wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2023 – 06:34 PM EDT

PDB ID	:	3AOB
Title	:	Structures of the multidrug exporter AcrB reveal a proximal multisite drug-binding pocket
Authors	:	Nakashima, R.; Sakurai, K.; Yamaguchi, A.
Deposited on	:	2010-09-23
Resolution	:	3.35 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:

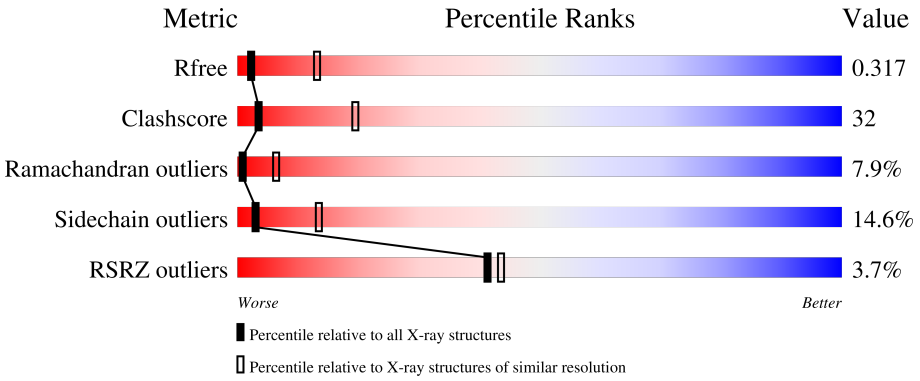
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	A	1053	3% 44% 42% 10%
1	B	1053	4% 39% 47% 11%
1	C	1053	4% 42% 43% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23385 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.

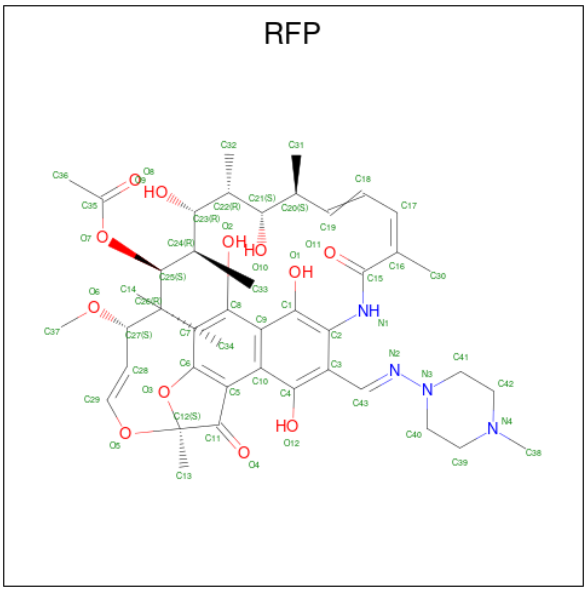
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
B	1051	HIS	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
C	1050	HIS	-	expression tag	UNP P31224
C	1051	HIS	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

- Molecule 2 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 59 43 4 12	0	0

- Molecule 3 is water.

