



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 12:16 am BST

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](mailto: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 following versions of software and data (see [references ⓘ](#)) 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) : 2.11

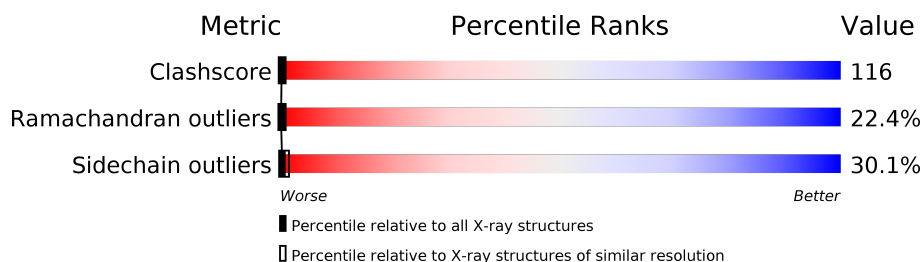
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1053	
1	B	1053	
1	C	1053	

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

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.

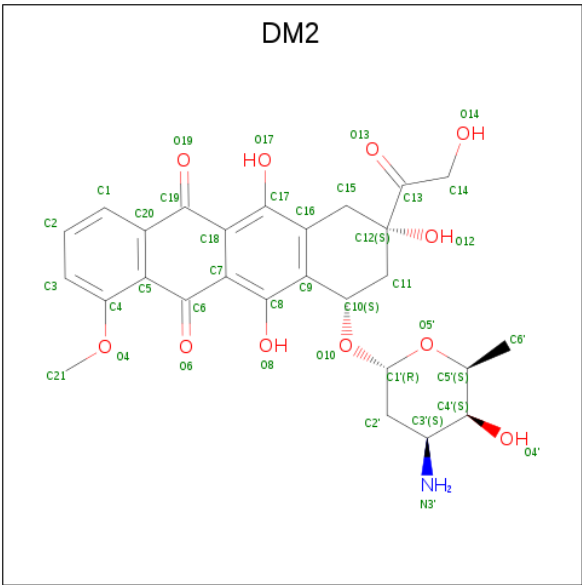
- Molecule 1 is a protein called ACRB.

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<sub>27</sub>H<sub>29</sub>NO<sub>11</sub>).



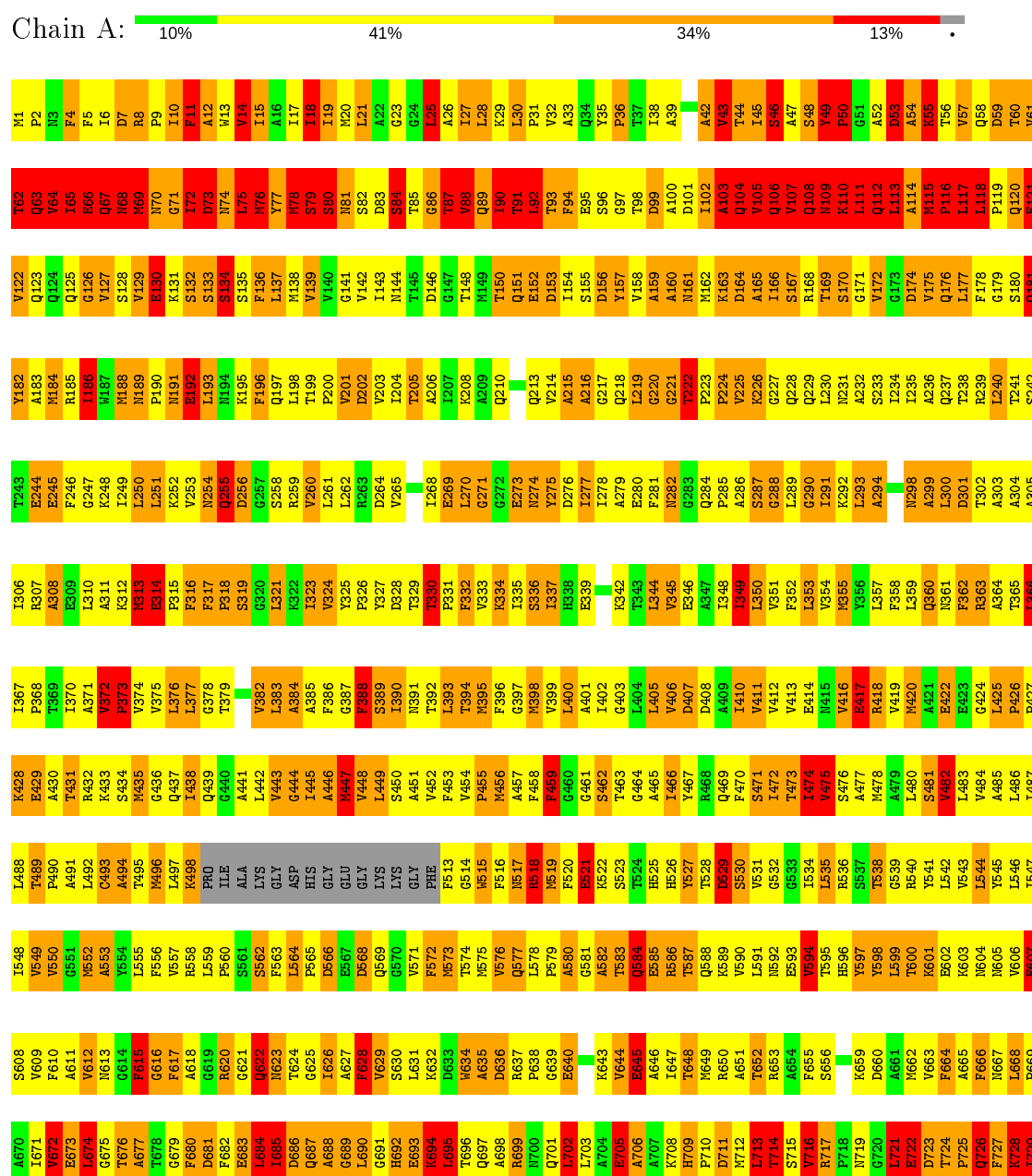
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	27	1	11		

