expression tag	UNP A0A482LRD5
AAA	17	ASN	-	expression tag	UNP A0A482LRD5
AAA	18	LEU	-	expression tag	UNP A0A482LRD5
AAA	19	TYR	-	expression tag	UNP A0A482LRD5
AAA	20	PHE	-	expression tag	UNP A0A482LRD5
AAA	21	GLN	-	expression tag	UNP A0A482LRD5
AAA	22	GLY	-	expression tag	UNP A0A482LRD5
BBB	6	MET	-	initiating methionine	UNP A0A482LRD5
BBB	7	HIS	-	expression tag	UNP A0A482LRD5
BBB	8	HIS	-	expression tag	UNP A0A482LRD5
BBB	9	HIS	-	expression tag	UNP A0A482LRD5
BBB	10	HIS	-	expression tag	UNP A0A482LRD5
BBB	11	HIS	-	expression tag	UNP A0A482LRD5
BBB	12	HIS	-	expression tag	UNP A0A482LRD5
BBB	13	SER	-	expression tag	UNP A0A482LRD5

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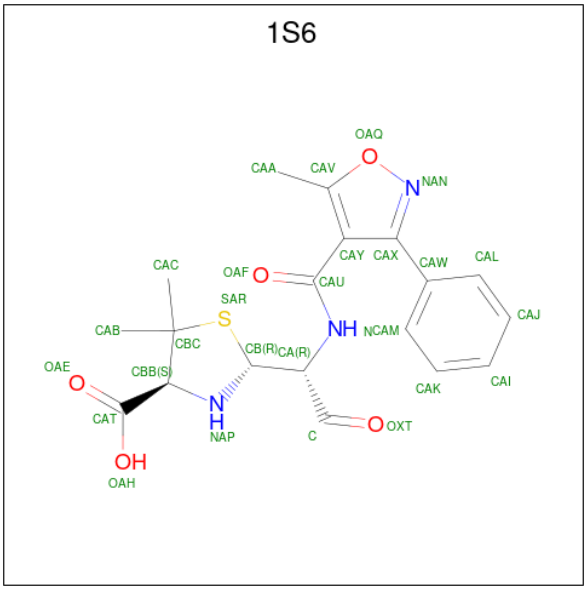
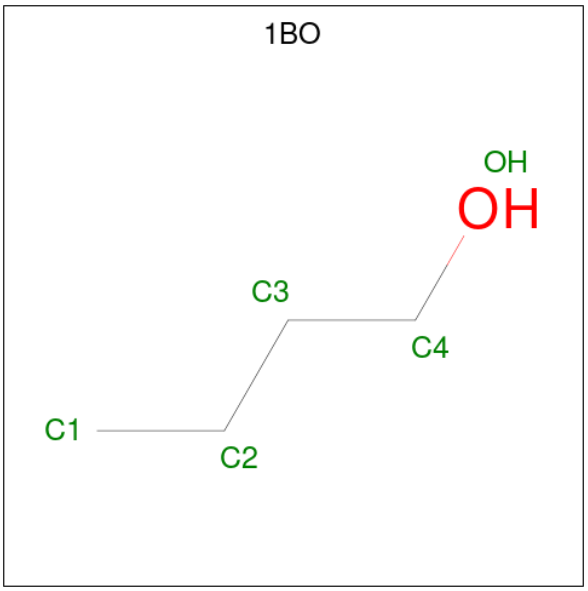
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	14	ALA	-	expression tag	UNP A0A482LRD5
BBB	15	GLY	-	expression tag	UNP A0A482LRD5
BBB	16	GLU	-	expression tag	UNP A0A482LRD5
BBB	17	ASN	-	expression tag	UNP A0A482LRD5
BBB	18	LEU	-	expression tag	UNP A0A482LRD5
BBB	19	TYR	-	expression tag	UNP A0A482LRD5
BBB	20	PHE	-	expression tag	UNP A0A482LRD5
BBB	21	GLN	-	expression tag	UNP A0A482LRD5
BBB	22	GLY	-	expression tag	UNP A0A482LRD5

