



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 09:40 pm GMT

PDB ID : 2DRD  
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 : 3.10 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

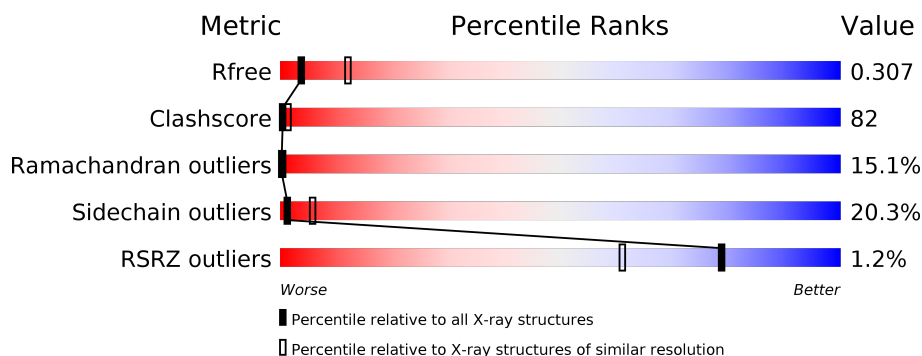
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	111664	1115 (3.12-3.08)
Clashscore	122126	1042 (3.10-3.10)
Ramachandran outliers	120053	1010 (3.10-3.10)
Sidechain outliers	120020	1010 (3.10-3.10)
RSRZ outliers	108989	1089 (3.12-3.08)

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.

Mol	Chain	Length	Quality of chain
1	A	1053	<div> <div>19%</div> <div>49%</div> <div>24%</div> <div>5%</div> <div>•</div> </div>
1	B	1053	<div> <div>17%</div> <div>53%</div> <div>23%</div> <div>•</div> <div>•</div> </div>
1	C	1053	<div> <div>2%</div> <div>19%</div> <div>50%</div> <div>23%</div> <div>6%</div> <div>•</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23355 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.

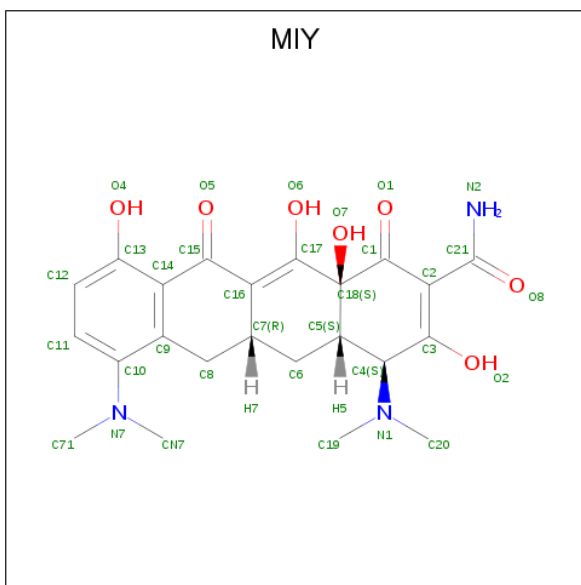
- Molecule 1 is a protein called ACRB.

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 (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: C<sub>23</sub>H<sub>27</sub>N<sub>3</sub>O<sub>7</sub>).

