



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:38 AM GMT

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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

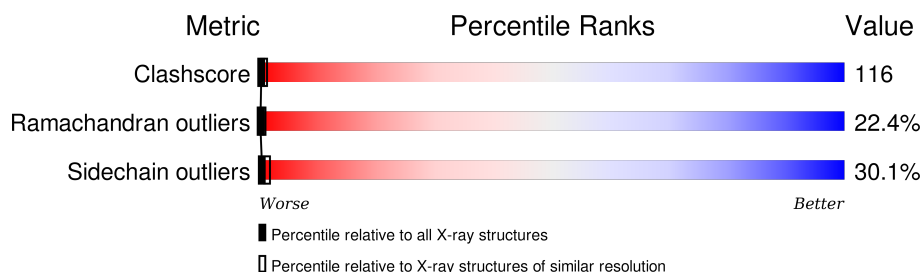
# 1 Overall quality at a glance

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	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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. 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  $\leq 5\%$ . 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.

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.

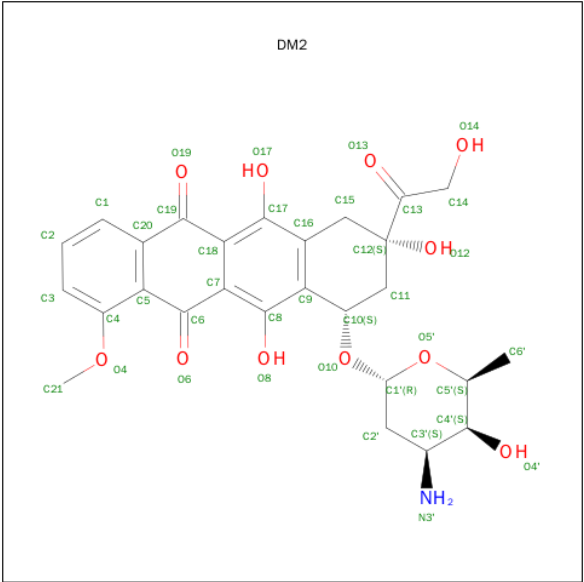
- Molecule 1 is a protein called ACRB.

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>).