- Molecule 2 is (2R,4S)-5,5-dimethyl-2-[(1R)-1-{[(5-methyl-3-phenyl-1,2-oxazol-4-yl)carbonyl]amino}-2-oxoethyl]-1,3-thiazolidine-4-carb oxylic acid (three-letter code: 1S6) (formula: $C_{19}H_{21}N_3O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	S	0	0
			47	19	19	3	5	1		
2	BBB	1	Total	C	H	N	O	S	0	0
			47	19	19	3	5	1		

- Molecule 3 is 1-BUTANOL (three-letter code: 1BO) (formula: $C_4H_{10}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C H O 15 4 10 1	0	0
3	AAA	1	Total C H O 15 4 10 1	0	0
3	BBB	1	Total C H O 15 4 10 1	0	0
3	BBB	1	Total C H O 15 4 10 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Cl 1 1	0	0

- Molecule 5 is water.

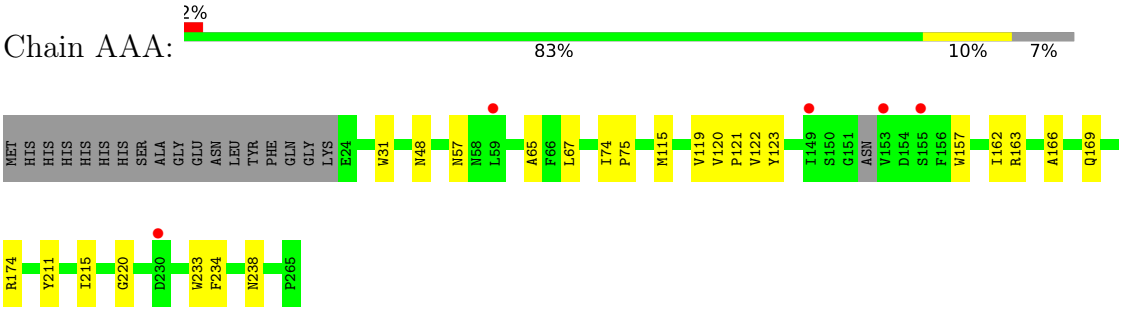
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	30	Total O 30 30	0	0
5	BBB	34	Total O 34 34	0	0

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.

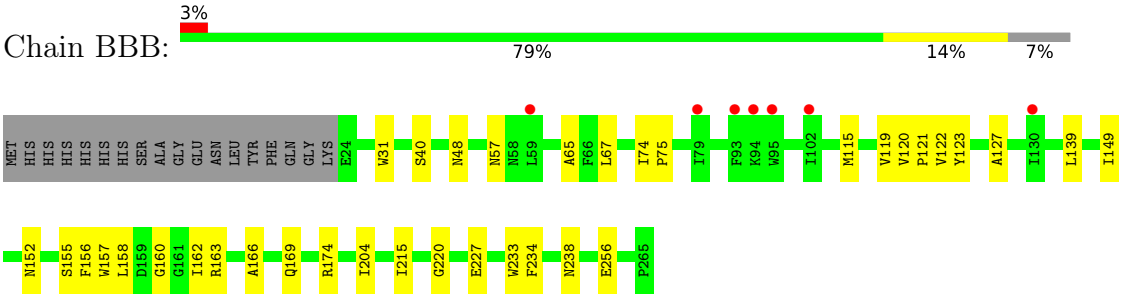
• Molecule 1: Beta-lactamase

Chain AAA:



• Molecule 1: Beta-lactamase

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.83Å 105.48Å 124.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.76 – 2.32 53.76 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.2 (53.76-2.32) 99.2 (53.76-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.235 , 0.289 0.241 , 0.293	Depositor DCC
R_{free} test set	1266 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 34.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8055	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1BO, ALY, 1S6, CL

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	AAA	0.71	0/2010	0.85	0/2716
1	BBB	0.71	0/2019	0.85	0/2730
All	All	0.71	0/4029	0.85	0/5446

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

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	AAA	1975	1936	1927	13	0
1	BBB	1983	1942	1934	20	0
2	AAA	28	19	19	1	0
2	BBB	28	19	19	1	0
3	AAA	10	20	20	0	0
3	BBB	10	20	20	0	0
4	AAA	1	0	0	0	0
5	AAA	30	0	0	0	0
5	BBB	34	0	0	2	0
All	All	4099	3956	3939	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 4.