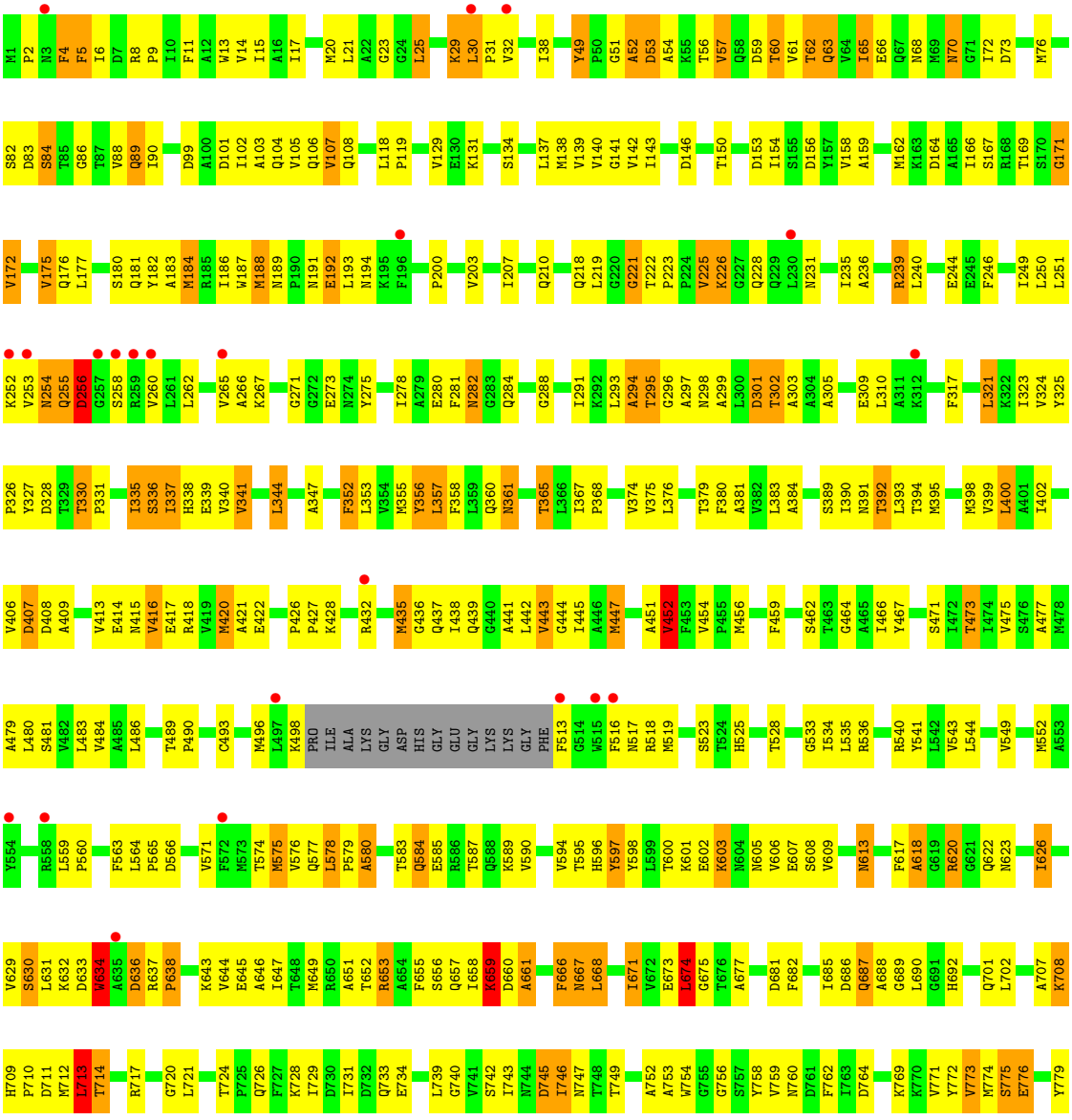
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0

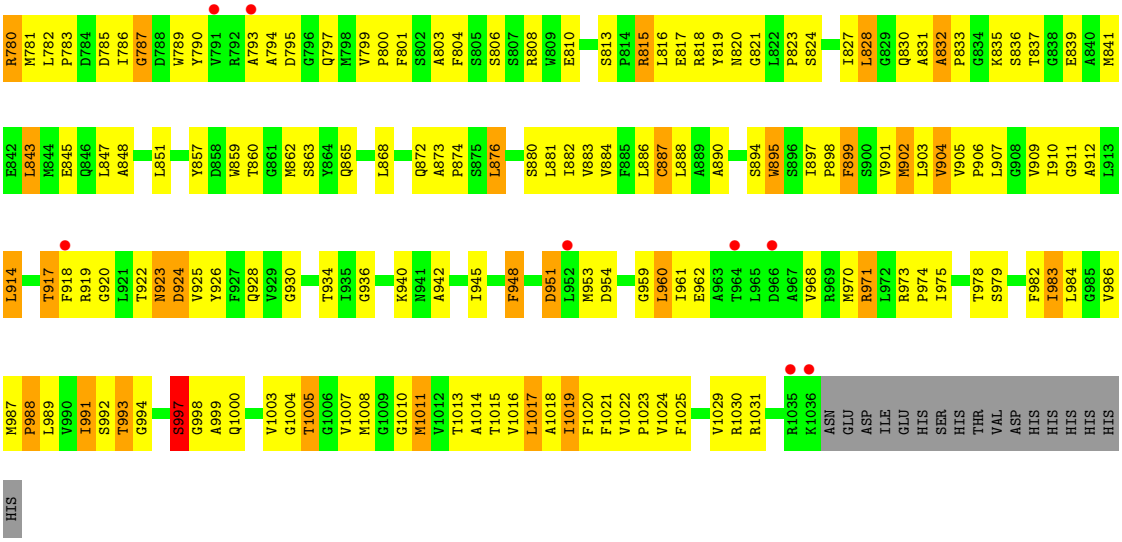
3 Residue-property plots (i)

