wwPDB X-ray Structure Validation Summary Report (i)

Mar 4, 2024 – 11:55 PM EST

PDB ID	:	2DR6
Title	:	Crystal structure of a multidrug transporter reveal a functionally rotating mechanism
Authors	:	Murakami, S.; Nakashima, R.; Yamashita, E.; Matsumoto, T.
Deposited on	:	2006-06-08
Resolution	:	3.30 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 (1)) were used in the production of this report:

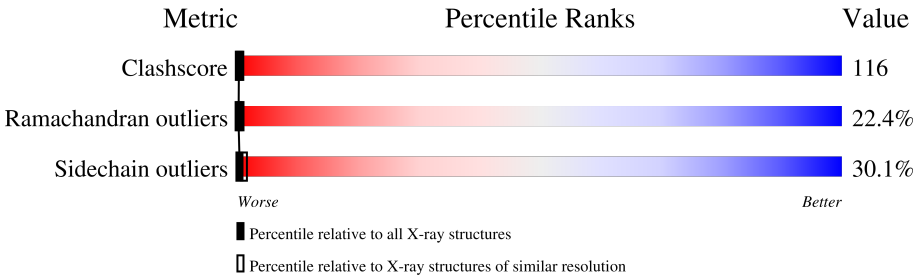
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.30 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	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1053	10% 41% 34% 13% .
1	B	1053	10% 46% 31% 10% .
1	C	1053	9% 39% 34% 15% .

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
2	DM2	A	2002	X	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23361 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.

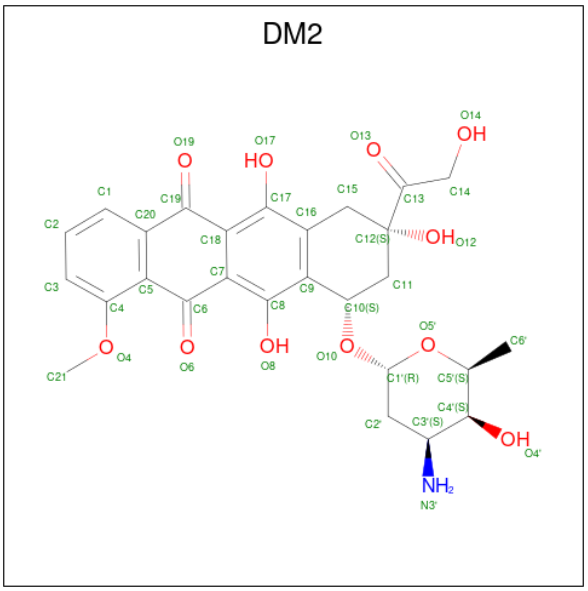
- Molecule 1 is a protein called ACRB.

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 DOXORUBICIN (three-letter code: DM2) (formula: $C_{27}H_{29}NO_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	39	27	1	11	0	0