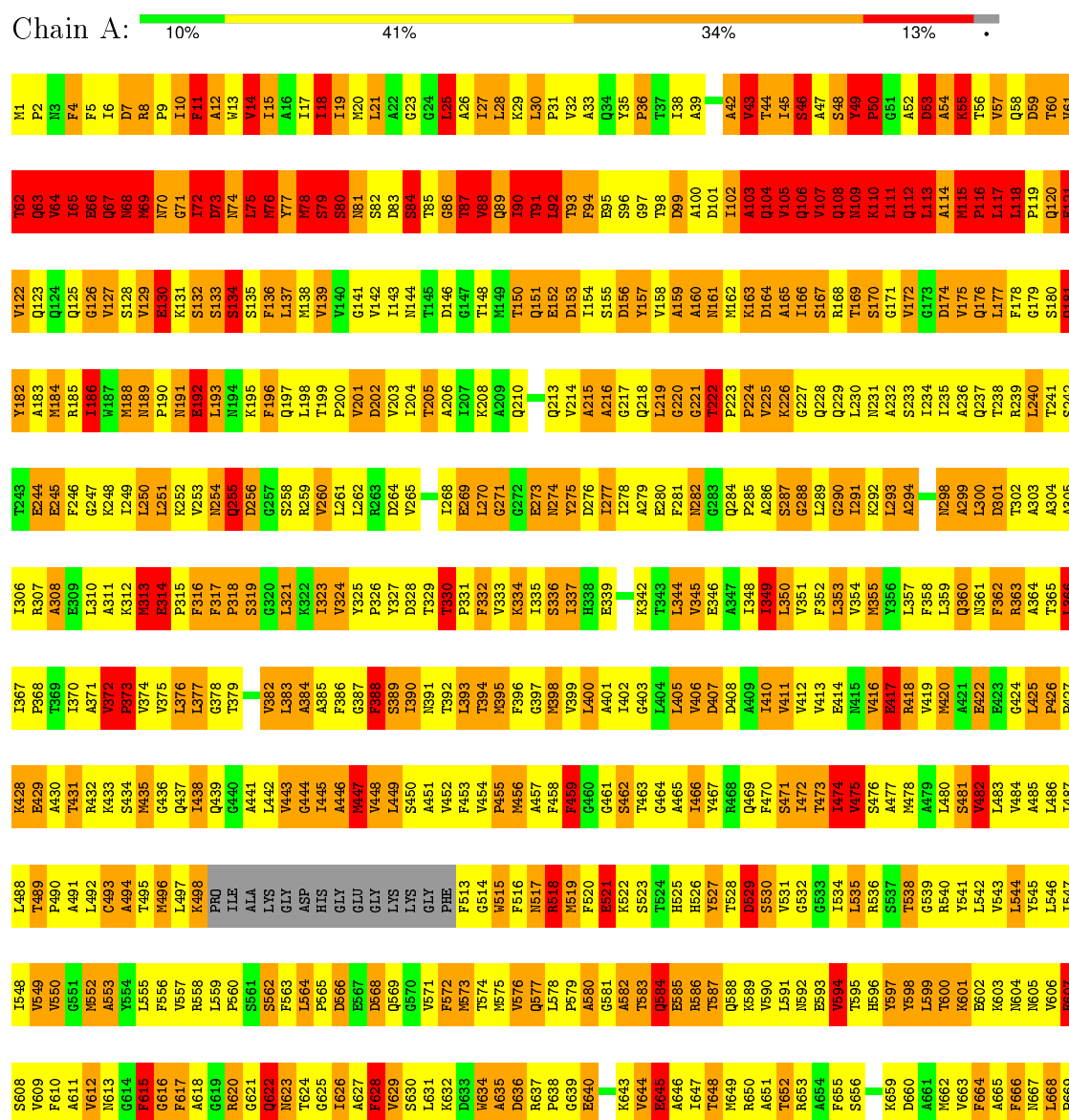
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	27	1	11		