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:BBB:48:ASN:HB2	1:BBB:233:TRP:CH2	2.34	0.62
1:BBB:152:ASN:HB2	1:BBB:155:SER:OG	1.99	0.62
1:BBB:120:VAL:N	1:BBB:121:PRO:HD2	2.16	0.61
1:AAA:48:ASN:HB2	1:AAA:233:TRP:CH2	2.36	0.60
1:AAA:120:VAL:N	1:AAA:121:PRO:HD2	2.15	0.60
1:BBB:115:MET:HG2	1:BBB:123:TYR:OH	2.03	0.58
1:BBB:67:LEU:HD11	1:BBB:215:ILE:HD12	1.87	0.56
1:AAA:115:MET:HG2	1:AAA:123:TYR:OH	2.05	0.55
1:BBB:40:SER:HB2	5:BBB:414:HOH:O	2.05	0.55
1:AAA:65:ALA:HB1	1:AAA:163:ARG:HB3	1.89	0.55
1:BBB:256:GLU:HG2	5:BBB:429:HOH:O	2.08	0.53
1:BBB:139:LEU:HD12	1:BBB:149:ILE:HG22	1.92	0.51
1:BBB:220:GLY:O	1:BBB:238:ASN:HA	2.12	0.49
1:AAA:174:ARG:HA	1:AAA:234:PHE:CE2	2.49	0.48
1:AAA:220:GLY:O	1:AAA:238:ASN:HA	2.13	0.48
1:BBB:65:ALA:HB1	1:BBB:163:ARG:HB3	1.95	0.48
1:BBB:158:LEU:HD23	2:BBB:301:1S6:CAA	2.44	0.47
1:AAA:166:ALA:O	1:AAA:169:GLN:HB2	2.16	0.46
1:AAA:31:TRP:HB2	1:AAA:57:ASN:HB3	1.98	0.45
1:BBB:174:ARG:HA	1:BBB:234:PHE:CE2	2.51	0.45
1:BBB:74:ILE:HB	1:BBB:75:PRO:CD	2.47	0.45
1:AAA:119:VAL:HG12	1:AAA:122:VAL:HG23	1.99	0.45
1:AAA:157:TRP:HA	1:AAA:162:ILE:CG2	2.47	0.44
1:AAA:211:TYR:CD2	2:AAA:301:1S6:H18	2.53	0.44
1:BBB:204:ILE:HB	1:BBB:227:GLU:HB2	2.00	0.44
1:BBB:119:VAL:HG12	1:BBB:122:VAL:HG23	1.99	0.43
1:AAA:74:ILE:HB	1:AAA:75:PRO:CD	2.48	0.42
1:BBB:31:TRP:HB2	1:BBB:57:ASN:HB3	2.01	0.42
1:BBB:166:ALA:O	1:BBB:169:GLN:HB2	2.19	0.42
1:AAA:67:LEU:HD11	1:AAA:215:ILE:HD12	2.01	0.41
1:BBB:156:PHE:HA	1:BBB:160:GLY:HA3	2.03	0.41
1:BBB:127:ALA:HB2	1:BBB:157:TRP:CH2	2.56	0.40
1:BBB:157:TRP:HA	1:BBB:162:ILE:CG2	2.51	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	AAA	236/260 (91%)	223 (94%)	13 (6%)	0	100	100
1	BBB	239/260 (92%)	227 (95%)	12 (5%)	0	100	100
All	All	475/520 (91%)	450 (95%)	25 (5%)	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	AAA	209/225 (93%)	209 (100%)	0	100	100
1	BBB	210/225 (93%)	210 (100%)	0	100	100
All	All	419/450 (93%)	419 (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

