



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 09:51 PM UTC

PDB ID : 2DR6 / pdb_00002dr6
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.

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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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

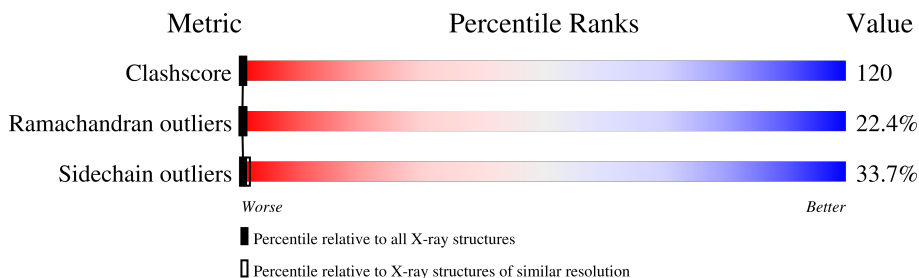
1 Overall quality at a glance

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	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1053	6% 35% 38% 18% .
1	B	1053	7% 37% 37% 16% .
1	C	1053	7% 33% 39% 19% .

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.

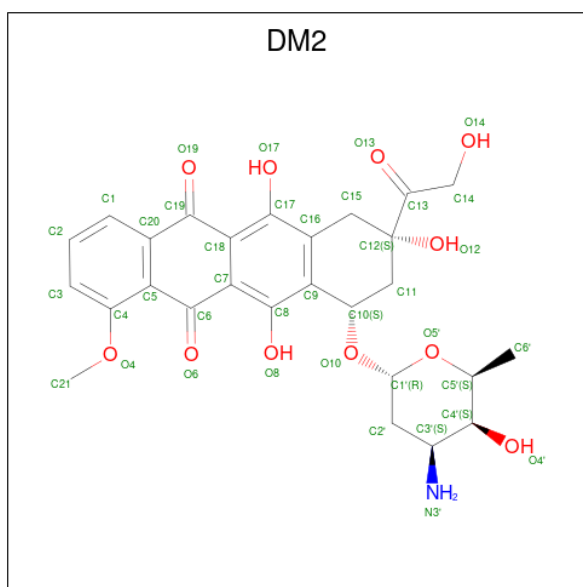
- Molecule 1 is a protein called ACRB.

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

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 (CCD ID: DM2) (formula: C₂₇H₂₉NO₁₁).



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

F1025	L965	V985	E845	D785	P725	A685	R685	Y845
F1026	D966	P906	Q846	I786	Q726	F666	V606	L846
V1027	A967	L907	L847	G787	F727	M667	E607	I547
V1028	V968	G908	A848	D788	K728	L668	S608	I548
V1029	R969	V909	S849	W789	I729	P669	V609	V549
R1030	M970	I910	K850	Y790	R730	A670	F610	V550
R1031	R971	G911	L851	W791	I731	I671	A611	G551
	L972	A912	P852	R792	D732	V672	V612	M552
S1034	R973	L913	T853	A793	Q733	E673	M613	A553
R1035	P974	L914	K854	A794	L674	L674	G614	Y554
R1036	I975	A915	V855	K795	K735	G675	F615	L555
ASN	L976	A916	G856	G796	A736	I676	A616	F556
GLU	M977	T917	Y857	Q797	Q737	A677	V617	V657
ASP	T978	F918	D858	W798	A738	T678	R618	R558
ILE	S979	R919	W859	V799	L739	G679	G619	L559
GLU	L980	G920	T860	P800	G740	F680	R620	P660
HIS	L981	G921	K861	F801	I741	D681	G621	S661
SER	F982	T922	M862	S802	S742	F682	Q622	S662
HIS	I983	N923	S863	A803	I743	E683	M623	F563
THR	L984	D924	V864	F804	N744	L684	T624	L564
VAL	G985	V925	Q865	S805	D745	G685	G625	P565
ASP	V986	Y926	E866	S806	I746	D686	I626	D566
HIS	P987	F927	R867	S807	N747	A687	A627	E567
HIS	P988	Q928	L868	R808	T748	A688	F628	D568
HIS	L989	V929	S869	W809	T749	G689	V629	Q569
HIS	V990	G930	G870	E810	L750	L690	S630	G570
HIS	I991	L931	M871	G811	G751	G691	L631	V571
HIS	S992	L932	K872	G812	A752	H692	K632	F572
	T993	T933	A873	S813	A753	E693	D633	M573
	G994	T934	R874	P814	V754	K694	W634	T574
	A995	I935	S875	R815	G755	L695	A635	M575
	G996	G936	L876	L816	G756	T696	D636	V576
	G997	L937	R877	E817	S757	Q697	R637	Q577
	A998	S938	A878	R818	Y758	A698	P638	L578
	A999	A939	R879	Y819	V759	R699	G639	P579
	Q1000	K940	S880	N820	N760	E640	E640	A580
	N1001	N941	L881	G821	D761	Q701	E641	G581
	A1002	A942	I882	L822	F762	L702	M642	A582
V1003	I943	I943	V883	P823	I763	L703	K643	T583
G1004	L944	L944	W884	S824	D764	V644	V644	Q584
T1005	I945	F885	F885	M825	R765	E705	E645	E585
G1006	V946	L886	L886	E826	G766	A706	A646	R586
V1007	E947	C887	C887	I827	R767	A707	I647	T587
M1008	F948	L888	L888	L828	V768	K708	T648	Q588
G1009	A949	A889	A889	G829	K769	H709	M649	K589
G1010	K950	A890	A890	Q830	K770	P710	R650	V590
M1011	D951	L891	L891	A831	V771	D711	A651	L591
V1012	L952	Y892	A832	A832	Y772	M712	T652	N592
T1013	M953	S893	P833	P833	V773	L713	R653	E593
A1014	D954	S894	G834	G834	M774	T714	A654	V594
T1015	K955	W895	K835	K835	S775	S715	F655	T595
V1016	E956	S896	S836	E776	V716	S656	G656	H596
L1017	G957	L897	T837	A777	Q657	Q657	Q657	Y597
A1018	K958	P898	G838	K778	P718	T658	T658	Y598
I1019	G959	F899	F839	Y779	N719	K659	L599	L599
F1020	I960	S900	A840	R780	G720	D660	T600	T600
F1021	I961	P901	M841	M781	L721	A661	A661	K601
V1022	E962	M902	E842	L782	M662	G662	M662	E602
P1023	A963	L903	L843	P783	K663	K663	K663	K603
V1024	T964	T964	M844	D784	T724	T724	F664	N604