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

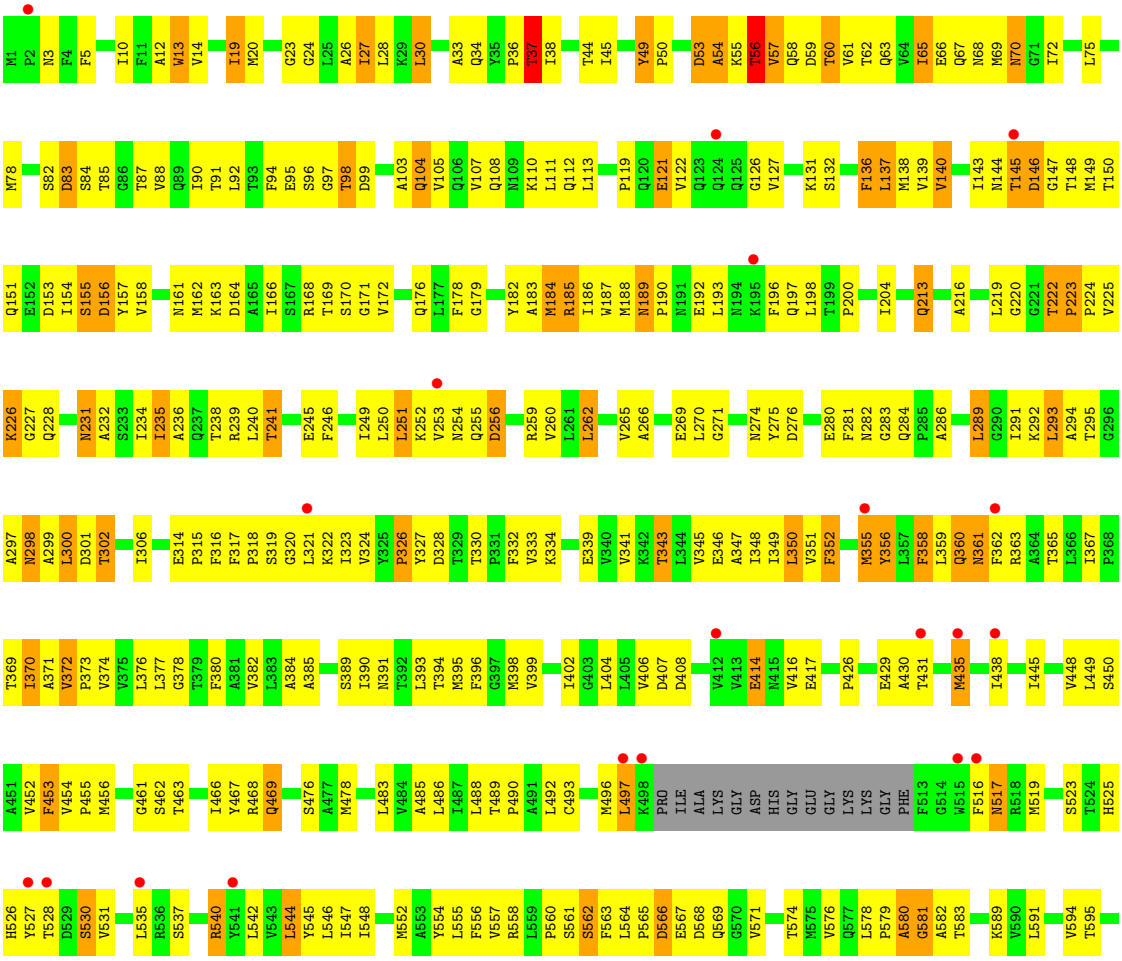
Chain A:

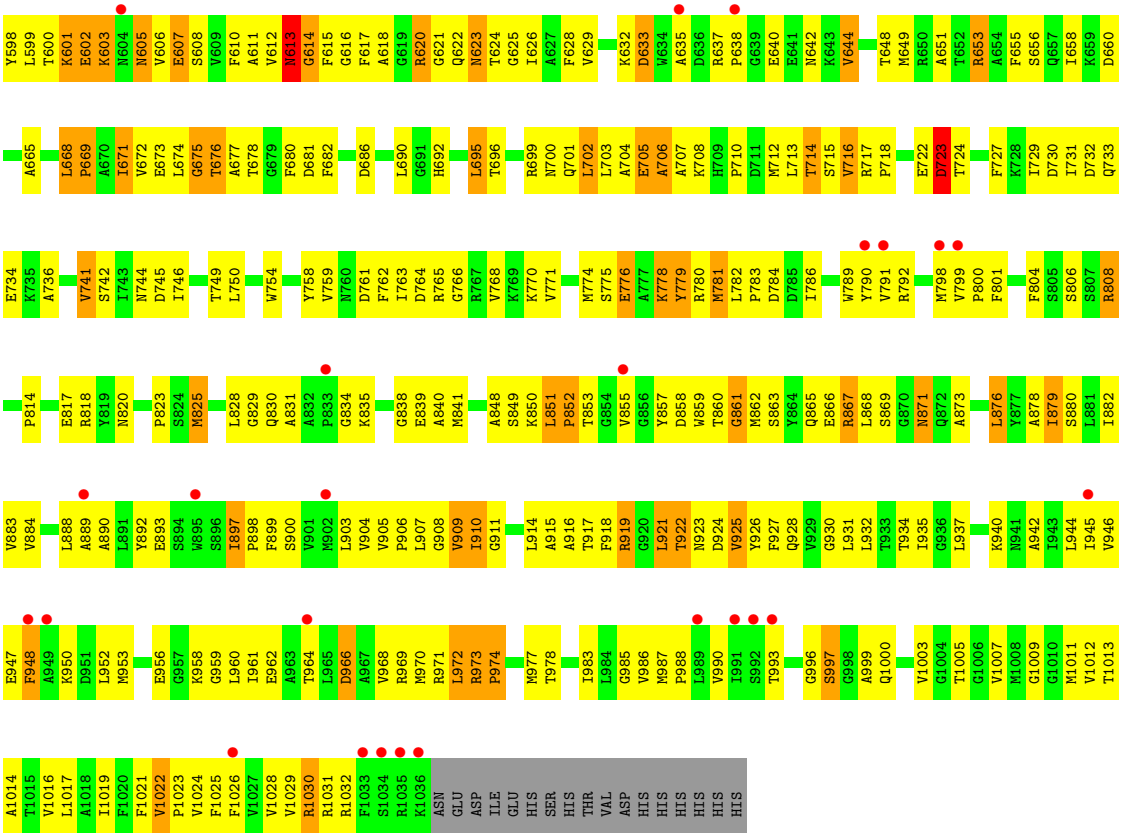




• Molecule 1: Acriflavine resistance protein B

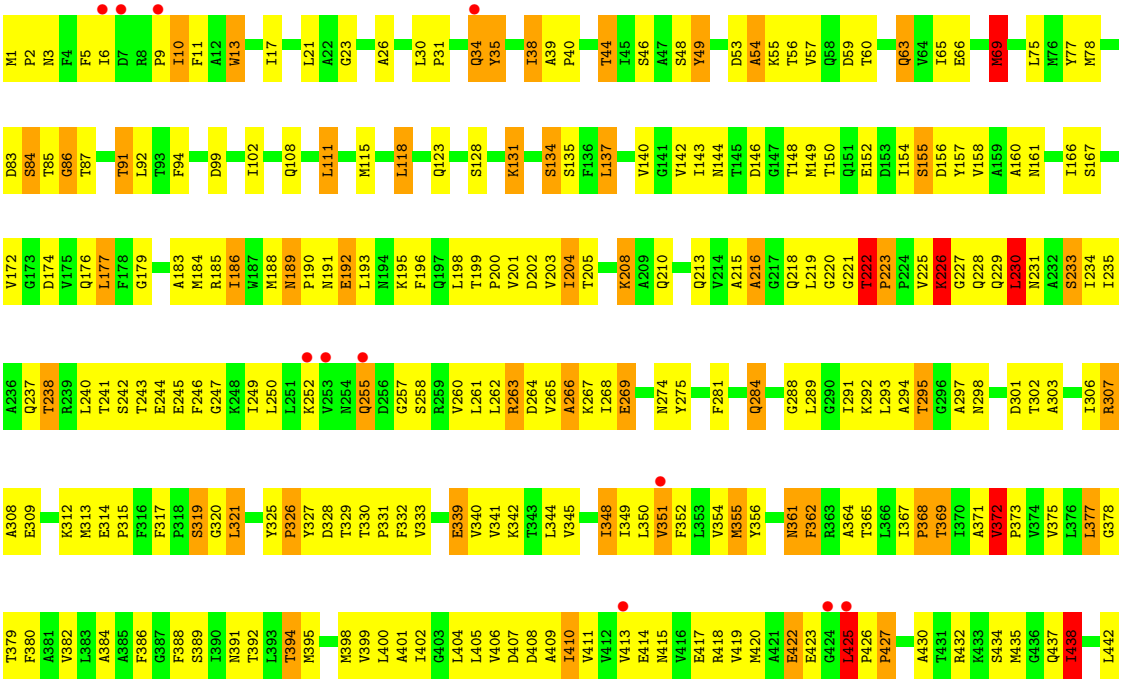
Chain B:

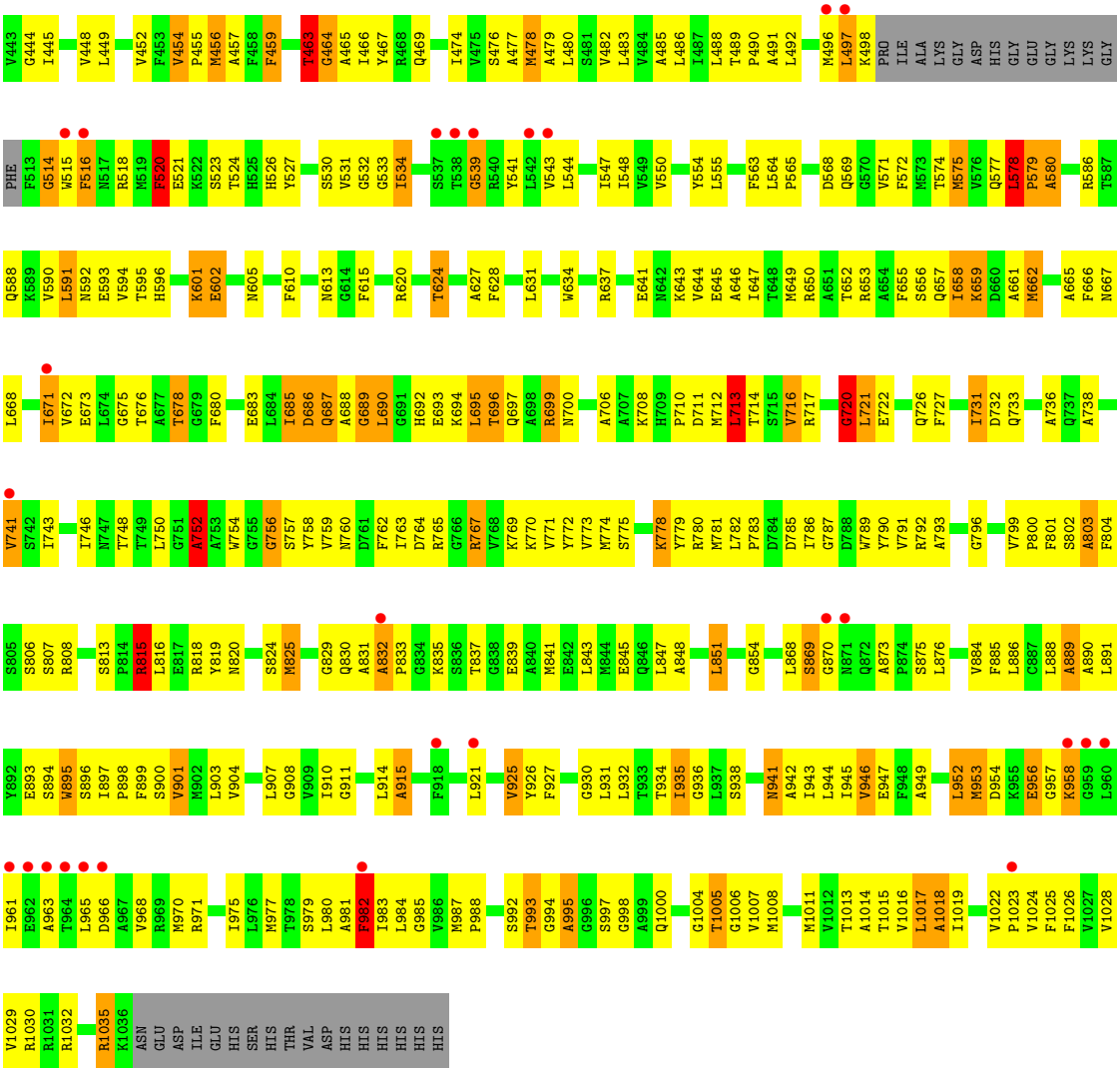




• Molecule 1: Acriflavine resistance protein B

Chain C:




V443 G444 I445 V448 L449 V452 F453 V454 P455 M456 A457 F458 F459 T463 G464 A465 I466 Y467 R468 Q469 I474 V475 S476 A477 M478 A479 L480 S481 V482 L483 V484 A485 L486 I487 L488 T489 P490 A491 L492 M496 L497 K498 PRO ILE ALA LYS GLY ASP HIS GLY GLU GLY LYS LYS GLY
PHE F513 G514 W515 F516 N517 R518 M519 F520 E521 K522 S523 T524 H525 H526 Y527 S530 V531 G532 G533 I534 S537 T538 G539 R540 Y541 L542 V543 L544 I547 I548 V549 V550 Y554 L555 F563 L564 P565 D568 Q569 G570 V571 F572 M573 T574 M575 V576 Q577 L578 P579 A580 R586 T587
Q588 K589 V590 L591 N592 E593 V594 T595 H596 K601 E602 N605 F610 N613 G614 F615 R620 T624 A627 F628 L631 W634 R637 E641 N642 K643 V644 E645 A646 I647 T648 M649 R650 A651 T652 R653 A654 F655 S656 Q657 I658 K659 D660 A661 M662 A665 F666 N667
L668 I671 V672 E673 L674 G675 T676 A677 T678 G679 F680 E683 L684 I685 D686 Q687 A688 G689 L690 G691 H692 E693 K694 L695 T696 Q697 A698 R699 N700 A706 A707 K708 H709 P710 D711 M712 L713 T714 S715 V716 R717 G720 L721 E722 Q726 F727 I731 D732 Q733 A736 Q737 A738
V741 S742 I743 I746 W747 T748 T749 L750 G751 A752 A753 W754 G755 G756 S757 Y758 V759 N760 D761 F762 I763 D764 R765 G766 R767 V768 K769 K770 V771 Y772 V773 M774 S775 K778 Y779 R780 M781 L782 P783 D784 D785 I786 G787 D788 W789 Y790 V791 R792 A793 G796 V799 P800 F801 S802 A803 F804
S805 S806 S807 R808 S813 P814 R815 L816 E817 R818 Y819 N820 S824 M825 G829 Q830 A831 A832 P833 G834 K835 S836 T837 G838 E839 A840 M841 E842 L843 M844 E845 Q846 L847 A848 L851 G854 L868 S869 G870 N871 Q872 A873 P874 S875 L876 V884 F885 L886 C887 L888 A889 A890 L891
V892 E893 S894 W895 S896 I897 P898 F899 S900 V901 M902 L903 V904 L907 G908 V909 I910 G911 L914 A915 F918 L921 V925 Y926 F927 G930 L931 L932 T933 T934 I935 G936 L937 S938 N941 A942 I943 L944 I945 V946 E947 F948 A949 L952 M953 D954 K955 E956 G957 K958 G959 L960
I961 E962 A963 T964 L965 D966 A967 V968 R969 M970 R971 I975 L976 M977 T978 S979 L980 A981 F982 I983 L984 G985 V986 M987 P988 S992 T993 G994 A995 G996 S997 G998 A999 Q1000 G1004 T1005 G1006 V1007 M1008 M1011 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 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 HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	223.90Å 134.31Å 161.77Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	48.91 – 3.35 48.91 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.91-3.35) 97.7 (48.91-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.64 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.261 , 0.326 0.256 , 0.317	Depositor DCC
R_{free} test set	3350 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	87.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 71.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	23385	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: RFP

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	0.62	0/7920	0.75	2/10756 (0.0%)
1	B	0.58	0/7920	0.76	4/10756 (0.0%)
1	C	0.62	0/7920	0.76	5/10756 (0.0%)
All	All	0.61	0/23760	0.76	11/32268 (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	C	0	2

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	356	TYR	N-CA-CB	-12.26	88.53	110.60
1	B	355	MET	CB-CA-C	10.91	132.23	110.40
1	C	321	LEU	CA-CB-CG	8.34	134.48	115.30
1	B	960	LEU	CA-CB-CG	6.20	129.56	115.30
1	B	352	PHE	CB-CA-C	6.12	122.65	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	221	GLY	Peptide
1	C	222	THR	Peptide

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	7774	0	7931	460	0
1	B	7774	0	7931	536	0
1	C	7774	0	7931	577	0
2	C	59	0	57	10	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	23385	0	23850	1518	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 32.

The worst 5 of 1518 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:447:MET:HB3	1:A:887:CYS:SG	1.82	1.20
1:C:222:THR:HG23	1:C:223:PRO:CD	1.73	1.17
1:C:815:ARG:HG2	1:C:815:ARG:HH11	1.09	1.17
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.31	1.12
1:A:379:THR:HG21	1:A:477:ALA:HA	1.27	1.12

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	1018/1053 (97%)	769 (76%)	174 (17%)	75 (7%)	1 7
1	B	1018/1053 (97%)	742 (73%)	193 (19%)	83 (8%)	1 6
1	C	1018/1053 (97%)	754 (74%)	182 (18%)	82 (8%)	1 6
All	All	3054/3159 (97%)	2265 (74%)	549 (18%)	240 (8%)	1 6