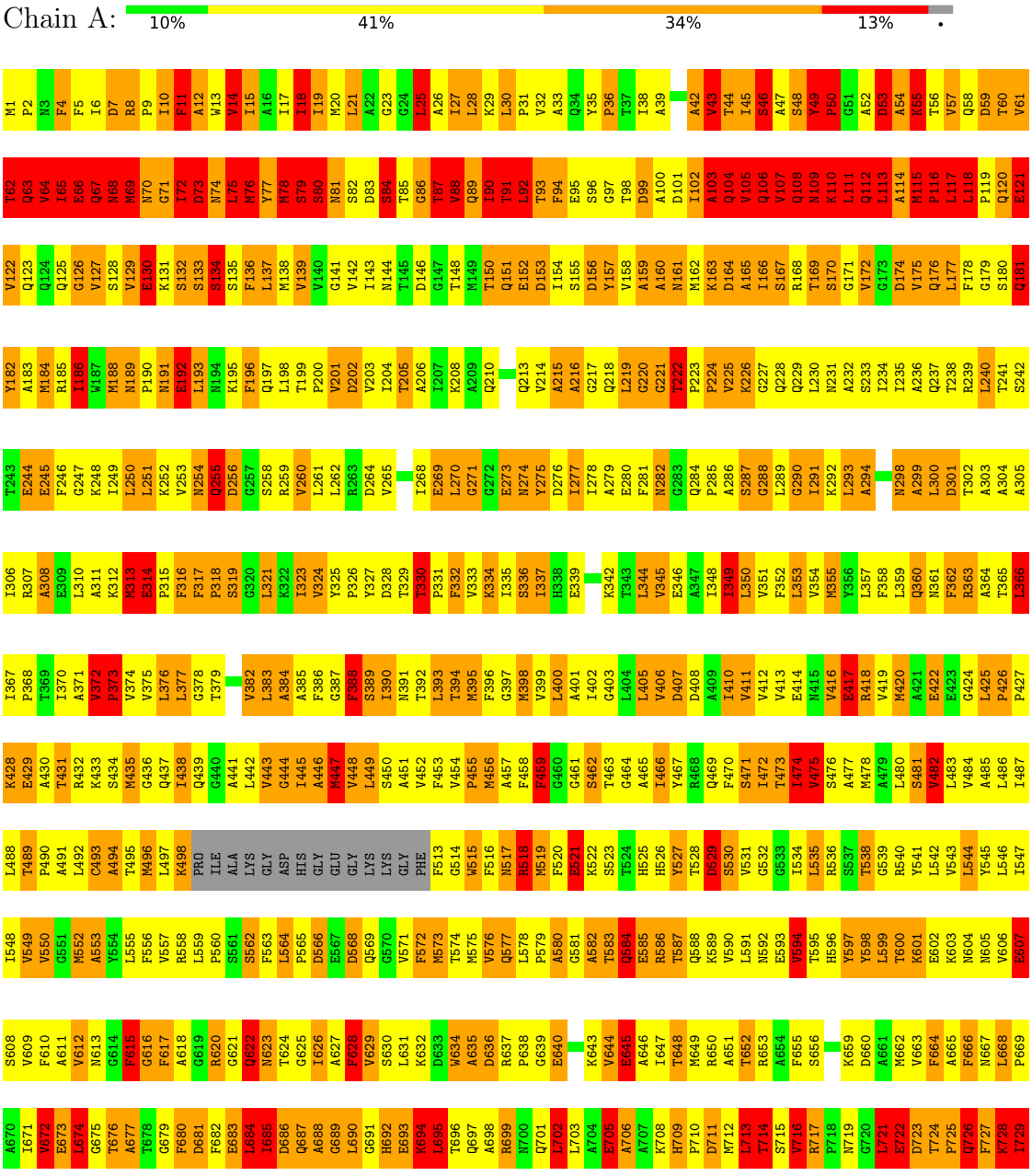
3 Residue-property plots (i)

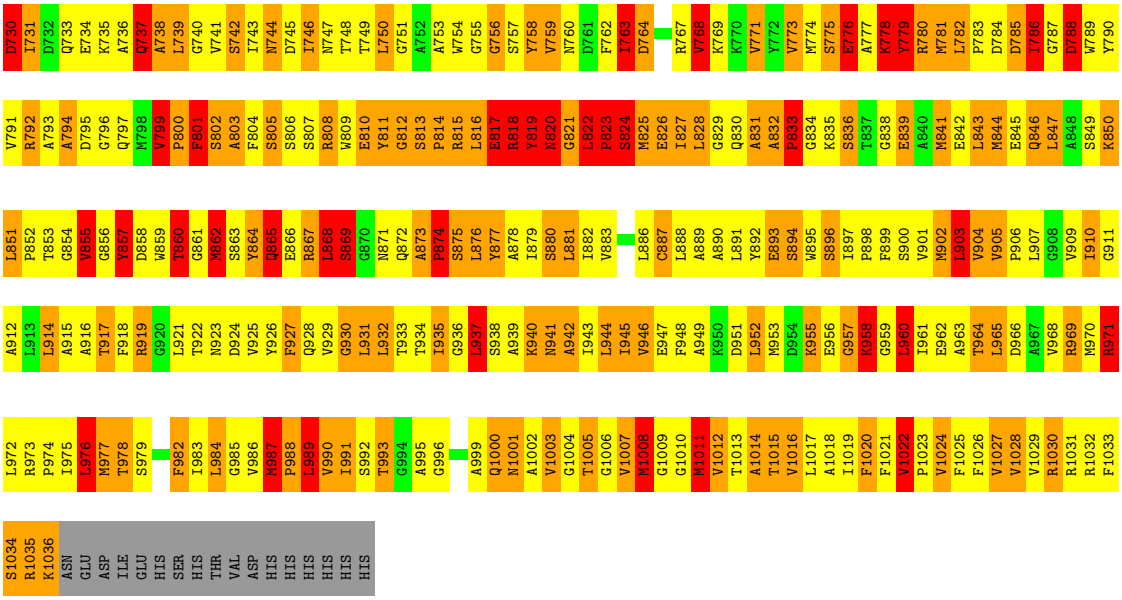
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