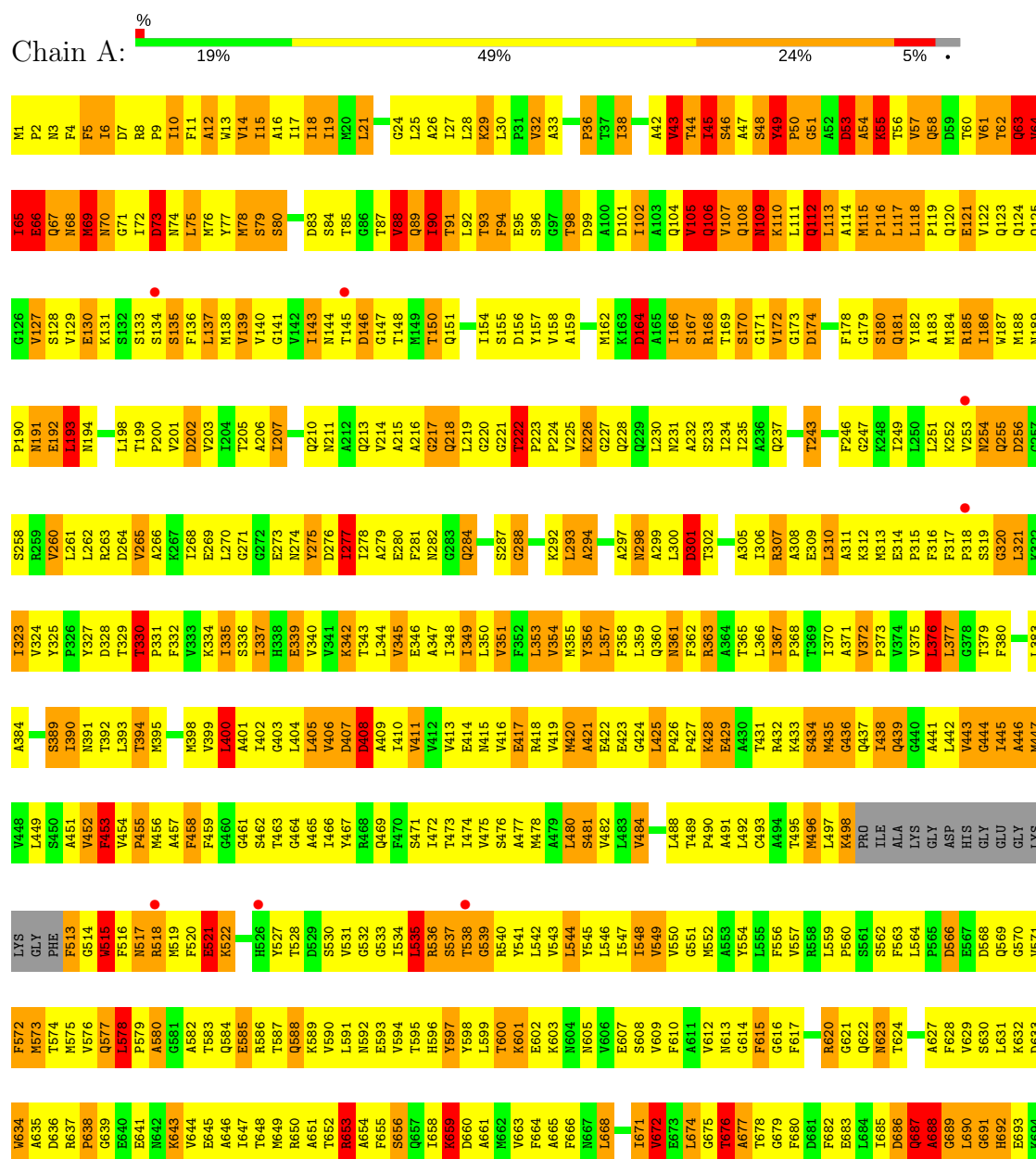


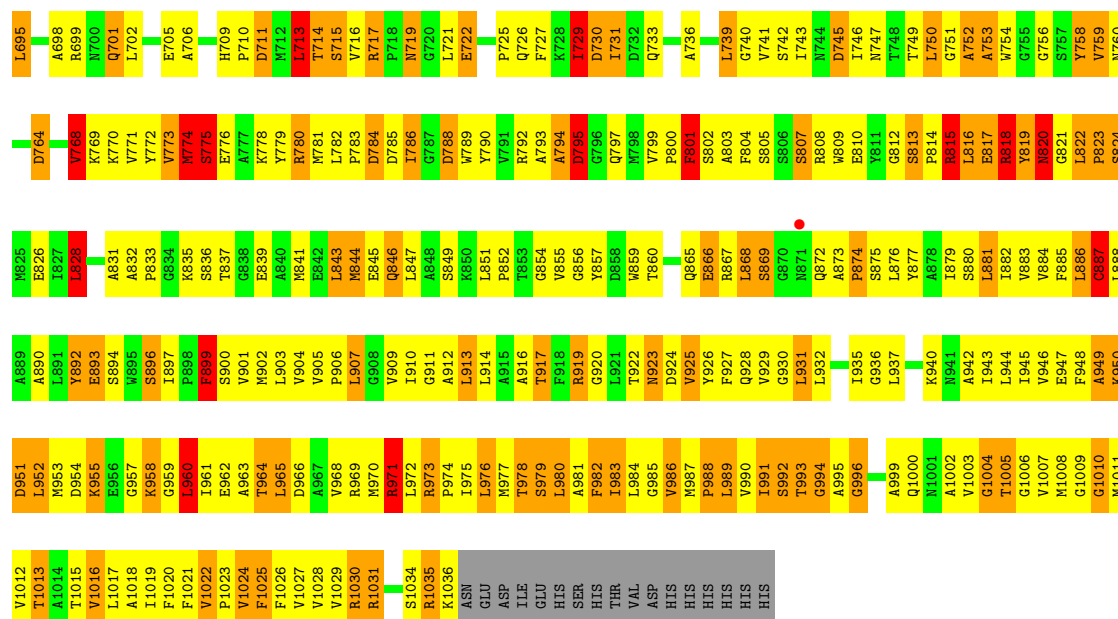
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	23	3	7		