4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	23361	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

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: 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	2.78	426/7920 (5.4%)	2.36	507/10756 (4.7%)
1	B	2.03	219/7920 (2.8%)	2.03	299/10756 (2.8%)
1	C	2.60	452/7920 (5.7%)	2.36	455/10756 (4.2%)
All	All	2.49	1097/23760 (4.6%)	2.26	1261/32268 (3.9%)

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 1097 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	VAL	CA-CB	52.28	2.25	1.54
1	A	66	GLU	N-CA	33.62	1.89	1.46
1	A	69	MET	N-CA	28.47	1.82	1.46
1	A	68	ASN	CA-CB	28.41	2.01	1.53
1	A	114	ALA	CA-C	-27.40	1.29	1.52

The worst 5 of 1261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	818	ARG	NE-CZ-NH2	-25.73	96.04	119.20
1	A	114	ALA	N-CA-C	-25.55	77.12	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	773	VAL	N-CA-C	-17.56	83.53	108.11
1	C	788	ASP	N-CA-C	-16.21	92.64	113.72
1	B	1007	VAL	CB-CA-C	-16.17	94.69	110.70

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	1982	0
1	B	7774	0	7931	1906	0
1	C	7774	0	7930	1981	0
2	A	39	0	27	23	0
All	All	23361	0	23816	5679	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 120.

The worst 5 of 5679 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%)	557 (67%)	276 (33%)	0	1
1	B	833/859 (97%)	566 (68%)	267 (32%)	0	1
1	C	833/859 (97%)	535 (64%)	298 (36%)	0	1
All	All	2499/2577 (97%)	1658 (66%)	841 (34%)	0	1

5 of 841 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	703	LEU
1	C	87	THR
1	C	879	ILE
1	B	760	ASN
1	B	702	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	744	ASN
1	C	108	GLN
1	C	797	GLN
1	B	830	GLN
1	B	1001	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 oligosaccharides 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	-	42,43,43	4.57	24 (57%)	56,67,67	4.21	35 (62%)

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	-13.35	1.16	1.38
2	A	2002	DM2	C1-C20	10.83	1.56	1.39
2	A	2002	DM2	C8-C9	8.64	1.54	1.40
2	A	2002	DM2	C5-C4	8.63	1.55	1.40
2	A	2002	DM2	C20-C5	8.42	1.53	1.41