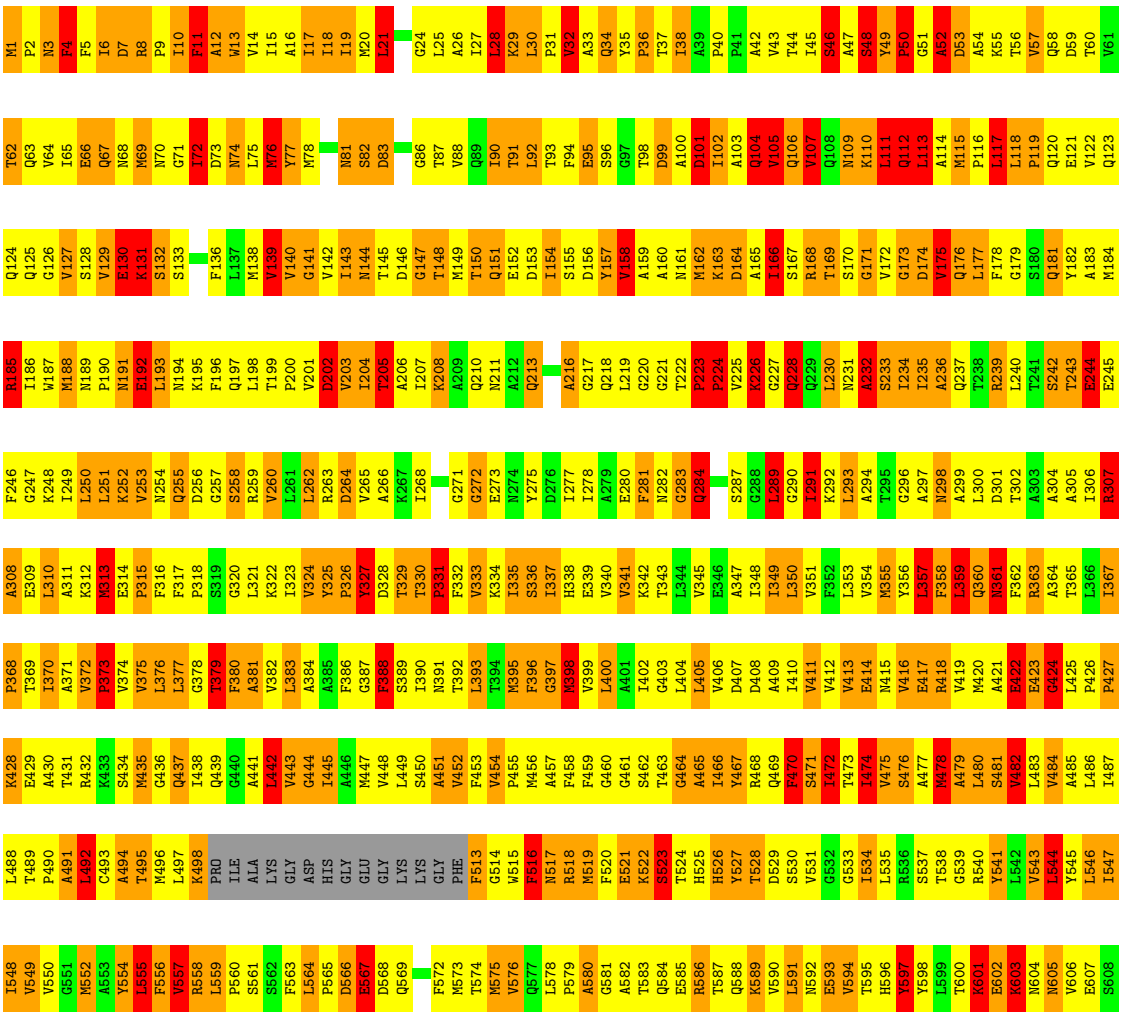
Chain A:

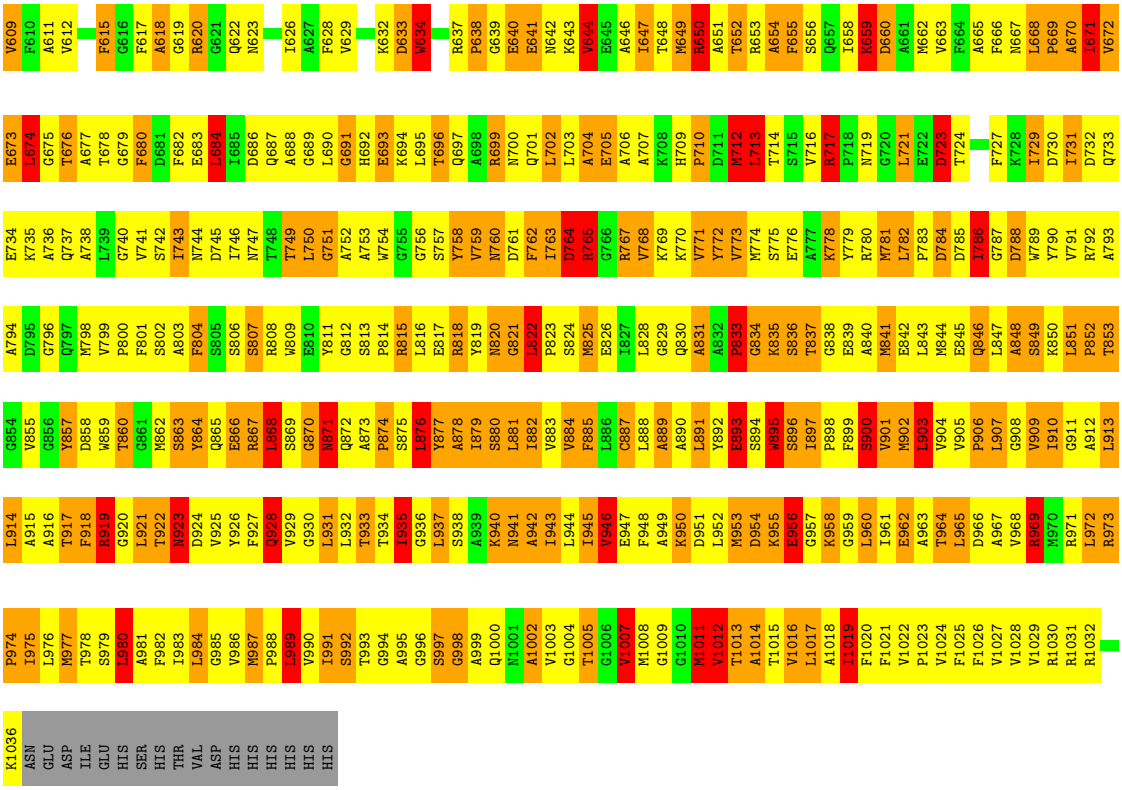




• Molecule 1: ACRB

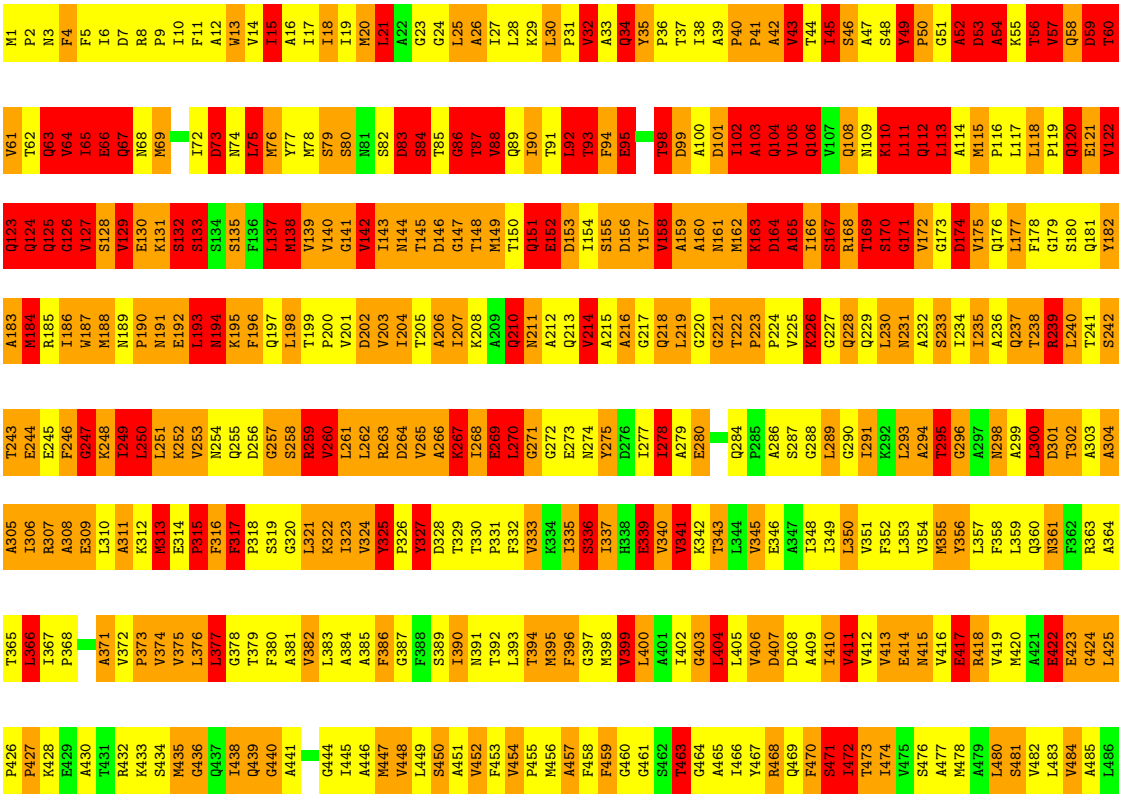
Chain B:

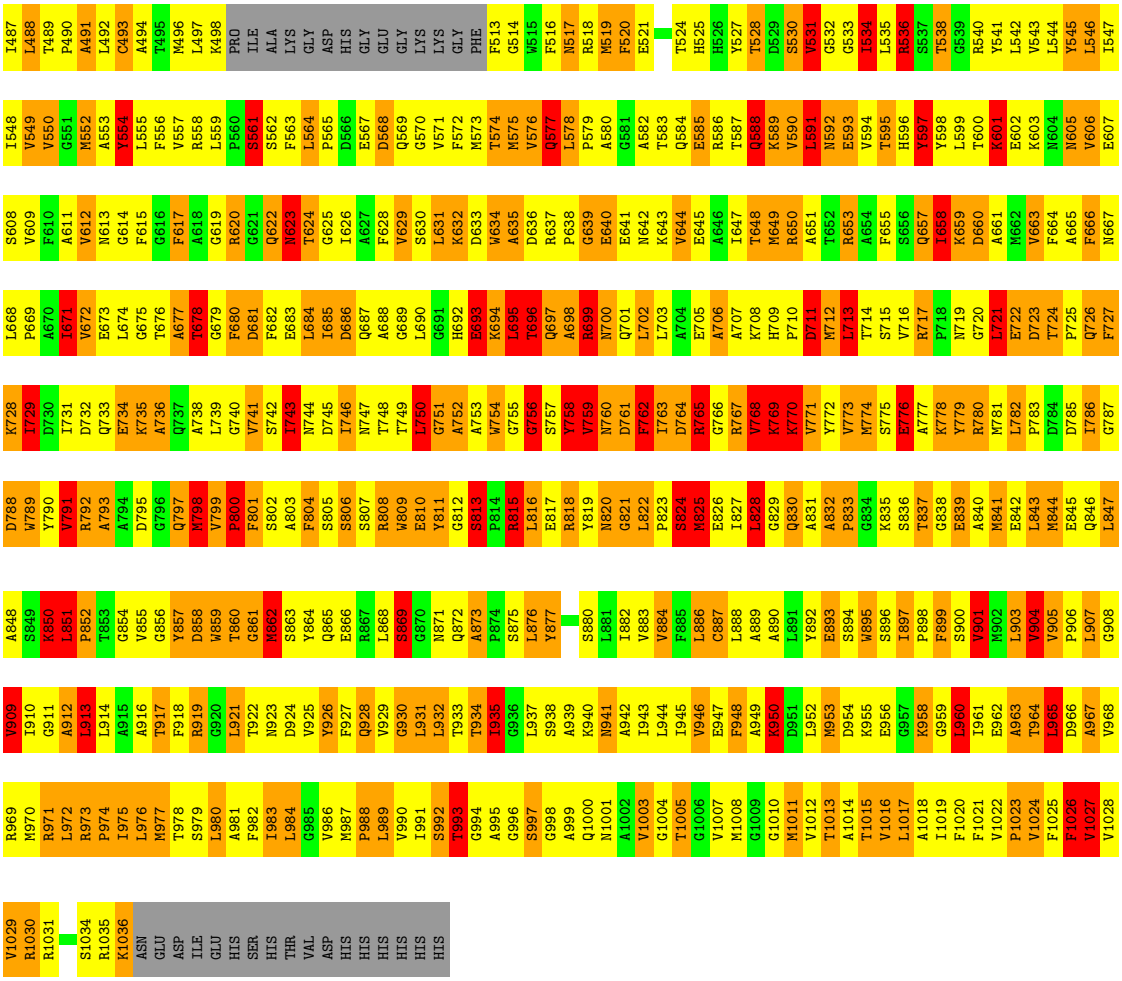




• Molecule 1: ACRB

Chain C:




I487 L488 T489 P490 A491 L492 C493 A494 T495 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 T524 H525 H526 Y527 T528 D529 S530 V531 G532 G533 I534 L535 R536 S537 T538 G539 R540 Y541 L542 V543 L544 Y545 L546 I547
I548 V549 V550 G551 M552 A553 Y554 L555 F556 V557 R558 L559 P560 S561 S562 F563 L564 P565 D566 E567 D568 Q569 G570 V571 F572 M573 T574 M575 V576 Q577 L578 P579 A580 G581 A582 T583 Q584 E585 R586 T587 Q588 K589 V590 L591 N592 E593 V594 T595 H596 Y597 Y598 L599 T600 K601 E602 K603 N604 N605 V606 E607
S608 V609 F610 A611 V612 N613 G614 F615 G616 F617 A618 G619 R620 G621 Q622 N623 T624 G625 I626 A627 F628 V629 S630 L631 K632 D633 W634 A635 D636 R637 P638 G639 E640 E641 N642 K643 V644 E645 A646 I647 T648 M649 R650 A651 T652 R653 A654 F655 S656 Q657 I658 K659 D660 A661 H662 V663 F664 A665 F666 N667
L668 P669 A670 I671 V672 E673 L674 G675 T676 A677 T678 G679 F680 D681 F682 E683 L684 I685 D686 Q687 A688 G689 L690 G691 H692 E693 K694 L695 T696 Q697 A698 R699 N700 Q701 L702 L703 A704 E705 A706 A707 K708 H709 P710 D711 M712 L713 T714 S715 V716 R717 P718 N719 G720 L721 E722 D723 T724 P725 Q726 F727
K728 I729 D730 I731 D732 Q733 E734 K735 A736 Q737 A738 L739 G740 V741 S742 I743 N744 D745 I746 N747 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 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 W809 E810 Y811 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 G870 N871 Q872 A873 P874 S875 L876 Y877 S880 L881 I882 V883 V884 F885 L886 C887 L888 A889 A890 L891 Y892 E893 S894 W895 S896 I897 P898 F899 S900 V901 M902 L903 V904 V905 P906 L907 G908
V909 I910 G911 A912 L913 L914 A915 A916 T917 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 E956 G957 K958 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 S1034 R1035 K1036 ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.05Å 134.56Å 161.70Å 90.00° 98.08° 90.00°	Depositor
Resolution (Å)	10.00 – 3.30	Depositor
% Data completeness (in resolution range)	94.2 (10.00-3.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.298 , 0.359	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23361	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DM2