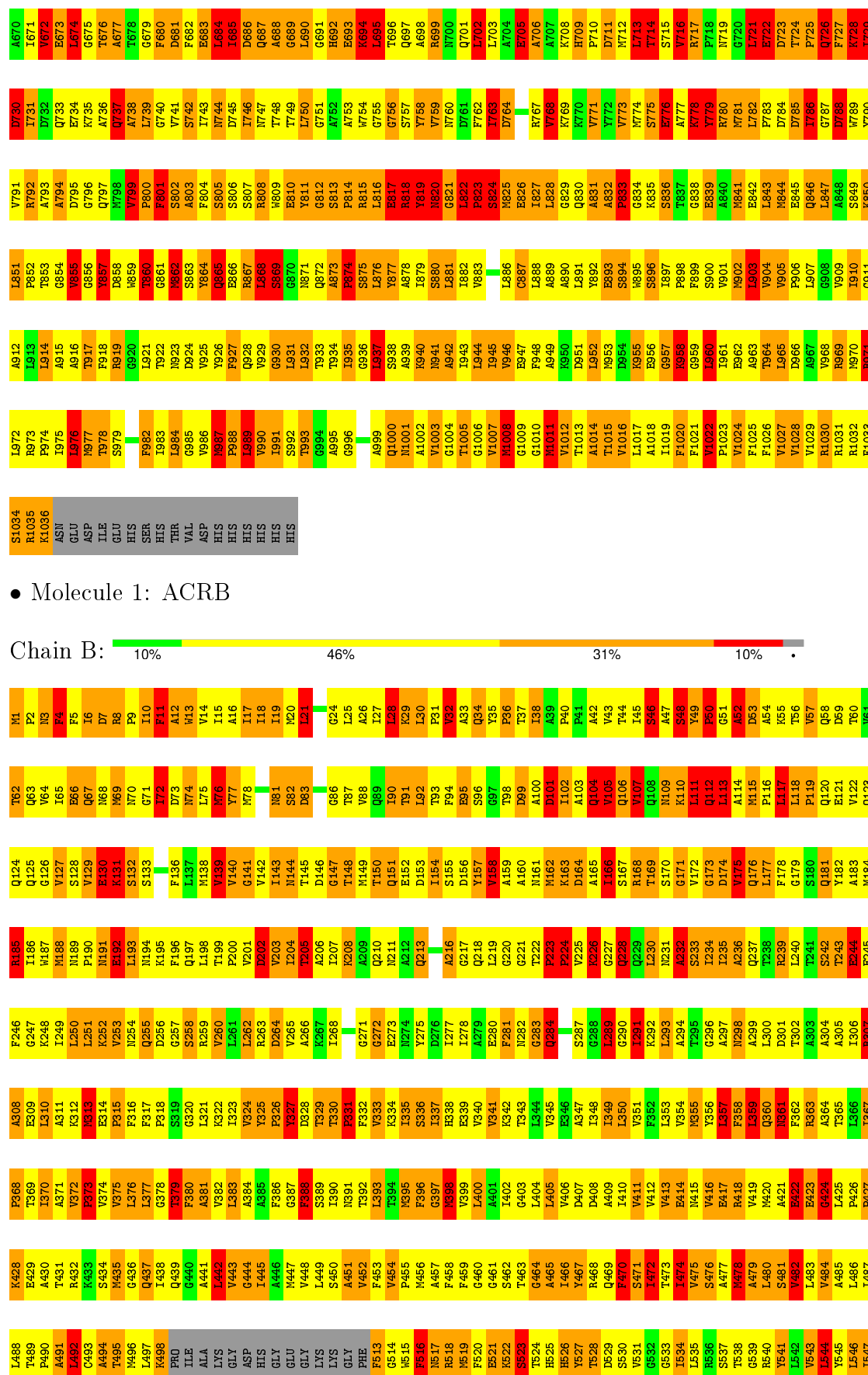
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