5 of 240 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	VAL
1	A	188	MET
1	A	239	ARG
1	A	256	ASP
1	A	293	LEU

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	833/859 (97%)	712 (86%)	121 (14%)	3 14
1	B	833/859 (97%)	705 (85%)	128 (15%)	2 12
1	C	833/859 (97%)	718 (86%)	115 (14%)	3 15
All	All	2499/2577 (97%)	2135 (85%)	364 (15%)	3 13

5 of 364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	876	LEU
1	C	255	GLN
1	B	925	VAL
1	C	75	LEU
1	C	361	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	151	GLN
1	C	588	GLN
1	C	189	ASN
1	C	237	GLN
1	C	872	GLN

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)

1 ligand is 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	RFP	C	2002	-	63,63,63	1.98	3 (4%)	94,94,94	1.83	14 (14%)

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	RFP	C	2002	-	-	16/60/85/85	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2002	RFP	O4-C11	13.30	1.43	1.21
2	C	2002	RFP	O7-C35	5.55	1.47	1.35
2	C	2002	RFP	O5-C29	3.39	1.48	1.39

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2002	RFP	O4-C11-C5	-8.76	115.09	131.81
2	C	2002	RFP	C41-C42-N4	5.45	116.96	110.80
2	C	2002	RFP	O7-C35-C36	4.49	119.35	111.09
2	C	2002	RFP	O4-C11-C12	-4.08	112.25	120.56
2	C	2002	RFP	O3-C6-C7	3.96	127.95	121.14

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2002	RFP	C2-C3-C43-N2
2	C	2002	RFP	C4-C3-C43-N2
2	C	2002	RFP	C26-C27-O6-C37
2	C	2002	RFP	C28-C27-O6-C37
2	C	2002	RFP	C36-C35-O7-C25

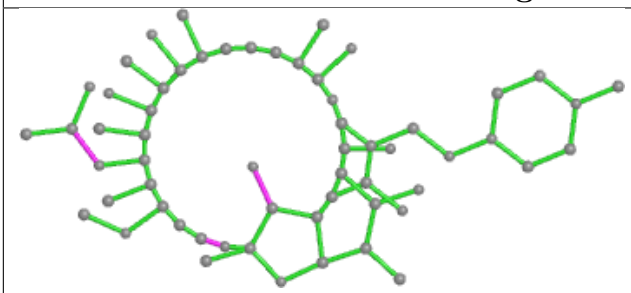
There are no ring outliers.

1 monomer is involved in 10 short contacts:

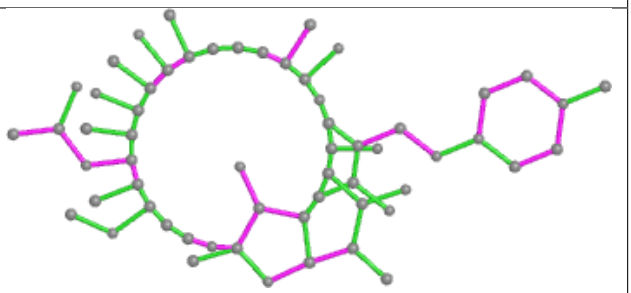
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2002	RFP	10	0

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.

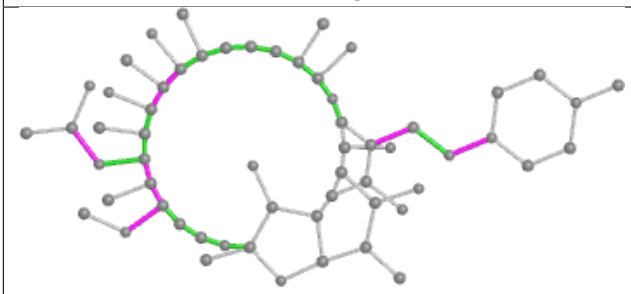
Ligand RFP C 2002



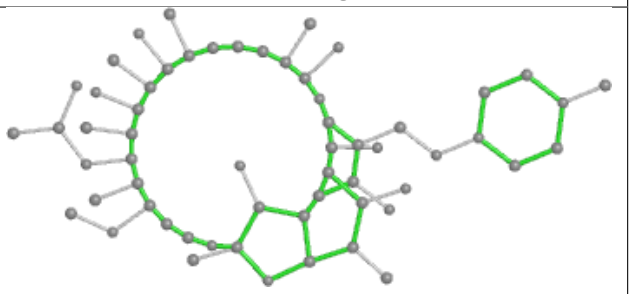
Bond lengths



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	A	1022/1053 (97%)	0.06	30 (2%) 51 54	40, 90, 124, 144	0
1	B	1022/1053 (97%)	0.21	45 (4%) 34 37	57, 97, 133, 162	0
1	C	1022/1053 (97%)	0.09	38 (3%) 41 43	35, 89, 138, 167	0
All	All	3066/3159 (97%)	0.12	113 (3%) 41 43	35, 92, 134, 167	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1036	LYS	6.1
1	C	538	THR	5.7
1	C	870	GLY	5.0
1	B	1034	SER	4.9
1	A	515	TRP	4.9

