wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2023 – 07:50 AM EDT

PDB ID	:	2RDD
Title	:	X-ray crystal structure of AcrB in complex with a novel transmembrane helix.
Authors	:	Tornroth-Horsefield, S.; Gourdon, P.; Horsefield, R.; Neutze, R.
Deposited on	:	2007-09-22
Resolution	:	3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

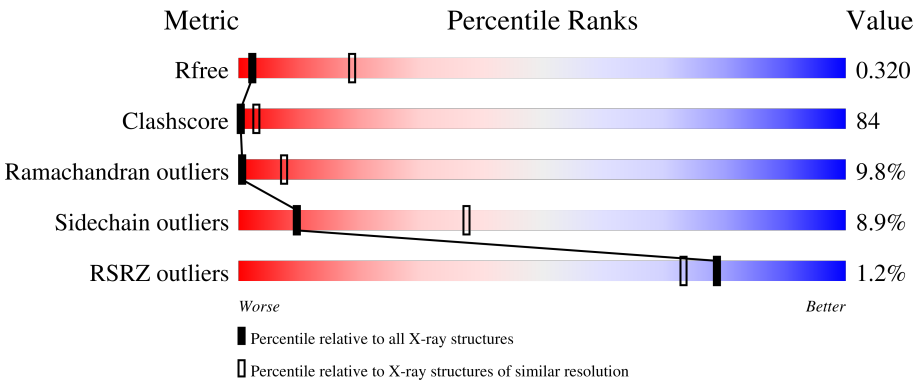
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.50 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))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	A	1049	% 21% 63% 13% • •
2	B	37	65% 32% •

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
3	AIC	A	1110	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8026 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.

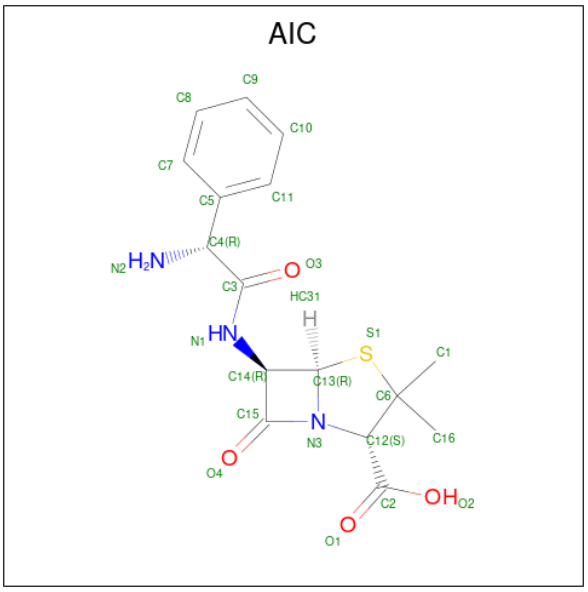
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1018	7760	5000	1281	1435	44	0	0	0

- Molecule 2 is a protein called UPF0092 membrane protein yajC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	37	218	138	39	38	3	23	0	0

- Molecule 3 is (2S,5R,6R)-6-{[(2R)-2-AMINO-2-PHENYLETHANOYL]AMINO}-3,3-DIMETHYL-7-OXO-4-THIA-1-AZABICYCLO[3.2.0]HEPTANE-2-CARBOXYLIC ACID (three-letter code: AIC) (formula: $C_{16}H_{19}N_3O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	24	16	3	4	1	0	0

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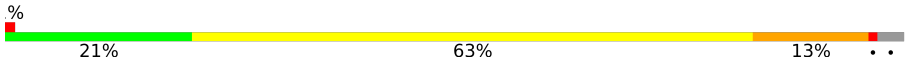
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	24	16	3	4	1	0	0