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	2.18	252/7920 (3.2%)	1.95	258/10756 (2.4%)
1	B	1.57	63/7920 (0.8%)	1.59	113/10756 (1.1%)
1	C	2.04	222/7920 (2.8%)	1.89	245/10756 (2.3%)
All	All	1.95	537/23760 (2.3%)	1.82	616/32268 (1.9%)

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	1	31
1	B	0	11
1	C	0	19
All	All	1	61

The worst 5 of 537 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	VAL	CA-CB	33.72	2.25	1.54
1	A	818	ARG	CZ-NH1	27.46	1.68	1.33
1	A	66	GLU	N-CA	21.61	1.89	1.46
1	A	66	GLU	CD-OE1	18.81	1.46	1.25
1	A	68	ASN	CA-CB	18.59	2.01	1.53

The worst 5 of 616 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	818	ARG	NE-CZ-NH2	-48.52	96.04	120.30
1	C	767	ARG	NE-CZ-NH1	-25.67	107.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	LEU	CB-CG-CD1	-25.55	67.57	111.00
1	C	164	ASP	CB-CG-OD2	-20.31	100.02	118.30
1	A	99	ASP	CB-CG-OD1	-17.20	102.82	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	61	VAL	CA

5 of 61 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	THR	Peptide
1	A	64	VAL	Peptide,Mainchain
1	A	65	ILE	Peptide
1	A	68	ASN	Sidechain
1	A	69	MET	Peptide

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	7774	0	7928	1898	0
1	B	7774	0	7931	1841	0
1	C	7774	0	7930	1919	0
2	A	39	0	27	23	0
All	All	23361	0	23816	5470	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 116.

The worst 5 of 5470 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:118:LEU:CD2	1:A:118:LEU:CG	1.75	1.64
1:C:60:THR:CB	1:C:60:THR:CG2	1.75	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:CA	1:C:88:VAL:CB	1.80	1.59
1:C:767:ARG:CB	1:C:767:ARG:CG	1.78	1.59
1:C:65:ILE:CB	1:C:65:ILE:CG2	1.77	1.59

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	1018/1053 (97%)	530 (52%)	251 (25%)	237 (23%)	0	0
1	B	1018/1053 (97%)	558 (55%)	238 (23%)	222 (22%)	0	0
1	C	1018/1053 (97%)	565 (56%)	229 (22%)	224 (22%)	0	0
All	All	3054/3159 (97%)	1653 (54%)	718 (24%)	683 (22%)	0	0

5 of 683 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	54	ALA
1	A	63	GLN
1	A	64	VAL
1	A	66	GLU

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%)	592 (71%)	241 (29%)	0 1
1	B	833/859 (97%)	594 (71%)	239 (29%)	0 1
1	C	833/859 (97%)	560 (67%)	273 (33%)	0 1
All	All	2499/2577 (97%)	1746 (70%)	753 (30%)	0 1

5 of 753 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	962	GLU
1	C	280	GLU
1	B	1016	VAL
1	B	960	LEU
1	C	124	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	700	ASN
1	C	74	ASN
1	C	830	GLN
1	B	733	GLN
1	B	871	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)

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	DM2	A	2002	-	41,43,43	4.31	24 (58%)	55,67,67	4.17	34 (61%)

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	DM2	A	2002	-	1/1/9/9	4/13/60/60	0/5/5/5

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	DM2	C2-C3	-10.86	1.16	1.38
2	A	2002	DM2	C1-C20	10.33	1.56	1.39
2	A	2002	DM2	C5-C4	8.54	1.55	1.40
2	A	2002	DM2	C20-C5	8.38	1.53	1.41
2	A	2002	DM2	C8-C9	7.95	1.54	1.40