#### • Molecule 1: ACRB





• Molecule 1: ACRB



V1029	R669	R608	A848	D788	K728	L668	S608	L548	L487	P426
R1030	P970	I910	S849	W789	I729	P669	V609	V649	L488	P427
R1031	R971	G911	R850	W790	D730	A670	F610	V650	T489	K428
	L972	A912	L851	V791	I731	L671	A611	S551	P490	E428
S1034	R973	L913	P852	R792	D732	V672	V612	V652	A491	A430
R1035	P974	L914	T853	A793	Q733	B673	V613	A553	L492	T431
K1036	I975	A915	G854	A794	R734	L674	G614	S554	C993	R432
ASN	L976	A916	V855	D795	K735	G675	F615	L555	C993	K433
GLU	T977	T917	G856	D796	A736	T676	G616	T556	T495	S434
ASP	T978	F918	Y857	Q797	Q737	R738	F617	V557	M496	M435
ILE	S979	R919	D858	W798	I738	T678	A618	R558	L497	Q436
GLU	L980	G920	W859	V799	L739	G679	G619	L559	K498	Q437
HIS	A981	L921	T860	R800	R740	F680	R620	P560	P498	T438
SER	F982	T922	G861	F801	V741	D681	G621	S561	ILE	Q439
HIS	L983	N923	S862	S802	S742	F682	G622	S562	ALA	G440
THR	L984	D924	S863	A803	I743	F683	M623	F563	LVS	A441
VAL	G985	V925	Y864	F804	N744	L684	T624	L564	GLY	G444
ASP	V986	T926	Q865	S805	D745	T685	G625	P565	ASP	T445
HIS	N987	F927	E866	S806	I746	D686	I626	D566	HIS	T445
HIS	P988	Q928	R867	S807	I747	Q687	A627	E567	GLY	L446
HIS	V929	V929	L868	R808	T748	A688	F628	D568	GLU	M447
HIS	P990	G930	S869	W809	T749	G689	V629	Q569	GLY	Y448
HIS	I991	L931	G870	E810	L750	L690	S630	G570	LVS	L449
S992	T992	L932	N871	E811	G751	G691	L631	V571	LVS	S450
T993	T933	Q932	Q872	G812	A752	H692	K632	F572	GLY	A451
G994	T934	T934	A873	S813	A753	E693	D633	H573	PHE	V452
A995	T935	T935	F874	P814	G754	R694	W634	T574	F513	F453
G996	G936	G936	S875	R815	G755	L695	A635	N575	G514	V454
S997	L937	L937	L876	L816	G756	T696	D636	V576	W515	P455
G998	S938	S938	T877	E817	S757	Q697	R637	Q577	F516	M456
A999	A939	A939	R818	R818	Y758	A698	P638	L578	N517	A457
Q1000	V940	V940	S880	Y819	V759	R699	G639	F579	R518	F458
M1001	N941	N941	L881	M820	N760	N700	E640	A980	M519	F459
A1002	A942	A942	I882	G821	D761	Q701	B641	N581	F520	G460
V1003	I943	I943	V883	L822	F762	L702	M642	A582	E521	G461
G1004	L944	L944	V884	P823	I763	L703	K643	T583		
T1005	I945	I945	F885	S824	D764	A704	V644	Q584		
G1006	V946	V946	L886	R825	R765	E705	E645	E585	T524	T463
V1007	E947	E947	C887	E826	G766	A706	A646	R586	H525	G464
M1008	F948	F948	L888	I827	R767	A707	I647	T587	H526	A465
G1009	A949	A949	A889	L828	V768	K708	T648	Q588	T527	1466
G1010	Q950	Q950	A890	G829	K769	H709	M649	X589	D529	R467
M1011	D951	D951	L891	Q830	K770	P710	R650	V590	D529	R468
V1012	L952	L952	Y892	A831	V771	D711	A651	L591	S530	Q469
T1013	N953	N953	E893	A832	Y772	H712	T652	H592	V531	P470
A1014	D954	D954	S894	P833	V773	L713	R653	G593	G532	S471
T1015	K955	K955	W895	G834	M774	T714	A654	V594	G533	1472
V1016	E956	E956	S896	K835	S775	S715	F655	T595	1534	T473
L1017	G957	G957	T897	S836	E776	V716	S656	H596	L535	1474
A1018	K958	K958	P898	T837	A777	R717	Q657	H597	R536	V475
I1019	G959	G959	F899	G838	K778	F718	I658	V598	S537	S476
F1020	L960	L960	S900	E839	Y779	H719	R659	L599	T538	A477
F1021	I961	I961	V901	A840	R780	G720	D660	T600	G539	A478
V1022	E962	E962	H902	N841	M781	L721	A661	T600	R540	A479
P1023	A963	A963	L903	E842	L782	E722	M662	E602	Y541	L480
P1024	T964	T964	V904	L843	P783	D723	V663	V603	L542	S481
F1025	L965	L965	V905	N844	D784	T724	F664	H604	V543	V482
F1026	D966	D966	P906	E845	T785	P725	A665	H605	L544	L483
V1027	A967	A967	L907	Q846	I786	Q726	F666	V606	Y545	V484
V1028	V968	V968	G908	L847	G787	F727	M667	E607	L547	L486



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

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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

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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:CG	1:C:767:ARG:CB	1.78	1.59
1:C:65:ILE:CG2	1:C:65:ILE:CB	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	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	4.23	24 (58%)	55,67,67	4.04	32 (58%)

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	0/13/60/60	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	-11.10	1.16	1.38
2	A	2002	DM2	C3-C4	-7.29	1.24	1.39
2	A	2002	DM2	C2-C1	-6.93	1.24	1.38
2	A	2002	DM2	C17-C16	-5.52	1.31	1.40
2	A	2002	DM2	C18-C19	-2.45	1.41	1.47

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2002	DM2	C2-C1-C20	-8.92	102.65	119.87
2	A	2002	DM2	C3-C4-C5	-8.29	105.31	120.43
2	A	2002	DM2	O17-C17-C16	-5.31	102.29	118.11
2	A	2002	DM2	O13-C13-C12	-4.99	116.05	122.22
2	A	2002	DM2	C16-C9-C10	-4.04	113.19	120.89

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2002	DM2	C4'

There are no torsion outliers.

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

## 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](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.