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	ALY	AAA	73	1	10,11,12	0.40	0	7,12,14	0.34	0
1	ALY	BBB	73	1	10,11,12	0.42	0	7,12,14	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
1	ALY	AAA	73	1	-	0/9/10/12	-
1	ALY	BBB	73	1	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\#\|Z\| > 2$
2	1S6	AAA	301	1	22,30,30	0.90	1 (4%)	25,44,44	1.02	1 (4%)
3	1BO	AAA	303	-	4,4,4	0.22	0	3,3,3	0.11	0
2	1S6	BBB	301	1	22,30,30	0.88	2 (9%)	25,44,44	0.96	1 (4%)
3	1BO	AAA	302	-	4,4,4	0.62	0	3,3,3	0.42	0
3	1BO	BBB	302	-	4,4,4	0.42	0	3,3,3	0.32	0
3	1BO	BBB	303	-	4,4,4	0.26	0	3,3,3	0.30	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
2	1S6	AAA	301	1	-	4/12/37/37	0/3/3/3
3	1BO	AAA	303	-	-	0/2/2/2	-
2	1S6	BBB	301	1	-	3/12/37/37	0/3/3/3
3	1BO	AAA	302	-	-	2/2/2/2	-
3	1BO	BBB	302	-	-	1/2/2/2	-
3	1BO	BBB	303	-	-	0/2/2/2	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	301	1S6	OAH-CAT	-2.45	1.22	1.30
2	BBB	301	1S6	CAY-CAX	2.16	1.43	1.41
2	AAA	301	1S6	OAH-CAT	-2.03	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	301	1S6	CBC-SAR-CB	-3.91	85.63	93.99
2	AAA	301	1S6	CBC-SAR-CB	-3.84	85.78	93.99

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	1S6	C-CA-N-CAU
2	AAA	301	1S6	CAL-CAW-CAX-NAN
2	AAA	301	1S6	CAM-CAW-CAX-NAN
2	BBB	301	1S6	CAM-CAW-CAX-NAN
2	BBB	301	1S6	CAL-CAW-CAX-NAN
3	BBB	302	1BO	C1-C2-C3-C4
3	AAA	302	1BO	C2-C3-C4-OH
2	AAA	301	1S6	CB-CA-N-CAU
2	BBB	301	1S6	CB-CA-N-CAU
3	AAA	302	1BO	C1-C2-C3-C4

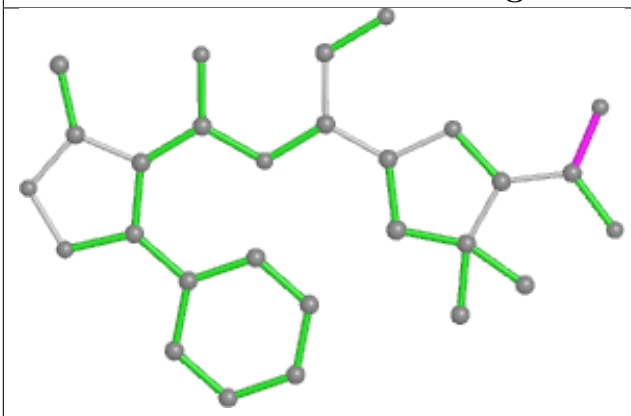
There are no ring outliers.

2 monomers are involved in 2 short contacts:

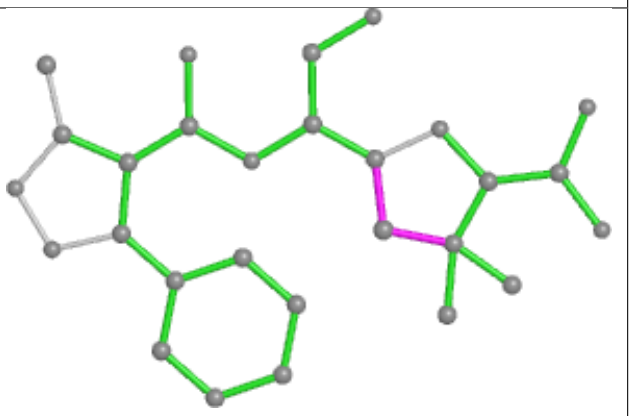
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	301	1S6	1	0
2	BBB	301	1S6	1	0

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.