### 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 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: ACRB







T1005	G1006	N941	I879	R818	G751	D686	G695	P560	ILE	L438
G1007	I943	A942	S880	Y819	A752	Q687	I626	S561	ALA	Q439
M1008	V883	I944	V883	N820	A753	G688	F628	S562	LYS	
G1009	I945	I945	F885	S824	W754	G689	F629	F563	GLY	L442
M1011	V946	V946	L886	M825	G755	L690	S630	L564	ASP	V443
V1012	E947	E947	C887	E826		G691	L631	P565	HIS	Q444
T1013	F948	F948	L888	L827	W759	H692	K632	D566	GLY	L445
A1014	A949	A949	L889	L828	N760	K693	D633	E567	GLU	A446
T1015	K950	K950	A889	L829	D761	L694	W634	D568	GLY	A447
V1016	D951	D951	A890	G829	F762	T696	A635	Q570	LYS	V448
L1017	L952	L952	L891	Q830	I763	Q697	D636	V571	GLY	L449
A1018	K953	K953	Y892	A831	D764	A698	R637	F572	PHF	S450
I1019	D954	D954	E893	A832	K765	R639	F638	H573	F513	A451
F1020	K958	K958	S894	P833	G766	N700	G639	T574	G514	V452
V1021	G959	G959	W895	G834	R767	Q701	E640	M575	G515	F453
P1022	L960	L960	S896	K835	V768	L702	E641	Q576	F516	V454
P1023	I961	I961	I897	S836	K769	L703	N642	Q577	N517	P455
V1024	E962	E962	P898	T837	K770	A704	K643	L578	R518	N456
F1025	A963	A963	F899	G838	V771	E705	V644	P579	M519	A457
F1026	T964	T964	S900	E839	Y772	A706	E645		F520	F458
V1027	L965	L965	V901	N840	W773	A707	A646	A582	E521	F459
V1028	D966	D966	V904	A841	M774	K708	L647	T583	G460	G461
V1029	A967	A967	G905	L843	E775	H709	T648	Q584	S523	S462
R1030	V968	V968	P906	M844	A777	D711	K650	E585	T524	T463
R1031	R969	R969	L907	E845	K778	M712		R586	H525	G464
R1032	M970	M970	G908	Q846	Y779	L713	R653	T587	H526	A465
F1033	R971	R971	V909	L847	K780	T714	A654	K589	Y527	L466
S1034	L972	L972	A910	A848	M781	S715	F655	V590	D529	V467
R1035	R973	R973	G911	S849	L782	V716	S656	L591	S530	R468
R1036	P974	P974	A912	K850	P783	K717	Q657	N592	V531	Q469
ASN	I975	I975	L913	L851	D784	P718	L658	E593	G532	F470
GLU	L976	L976	L914	P852	D785	M719	D659	V594	G533	S471
ASP	M977	M977	A915	T853	I786	G720	D660		I534	
ILE	T978	T978	A916	G854	G787	L721	R661	V597	G534	L474
GLU	S979	S979	T917	V855	D788	E722	M662	V598	R536	V475
HIS	L980	L980	F918	G856	Y789		V663	L599	S537	A477
SER	A981	A981	R919	Y857	Y790	Q726	F664	T600	T538	V478
HIS	F982	F982	G920	D858	W791	F727	A665	K601	G539	A479
THR	I983	I983	L921	W859	R792	K728	F666	E602	R540	L480
VAL	L984	L984	T922	T860	A793	I729	N667	K603	Y541	S481
ASP	G985	G985	N923	G861		D730	L668		L542	V482
HIS	V986	V986	D924	M862	W798	I731	P669	V606	V543	L483
HIS	M987	M987	V925	S863	V799	D732	A670	E507	L544	V484
HIS	P988	P988	Y926	Y864	P800	Q733	T671	S508	Y545	V485
HIS	L989	L989	F927	Q865	F801	E734	V672		L546	L486
HIS	V990	V990	Q928	E866		K735	E673	V612	T547	L487
HIS	I991	I991	V929	R867	F804	A736	L674	N613	T548	L488
HIS	S992	S992	G930	L868	S805	Q737	G675	G614	V549	T489
	T993	T993	L931	S869			T676	F615	V550	P490
	G994	G994	L932	G870	R808	S742	A677	G616	G551	A491
			T933	N871	W609	I743	T678	F617	M552	L492
	S997	S997	T934	K872		N744	G679	A618	A553	C493
	G998	G998	A873	R873		D745	F680	G619	Y554	A494
	A999	A999	G936	P874	S813	I746	D681	R620	L555	T495
Q1000	Q1000	Q1000	L937	S875	P614	N747	F682	G521	F556	M496
N1001	N1001	N1001	R815	L876	R815	T748	E683	Q522	V557	L497
			A939	Y877	L816	T749	L684	N623	R558	K498
	G1004	G1004	K940	A878	E817	L750	T685	T624	L559	PR0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.80Å 134.47Å 162.12Å 90.00° 98.17° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (10.00-3.10) 97.4 (10.00-3.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 3.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.255 , 0.310 0.248 , 0.307	Depositor DCC
$R_{free}$ test set	4181 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.1	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 97.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23355	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MIY