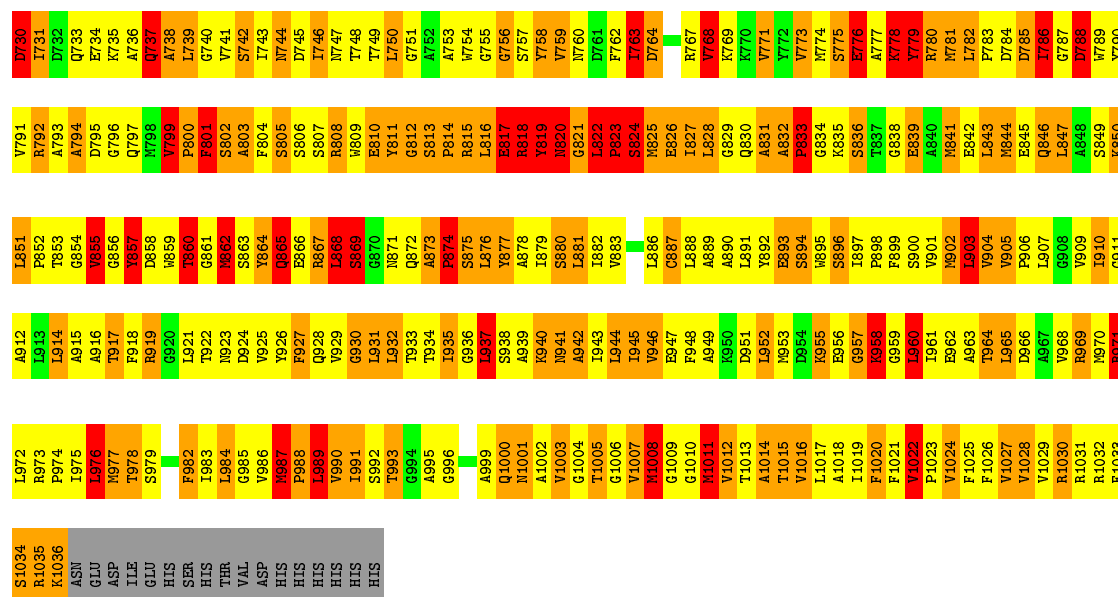
### 3 Residue-property plots

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. 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.