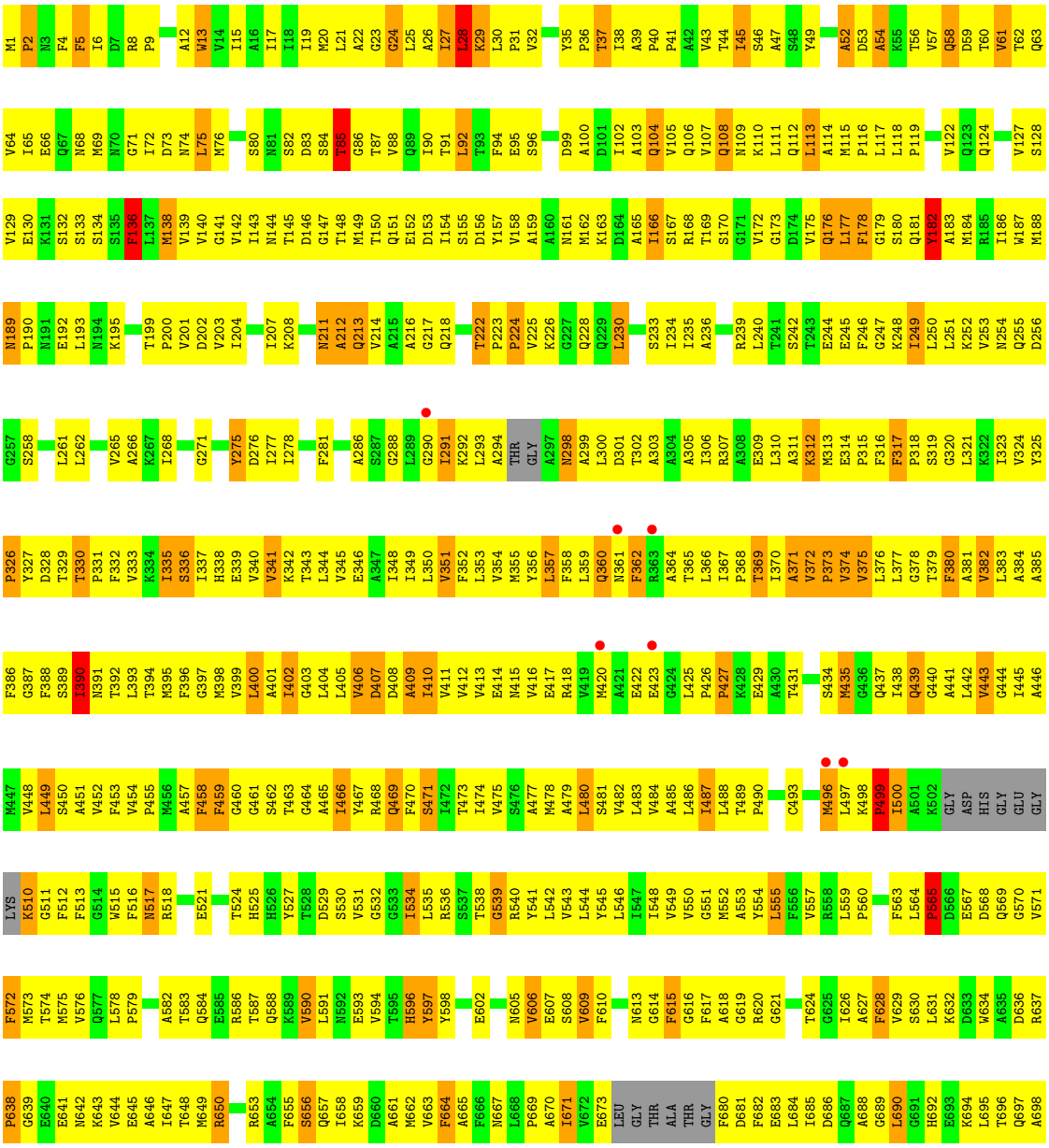
3 Residue-property plots (i)

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: Acriflavine resistance protein B

Chain A:





R699 N700 L703 A704 E705 A706 A707 K708 H709 P710 D711 M712 LEU THR SER V716 R717 P718 N719 G720 L721 T724 P725 Q726 F727 K728 I729 D730 Q733 A736 G740 V741 S742 I743 N744 D745 I746 N747 T748 T749 L750 G751 A752 A753 W754 Y758 V759 N760 D761 F762 I763 D764 R767