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2002	DM2	C3-C2-C1	12.49	137.98	120.25
2	A	2002	DM2	C2-C1-C20	-9.08	102.65	119.81
2	A	2002	DM2	C2-C3-C4	8.77	135.83	119.71
2	A	2002	DM2	O4-C4-C5	7.48	126.27	115.85
2	A	2002	DM2	C3-C4-C5	-7.32	105.31	120.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2002	DM2	C4'

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2002	DM2	C2'-C1'-O10-C10
2	A	2002	DM2	O5'-C1'-O10-C10
2	A	2002	DM2	C5-C4-O4-C21
2	A	2002	DM2	C11-C10-O10-C1'

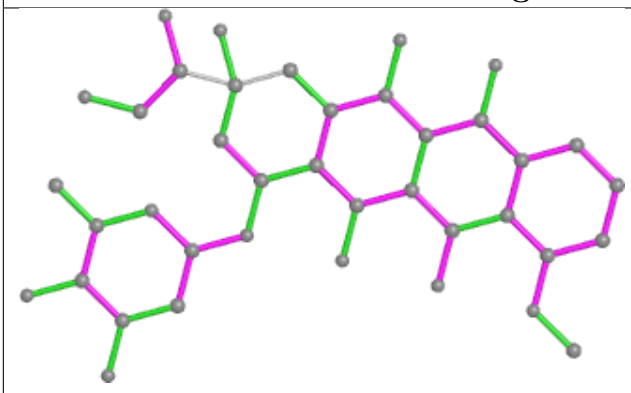
There are no ring outliers.

1 monomer is involved in 23 short contacts:

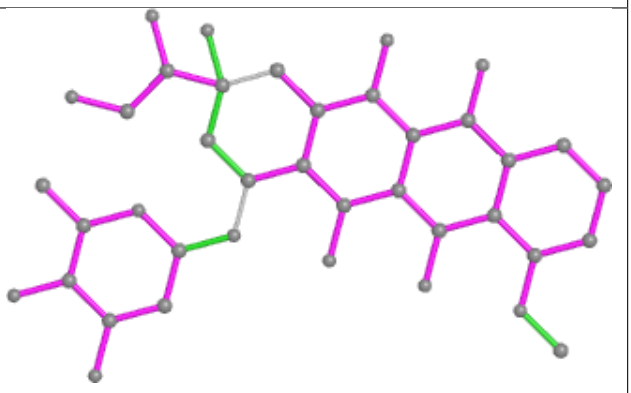
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2002	DM2	23	0

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.

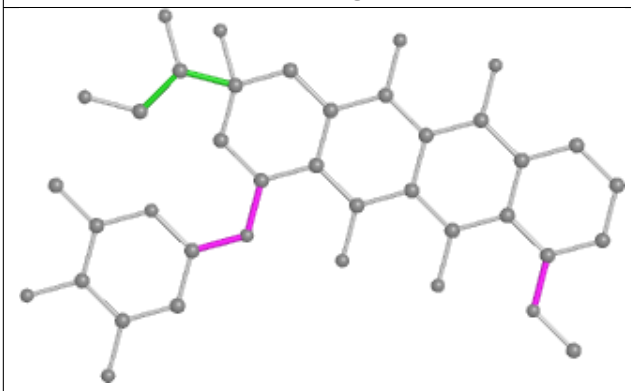
Ligand DM2 A 2002



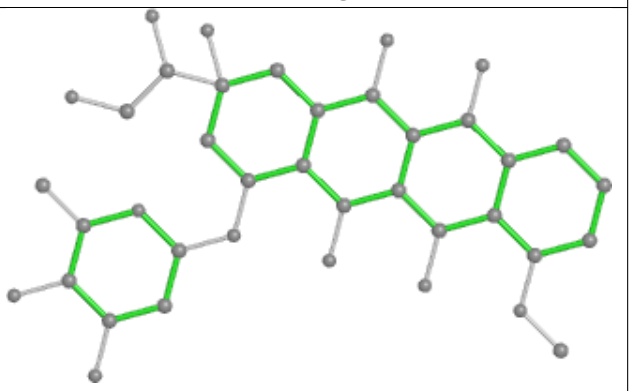
Bond lengths



Bond angles



Torsions



Rings

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.