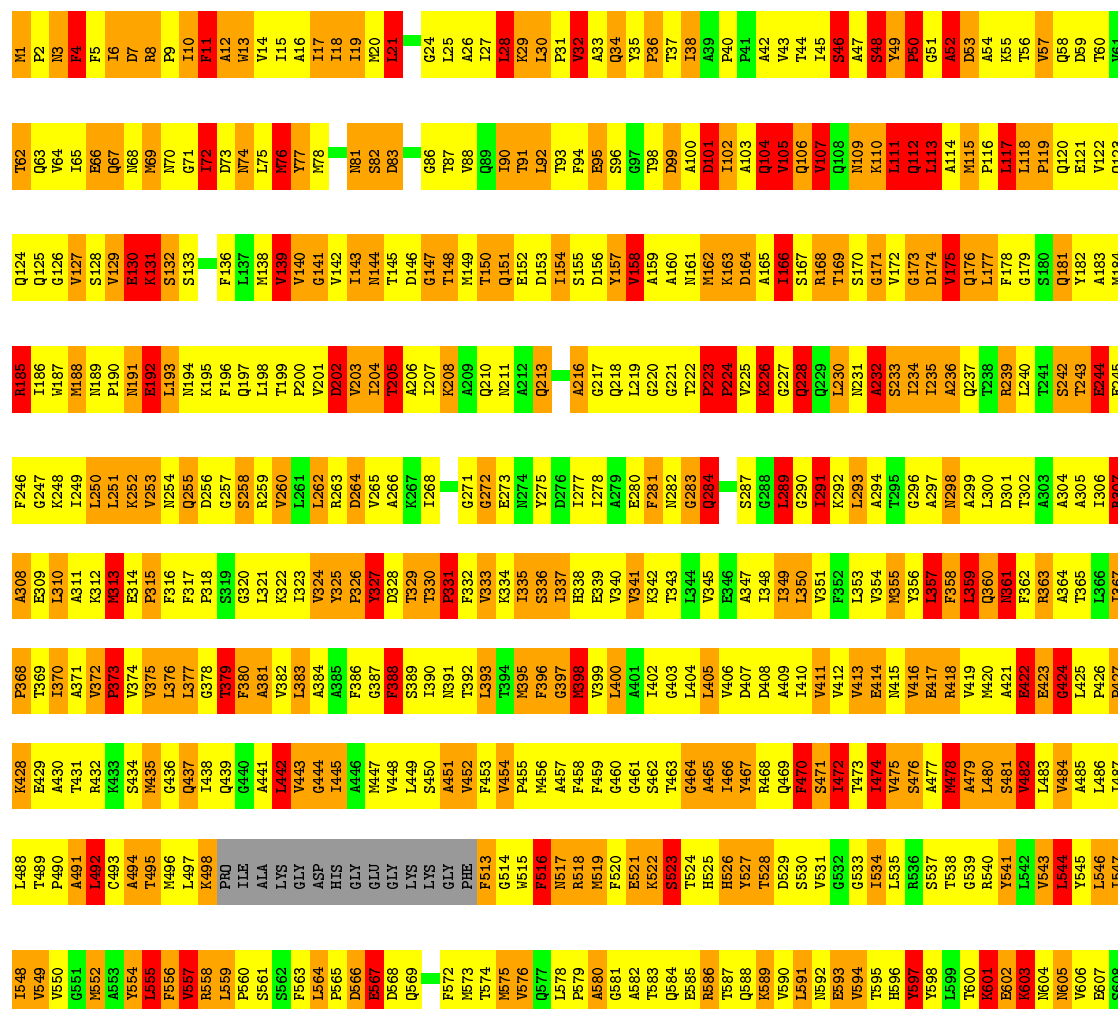
#### • Molecule 1: ACRB

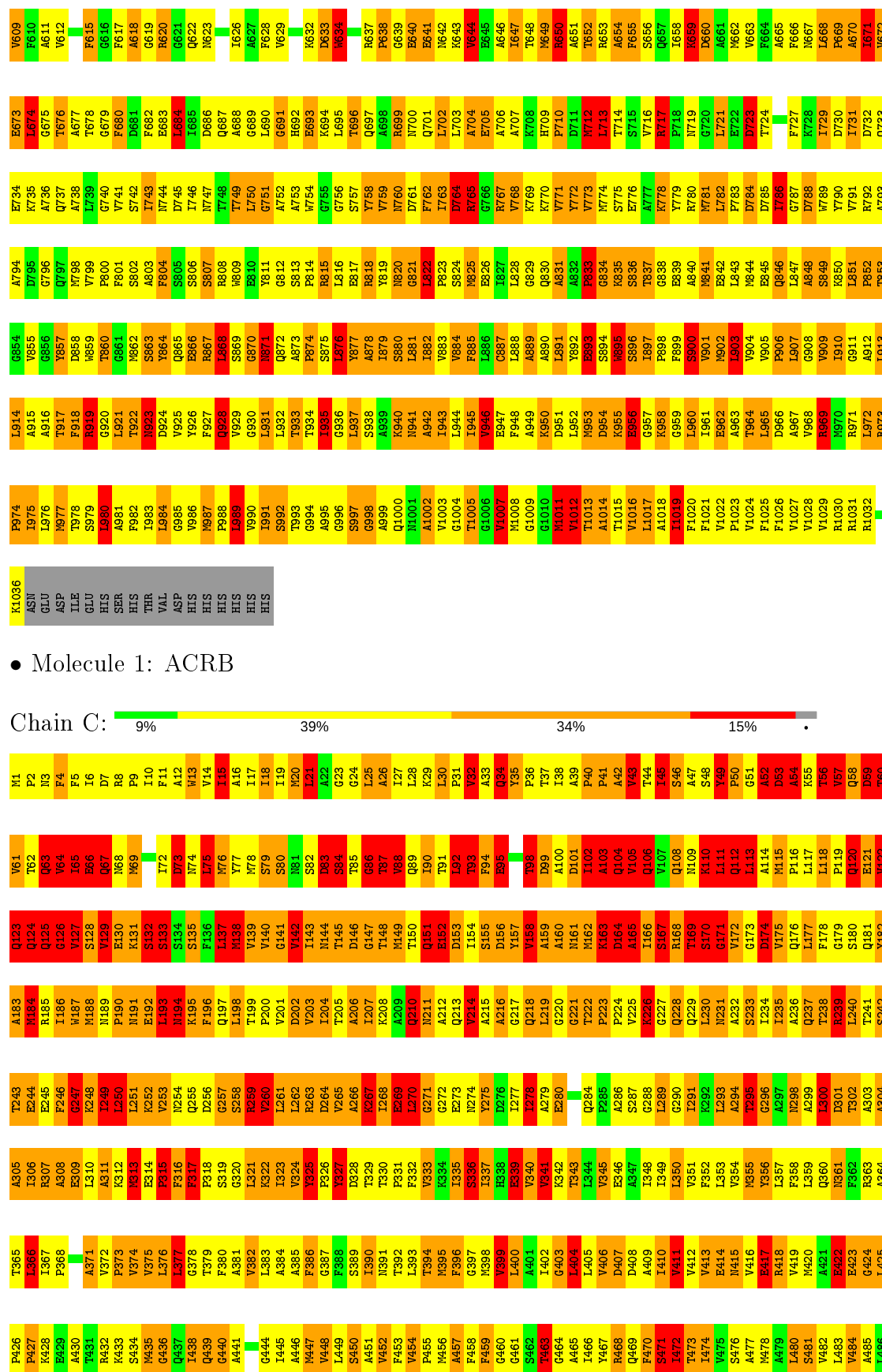




## ● Molecule 1: ACRB

Chain B: 10% 46% 31% 10%





• Molecule 1: ACRB

Y1029	R969	I909	A848	D788	K728	L688	S608	I548	L487
R1030	M970	I910	S849	M789	I729	P689	V609	V549	L488
R1031	R871	G911	R850	Y790	I730	A670	F610	T489	T489
	L872	A912	L851	Y791	I731	I671	A611	G551	P490
S1034	R973	L913	P852	R792	Q732	V672	N612	M552	A491
R1035	P974	L914	T853	A793	Q733	P673	N613	A492	A491
K1036	L975	A915	G854	A794	E734	L674	G614	C493	L492
ASN	L976	A916	V855	D795	K735	O675	F615	Y554	C493
GLU	M977	T917	V856	G796	A736	T676	G616	L555	A494
ASP	T978	F918	V857	Q797	Q737	A677	F617	F556	T495
ILE	S979	R919	D858	Y798	A738	T678	A618	V557	M496
GLU	L980	R920	V859	V799	L739	G679	G619	R558	L497
HIS	A981	L921	T860	P800	G740	F680	R620	L559	K498
SER	F982	T922	G861	F801	V741	D681	G621	P560	P490
HIS	L983	N923	R862	S802	S742	F682	Q622	S561	ILE
THR	L984	D924	S863	A803	I743	P683	Q623	S562	ALA
VAL	G985	V925	V864	A804	N744	L684	T624	F563	LYS
ASP	V986	Y926	Q865	S805	D745	I685	G625	L564	GLY
HIS	M987	F927	E866	S806	I746	D686	I626	P565	ASP
HIS	P988	Q928	R867	S807	N747	Q687	A627	D566	ASP
HIS	L989	V929	L868	R808	T748	A688	F628	E567	HIS