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

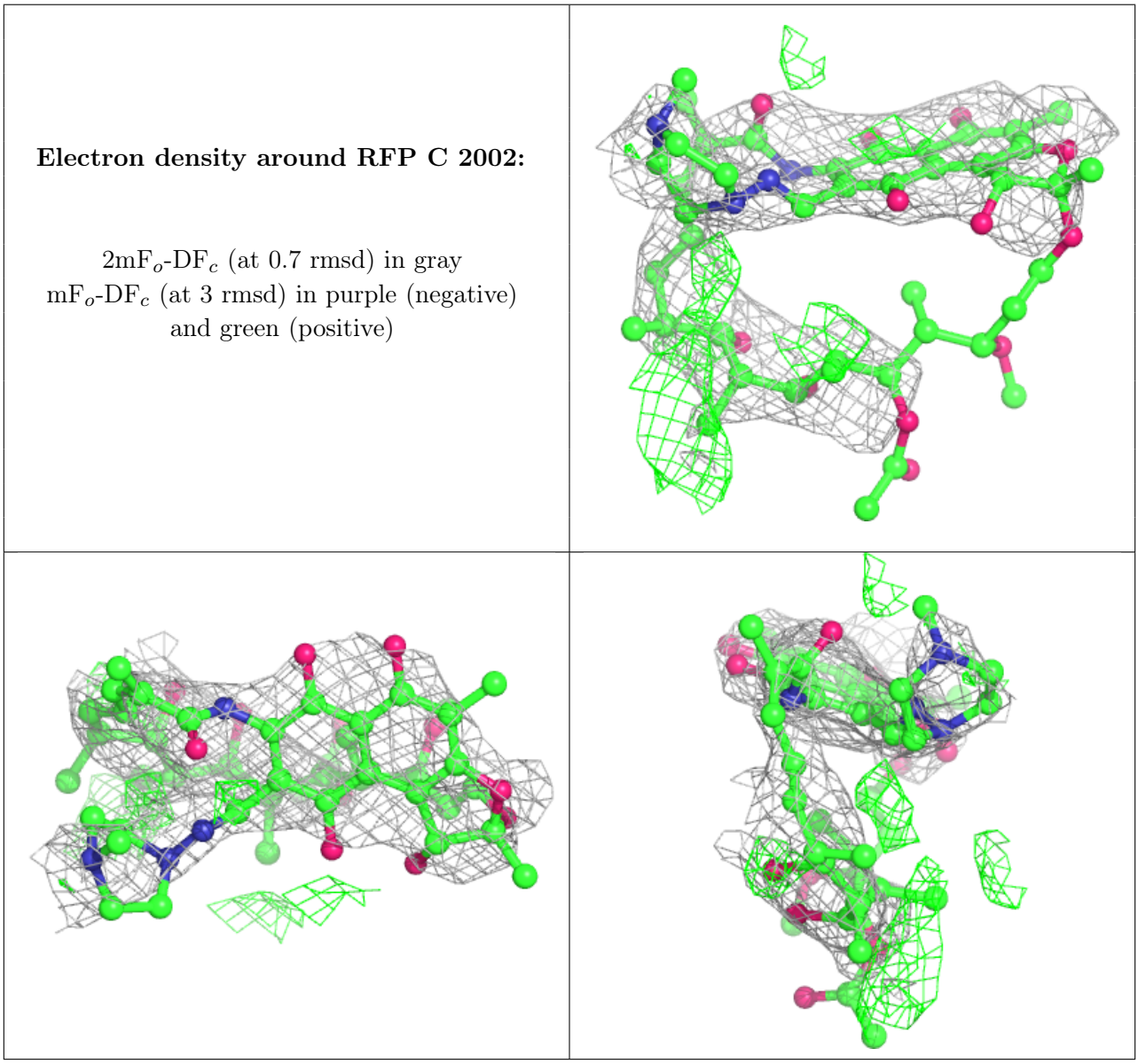
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	RFP	C	2002	59/59	0.83	0.34	100,104,105,105	59

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 RFP C 2002:

$2mF_o$-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.