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2002	DM2	C3-C2-C1	13.80	137.98	120.24
2	A	2002	DM2	C2-C1-C20	-9.49	102.65	119.80
2	A	2002	DM2	C2-C3-C4	8.93	135.83	119.60
2	A	2002	DM2	O4-C4-C5	7.36	126.27	115.84
2	A	2002	DM2	C3-C4-C5	-7.30	105.31	120.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2002	DM2	C4'

All (4) torsion outliers are listed below:

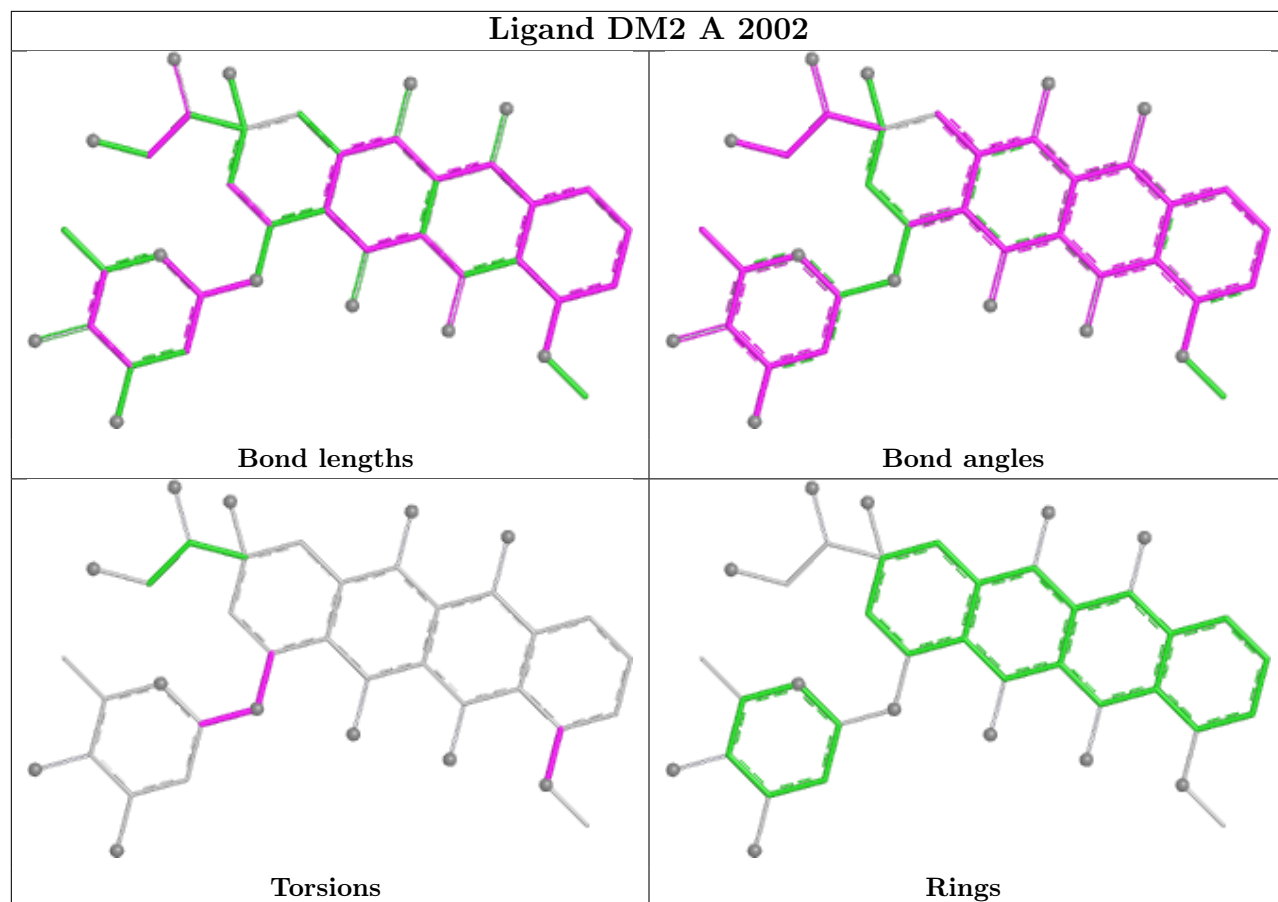
Mol	Chain	Res	Type	Atoms
2	A	2002	DM2	C2'-C1'-O10-C10
2	A	2002	DM2	O5'-C1'-O10-C10
2	A	2002	DM2	C5-C4-O4-C21
2	A	2002	DM2	C11-C10-O10-C1'

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.