HIS	V990	G930	S869	M809	T749	G689	V629	E568	GLY
HIS	I991	L931	G870	E810	L750	L690	S630	Q569	GLY
HIS	S992	L932	N871	Y811	G751	G691	L631	G570	LYS
	T993	T933	Q872	G812	A752	H632	K632	V571	LYS
	G994	T934	A873	S813	A753	E693	D633	F572	GLY
	A995	I995	P874	R814	M754	K694	M634	M573	PHE
	G996	G936	S875	R815	G755	L695	A635	T574	F513
	S997	L937	L876	L816	G756	T696	D636	M575	G514
	G998	S938	Y877	E817	S757	Q697	R637	V576	W515
	A999	A939		R818	A698	P638	P638	Q577	W516
	Q1000	K940	S880	Y819	V759	R699	G639	L578	N517
	N1001	N941	L881	M820	N760	M700	E640	P579	R518
	A1002	A942	T882	G821	D761	Q701	E641	A580	M519
	V1003	T943	V883	L822	F762	L702	N642	G581	F520
	G1004	L944	V884	P823	I763	L703	K643	A582	E521
	T1005	T945	F885	S824	D764	A704	V644	T583	
	G1006	V946	L886	M825	R765	E705	E645	Q584	T524
	V1007	E947	C887	E826	G766	A646	A646	E585	H525
	M1008	F948	L888	L827	A707	I647	L647	R586	H526
	G1009	A949	A889	L828	K708	T648	T648	T587	H527
	G1010	K950	A890	G829	K769	M649	K589	Q588	T528
	M1011	D951	L891	Q830	K770	P710	R650	D529	D529
	V1012	L952	T892	A831	V771	D711	A651	V590	S530
	T1013	M953	E893	A832	Y772	M712	T652	L591	R531
	A1014	D954	S894	P833	V773	L713	R653	M592	G532
	T1015	K955	V895	G834	M774	T714	A654	E593	G533