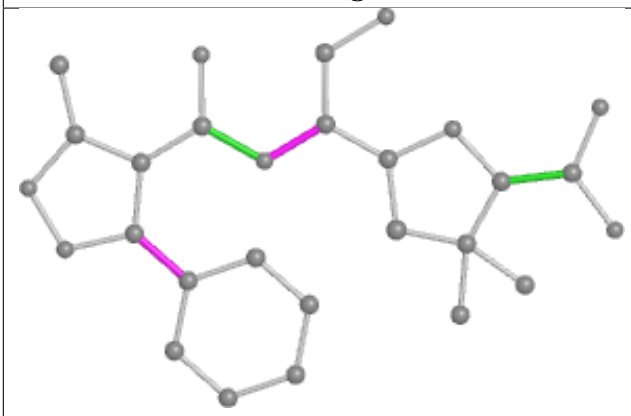
Ligand 1S6 AAA 301



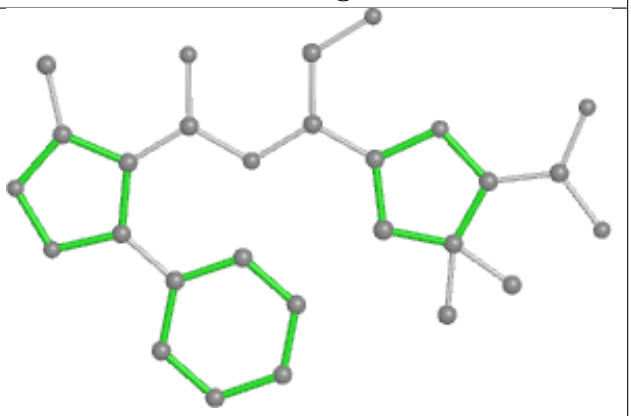
Bond lengths



Bond angles

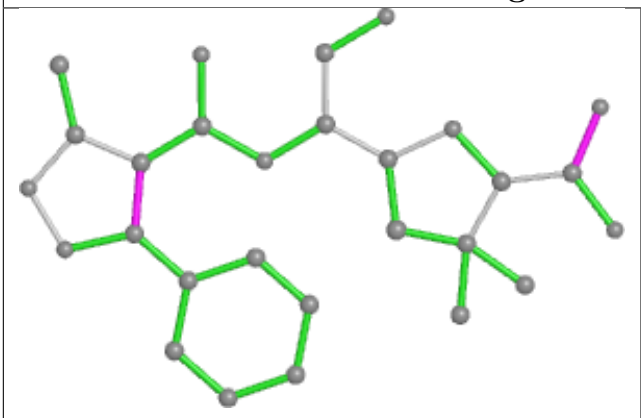


Torsions

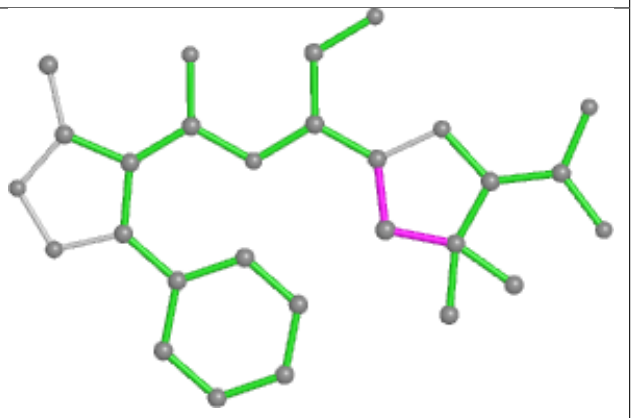


Rings

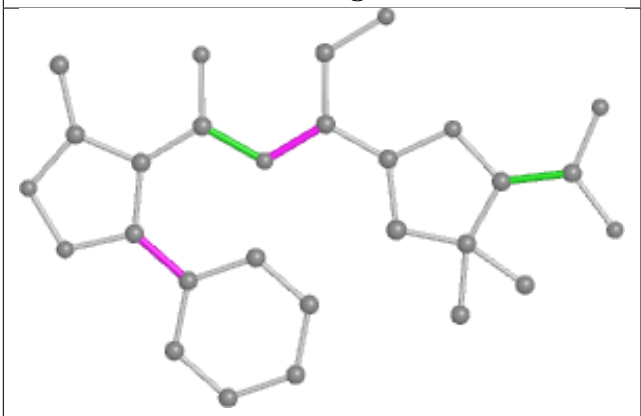
Ligand 1S6 BBB 301



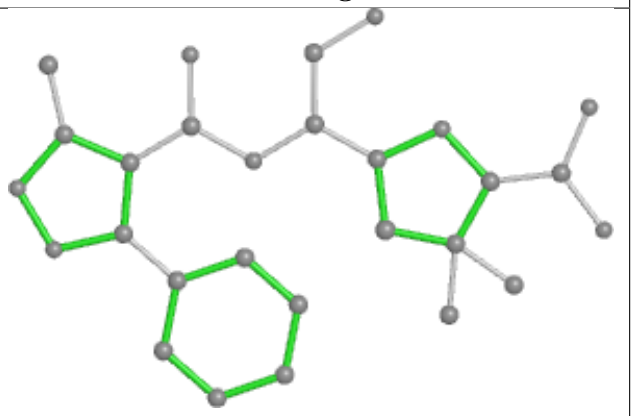
Bond lengths



Bond angles



Torsions



Rings

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

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^{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>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	240/260 (92%)	0.23	5 (2%)	63	70	28, 46, 80, 120	1 (0%)
1	BBB	241/260 (92%)	0.24	7 (2%)	51	59	30, 46, 81, 92	1 (0%)
All	All	481/520 (92%)	0.24	12 (2%)	57	64	28, 46, 81, 120	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	95	TRP	3.9
1	AAA	153	VAL	3.3
1	BBB	94	LYS	3.3
1	BBB	93	PHE	3.2
1	AAA	59	LEU	3.0
1	BBB	102	ILE	2.9
1	AAA	149	ILE	2.9