V768 K769 K770 V771 Y772 V773 M774 S775 E776 A777 K778 Y779 R780 M781 L782 P783 D784 D785 I786 G787 D788 W789 Y790 V791 R792 A793 A794 D795 G796 Q797 M798 V799 P800 F801 S802 A803 F804 S805 S806 S807 R808 G812 S813 P814 R815 L816 E817 R818 Y819 N820 G821 L822 P823 S824 M825 E826 I827 L828 G829

Q830 A831 A832 P833 G834 K835 S836 T837 G838 E839 A840 M841 E842 L843 M844 E845 Q846 L847 A848 S849 K850 L851 P852 T853 G854 V855 G856 Y857 D858 W859 T860 G861 M862 S863 Y864 Q865 E866 R867 L868 S869 Q872 A873 P874 S875 L876 Y877 A878 I879 S880 L881 I882 V883 V884 F885 L886 C887 L888 A889

E893 S894 W895 S896 I897 P898 F899 S900 V901 M902 L903 V904 V905 P906 L907 G908 V909 I910 G911 A912 L913 L914 A915 F918 R919 G920 L921 T922 N923 D924 V925 Y926 F927 Q928 V929 G930 L931 L932 T933 T934 I935 G936 L937 S938 A939 K940 N941 A942 I943 L944 I945 V946 E947 F948 A949 K950 D951 L952 M953

D954 K955 G959 L960 I961 E962 A963 T964 L965 D966 A967 V968 R969 M970 R971 L972 R973 P974 I975 L976 M977 T978 S979 L980 A981 F982 I983 L984 G985 V986 M987 P988 L989 V990 I991 S992 T993 G994 A995 G996 S997 G998 A999 Q1000 N1001 A1002 V1003 G1004 T1005 G1006 V1007 M1008 G1009 G1010 M1011 V1012 T1013 A1014 T1015

V1016 L1017 A1018 I1019 F1020 F1021 V1022 P1023 V1024 F1025 F1026 V1027 V1028 V1029 R1030 R1031 R1032 R1035 K1036 ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS

- Molecule 2: UPF0092 membrane protein yajC

Chain B: 65% 32%

S19 I33 F34 Y35 P41 Q42 Q43 K44 R45 T46 K47 E48 H49 K50 K51 L52 M53 D54 S55

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	145.10Å 145.10Å 511.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.50 72.55 – 3.50	Depositor EDS
% Data completeness (in resolution range)	88.0 (50.00-3.50) 88.1 (72.55-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.279 , 0.317 0.267 , 0.320	Depositor DCC
R_{free} test set	1182 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	101.4	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 62.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	8026	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 (i)

5.1 Standard geometry (i)

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

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	0.56	1/7905 (0.0%)	0.88	7/10728 (0.1%)
2	B	0.36	0/220	0.61	1/302 (0.3%)
All	All	0.56	1/8125 (0.0%)	0.87	8/11030 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	565	PRO	N-CD	5.72	1.55	1.47

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	41	PRO	N-CA-CB	5.75	110.20	103.30
1	A	469	GLN	CB-CA-C	5.42	121.23	110.40
1	A	510	LYS	C-N-CA	5.32	133.47	122.30
1	A	510	LYS	CA-C-N	-5.24	105.72	116.20
1	A	178	PHE	CB-CG-CD2	5.19	124.43	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7760	0	7920	1342	1
2	B	218	0	145	11	0
3	A	48	0	36	13	0
All	All	8026	0	8101	1352	1

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 84.

The worst 5 of 1352 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:A:49:TYR:CD2	1:A:52:ALA:HB2	1.67	1.27
1:A:462:SER:CB	1:A:865:GLN:HE22	1.51	1.24
1:A:670:ALA:O	1:A:671:ILE:HG12	1.33	1.22
1:A:499:PRO:O	1:A:500:ILE:HG13	1.30	1.22
1:A:448:VAL:HG21	1:A:888:LEU:CD2	1.70	1.22

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:CG1	1:A:105:VAL:CG1[2_445]	2.12	0.08

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	1008/1049 (96%)	678 (67%)	231 (23%)	99 (10%)	0 7
2	B	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1 9
All	All	1043/1086 (96%)	704 (68%)	237 (23%)	102 (10%)	0 7