	V1016	E956	S896	K835	S775	S715	F655	V594	I534
	L1017	G957	I897	S836	E776	V716	S656	T595	L535
	A1018	K958	P898	T837	A777	R717	Q657	H596	R536
	I1019	G959	F899	G838	K778	F718	L658	Y597	S537
	F1020	L960	S900	E839	Y779	M719	K659	Y598	T538
	V1021	T961	Y901	A840	R780	G720	D660	L599	G539
	T1022	E962	H902	M841	M781	L721	A661	R601	R540
	P1023	A963	L903	E842	L782	E722	M662	K601	Y541
	V1024	T964	V904	L843	P783	T723	V663	E602	L542
	F1025	L965	V905	M844	E784	T724	F664	K603	V543
	F1026	D966	P906	E845	D785	P725	A665	M604	L544
	V1027	A967	L907	Q846	T786	Q726	F666	N605	Y545
	V1028	V968	G908	L847	G787	F727	N667	L546	L546

## 4 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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(°)	Ideal(°)
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	Mainchain,Peptide
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:CG	1:A:118:LEU:CD2	1.75	1.64
1:C:60:THR:CG2	1:C:60:THR:CB	1.75	1.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:CB	1:C:88:VAL:CA	1.80	1.59
1:C:767:ARG:CB	1:C:767:ARG:CG	1.78	1.59
1:C:166:ILE:CG2	1:C:166:ILE:CB	1.81	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	398	MET
1	B	782	LEU
1	C	774	MET
1	B	437	GLN
1	B	601	LYS