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	1.56	90/7920 (1.1%)	1.40	68/10756 (0.6%)
1	B	1.30	22/7920 (0.3%)	1.26	50/10756 (0.5%)
1	C	1.54	90/7920 (1.1%)	1.44	86/10756 (0.8%)
All	All	1.47	202/23760 (0.9%)	1.37	204/32268 (0.6%)

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	0	2
1	B	0	1
1	C	0	4
All	All	0	7

The worst 5 of 202 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	819	TYR	CG-CD1	13.88	1.57	1.39
1	A	45	ILE	CA-CB	-12.79	1.25	1.54
1	A	818	ARG	CG-CD	12.35	1.82	1.51
1	C	167	SER	N-CA	11.14	1.68	1.46
1	A	819	TYR	CE2-CZ	10.84	1.52	1.38

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ASP	CB-CG-OD1	-15.00	104.80	118.30
1	C	126	GLY	N-CA-C	-11.22	85.04	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	686	ASP	CB-CG-OD2	10.96	128.16	118.30
1	A	717	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	C	686	ASP	CB-CG-OD1	-9.84	109.44	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	860	THR	Peptide
1	A	949	ALA	Peptide
1	B	706	ALA	Peptide
1	C	157	TYR	Sidechain
1	C	160	ALA	Mainchain

## 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	1270	0
1	B	7774	0	7931	1386	0
1	C	7774	0	7931	1315	0
2	A	33	0	25	2	0
All	All	23355	0	23818	3853	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 82.

The worst 5 of 3853 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:C:166:ILE:CA	1:C:166:ILE:CB	1.74	1.60
1:C:45:ILE:CA	1:C:45:ILE:CB	1.75	1.60
1:A:90:ILE:CG1	1:A:90:ILE:CD1	1.80	1.58
1:A:814:PRO:CG	1:A:814:PRO:CB	1.74	1.56
1:A:818:ARG:CD	1:A:818:ARG:CG	1.82	1.55

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%)	627 (62%)	225 (22%)	166 (16%)	0	0
1	B	1018/1053 (97%)	616 (60%)	246 (24%)	156 (15%)	0	0
1	C	1018/1053 (97%)	642 (63%)	236 (23%)	140 (14%)	0	1
All	All	3054/3159 (97%)	1885 (62%)	707 (23%)	462 (15%)	0	0

5 of 462 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	64	VAL
1	A	65	ILE
1	A	73	ASP
1	A	74	ASN

### 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%)	661 (79%)	172 (21%)	1	6
1	B	833/859 (97%)	665 (80%)	168 (20%)	1	6
1	C	833/859 (97%)	665 (80%)	168 (20%)	1	6
All	All	2499/2577 (97%)	1991 (80%)	508 (20%)	1	6

5 of 508 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	323	ILE
1	B	671	ILE
1	C	768	VAL
1	B	357	LEU
1	B	516	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	218	GLN
1	B	526	HIS
1	C	584	GLN
1	B	228	GLN
1	B	415	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 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	MIY	A	2001	-	35,36,36	1.25	3 (8%)	42,58,58	2.61	18 (42%)

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	MIY	A	2001	-	-	0/12/70/70	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	MIY	C4-C3	2.33	1.56	1.51
2	A	2001	MIY	C18-C17	2.88	1.54	1.52
2	A	2001	MIY	C4-N1	4.03	1.56	1.47

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	MIY	O6-C17-C16	-6.57	115.77	123.84
2	A	2001	MIY	O7-C18-C17	-4.18	102.92	110.09
2	A	2001	MIY	CN7-N7-C10	-3.95	102.99	115.24
2	A	2001	MIY	O5-C15-C14	-3.10	116.06	121.97
2	A	2001	MIY	C13-C14-C15	-3.03	117.03	121.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	MIY	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1022/1053 (97%)	-0.46	8 (0%) 86 72	3, 87, 108, 120	0
1	B	1022/1053 (97%)	-0.32	12 (1%) 79 61	42, 93, 108, 120	0
1	C	1022/1053 (97%)	-0.47	18 (1%) 68 46	5, 84, 109, 120	0
All	All	3066/3159 (97%)	-0.42	38 (1%) 79 61	3, 88, 108, 120	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1034	SER	4.9
1	C	870	GLY	4.7
1	C	514	GLY	3.7
1	C	538	THR	3.5
1	C	656	SER	3.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MIY	A	2001	33/33	0.82	0.32	112,122,129,131	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.