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ALA
1	A	108	GLN
1	A	182	TYR
1	A	222	THR
1	A	407	ASP

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	831/855 (97%)	757 (91%)	74 (9%)	9	37
2	B	10/36 (28%)	9 (90%)	1 (10%)	7	32
All	All	841/891 (94%)	766 (91%)	75 (9%)	9	37

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	775	SER
1	A	979	SER
1	A	801	PHE
1	A	887	CYS
1	A	298	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	A	569	GLN
1	A	871	ASN
1	A	525	HIS
1	A	605	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	AIC	A	1110	-	24,26,26	1.42	3 (12%)	35,40,40	1.85	9 (25%)
3	AIC	A	1109	-	24,26,26	1.40	3 (12%)	35,40,40	1.69	7 (20%)

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	AIC	A	1110	-	-	2/16/47/47	0/3/3/3
3	AIC	A	1109	-	-	6/16/47/47	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1109	AIC	C11-C5	2.42	1.43	1.39
3	A	1109	AIC	C6-C12	2.41	1.61	1.56
3	A	1110	AIC	C6-C12	2.41	1.61	1.56
3	A	1110	AIC	C11-C5	2.36	1.42	1.39
3	A	1110	AIC	C12-C2	2.27	1.55	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1110	AIC	C4-C3-N1	4.71	120.51	114.78
3	A	1110	AIC	C12-C6-S1	-4.68	96.17	104.10
3	A	1109	AIC	C4-C3-N1	4.66	120.45	114.78
3	A	1109	AIC	C12-C6-S1	-3.60	97.99	104.10
3	A	1110	AIC	C1-C6-S1	3.55	115.17	109.21

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1109	AIC	C6-C12-C2-O2
3	A	1109	AIC	N1-C3-C4-C5
3	A	1109	AIC	O3-C3-C4-C5
3	A	1109	AIC	N1-C3-C4-N2
3	A	1110	AIC	C6-C12-C2-O2

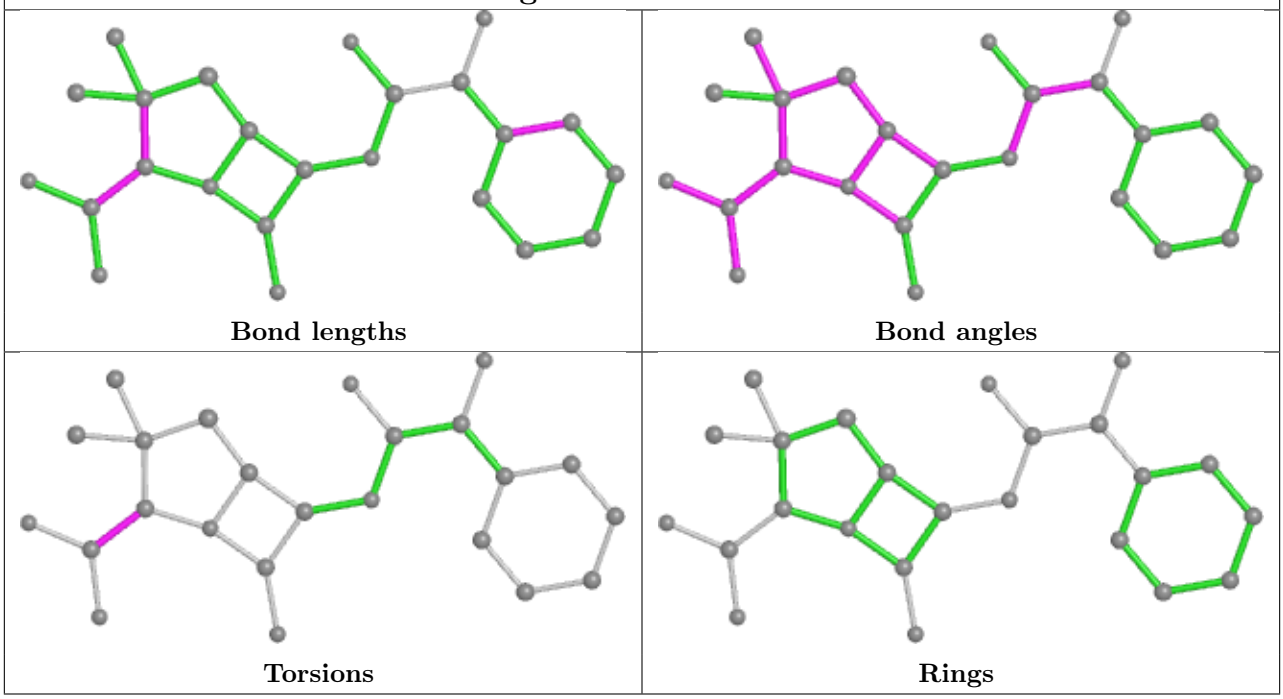
There are no ring outliers.