Some 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	361	ASN
1	B	700	ASN
1	C	692	HIS
1	B	415	ASN
1	B	584	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 carbohydrates 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(°)	Ideal(°)
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:

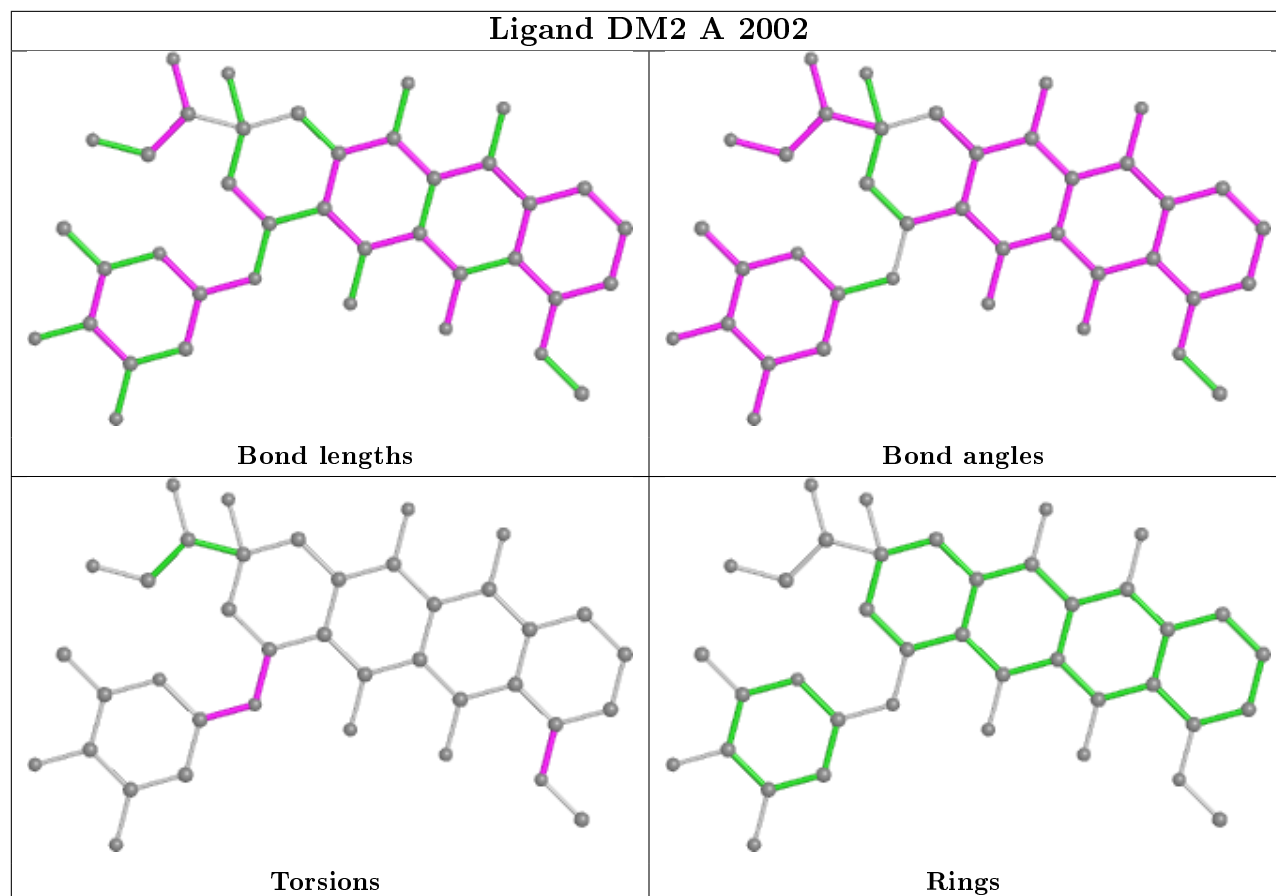
Mol	Chain	Res	Type	Atoms
2	A	2002	DM2	C2'-C1'-O10-C10
2	A	2002	DM2	O5'-C1'-O10-C10
2	A	2002	DM2	C5-C4-O4-C21
2	A	2002	DM2	C11-C10-O10-C1'

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 than 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.



## 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.