1	BBB	59	LEU	2.5
1	AAA	155	SER	2.4
1	AAA	230	ASP	2.3
1	BBB	79	ILE	2.2
1	BBB	130	ILE	2.0

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

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	B-factors(Å^2)	Q<0.9
1	ALY	AAA	73	12/13	0.96	0.14	28,33,49,51	0
1	ALY	BBB	73	12/13	0.97	0.14	37,43,47,47	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

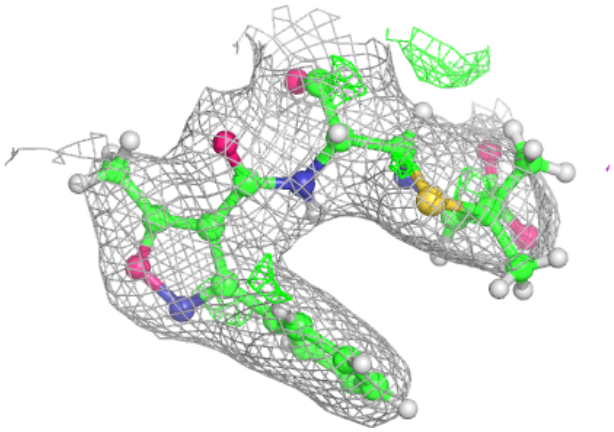
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

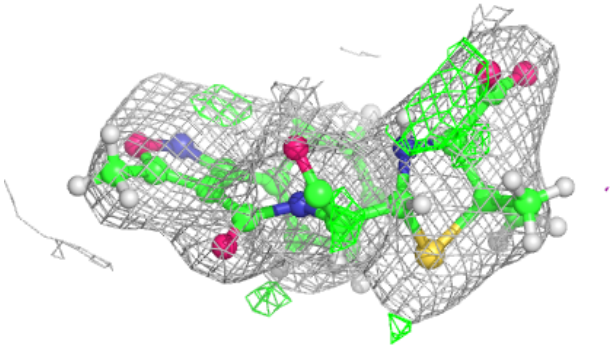
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	1BO	BBB	303	5/5	0.82	0.17	48,49,50,51	15
3	1BO	AAA	303	5/5	0.85	0.15	48,53,54,55	15
3	1BO	BBB	302	5/5	0.85	0.22	42,44,46,47	15
3	1BO	AAA	302	5/5	0.85	0.16	41,43,44,45	0
2	1S6	BBB	301	28/28	0.94	0.17	39,42,47,52	47
2	1S6	AAA	301	28/28	0.95	0.18	33,37,41,43	0
4	CL	AAA	304	1/1	0.99	0.15	27,27,27,27	0

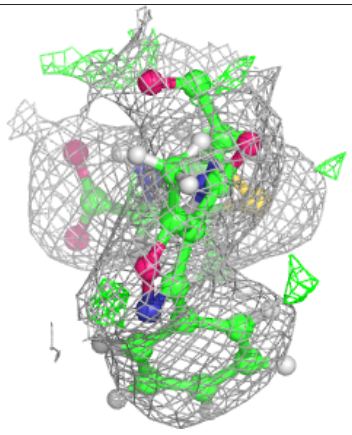
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1S6 BBB 301:

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

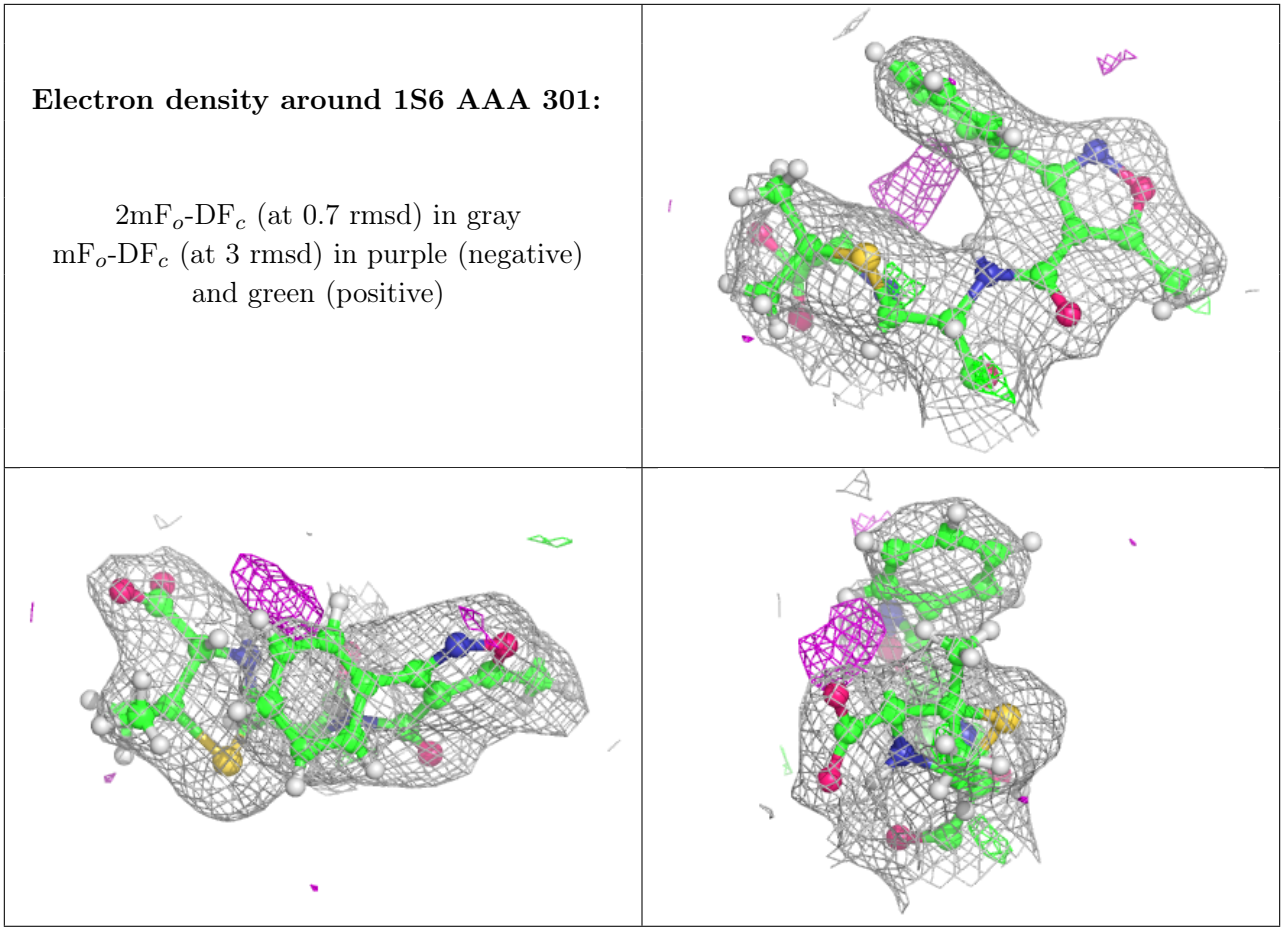






Electron density around 1S6 AAA 301:

$2mF_o$-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.