1 monomer is involved in 13 short contacts:

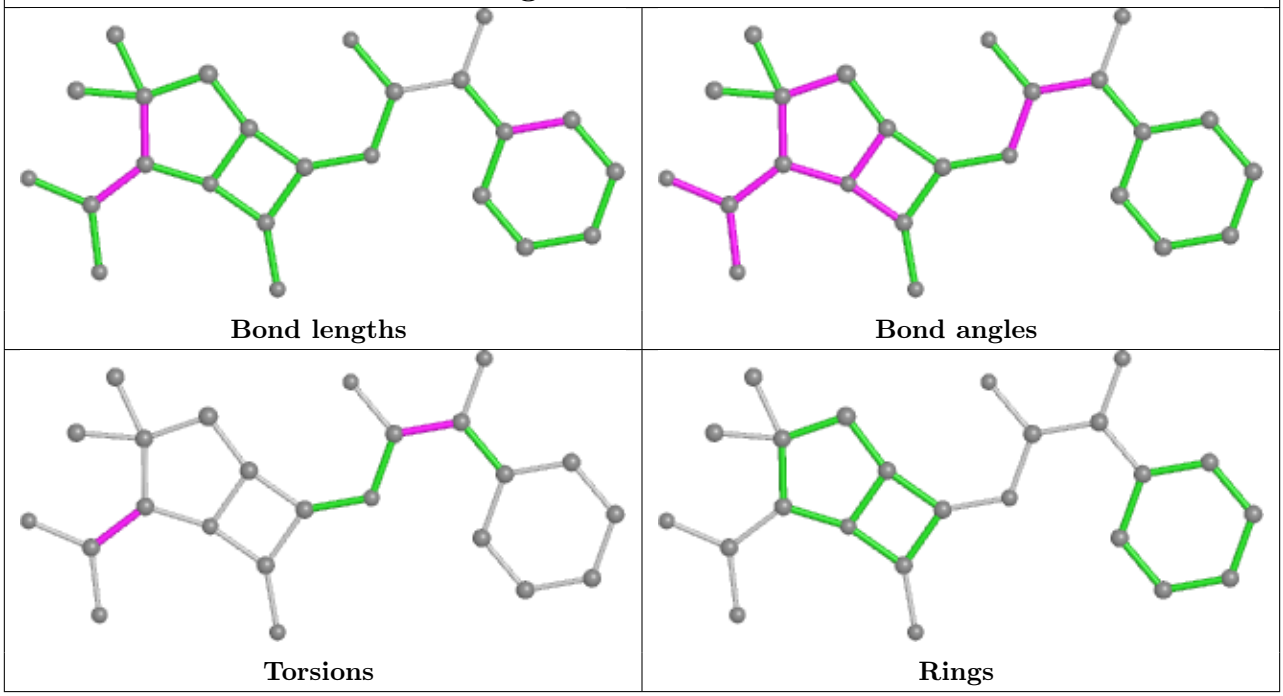
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1110	AIC	13	0

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 AIC A 1110



Ligand AIC A 1109



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 (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, 95th 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	A	1018/1049 (97%)	-0.14	13 (1%) 77 71	15, 61, 132, 173	0
2	B	37/37 (100%)	-0.79	0 100 100	49, 76, 135, 145	8 (21%)
All	All	1055/1086 (97%)	-0.16	13 (1%) 79 73	15, 62, 132, 173	8 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	830	GLN	3.3
1	A	836	SER	3.3
1	A	716	VAL	3.0
1	A	874	PRO	2.8
1	A	839	GLU	2.6

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 monosaccharides in this entry.

6.4 Ligands (i)

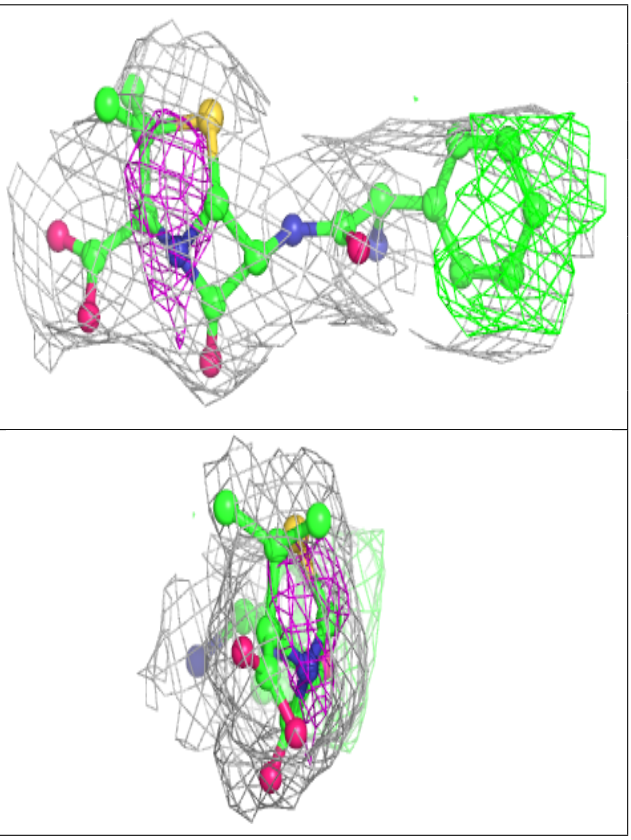
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	AIC	A	1109	24/24	0.80	0.27	49,49,49,49	0
3	AIC	A	1110	24/24	0.84	0.25	49,49,49,49	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.

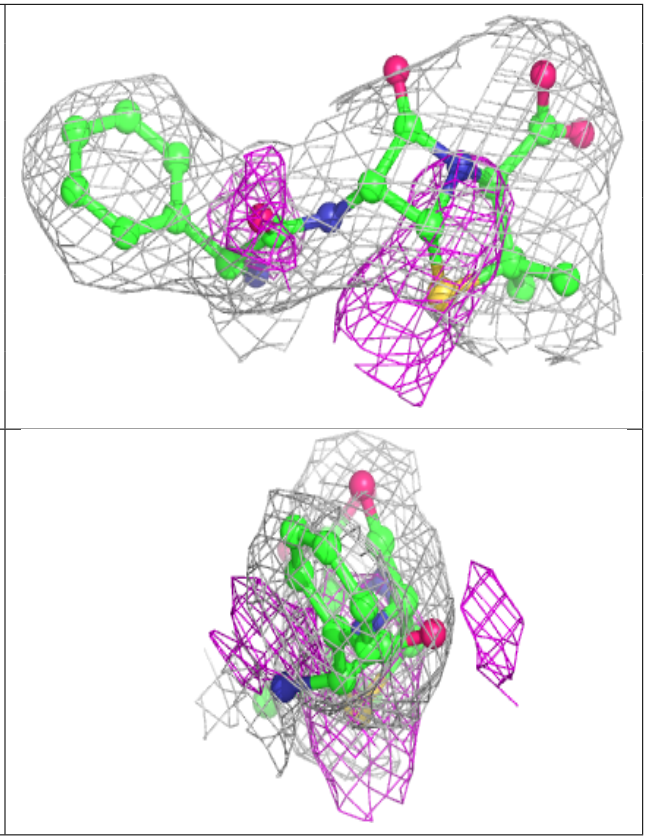
Electron density around AIC A 1109:

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 AIC A 1110:

$2mF_o$-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 (i)

There are no such residues in this entry.