



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 05:52 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

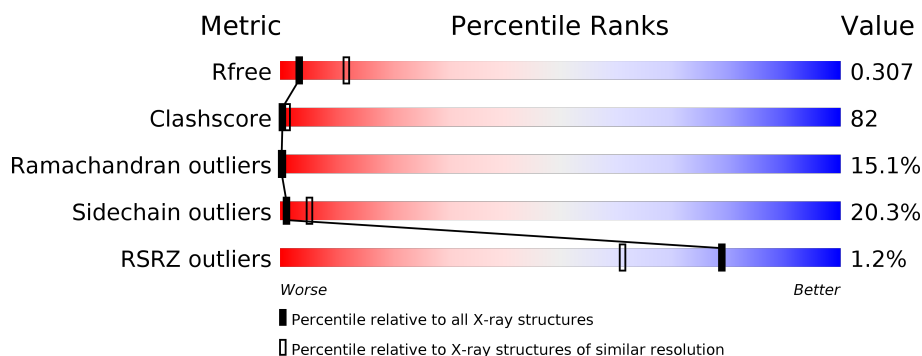
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

i

X-RAY DIFFRACTION

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 ≥ 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 $\leq 5\%$. 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	 19% 49% 24% 5%
1	B	1053	 17% 53% 23%
1	C	1053	 19% 50% 23% 6%

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.

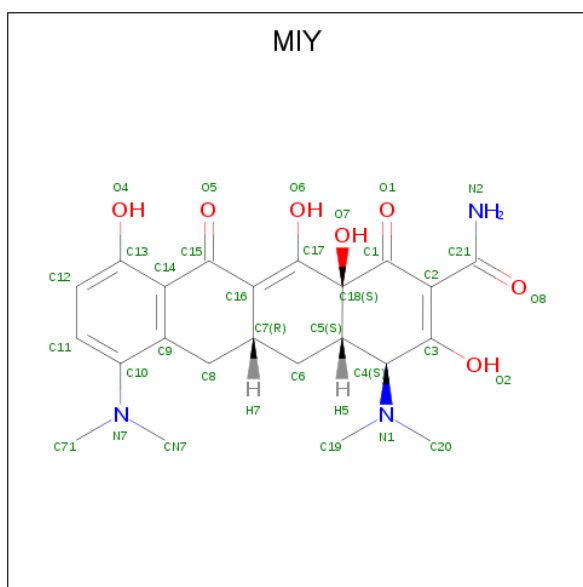
- Molecule 1 is a protein called ACRB.

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			

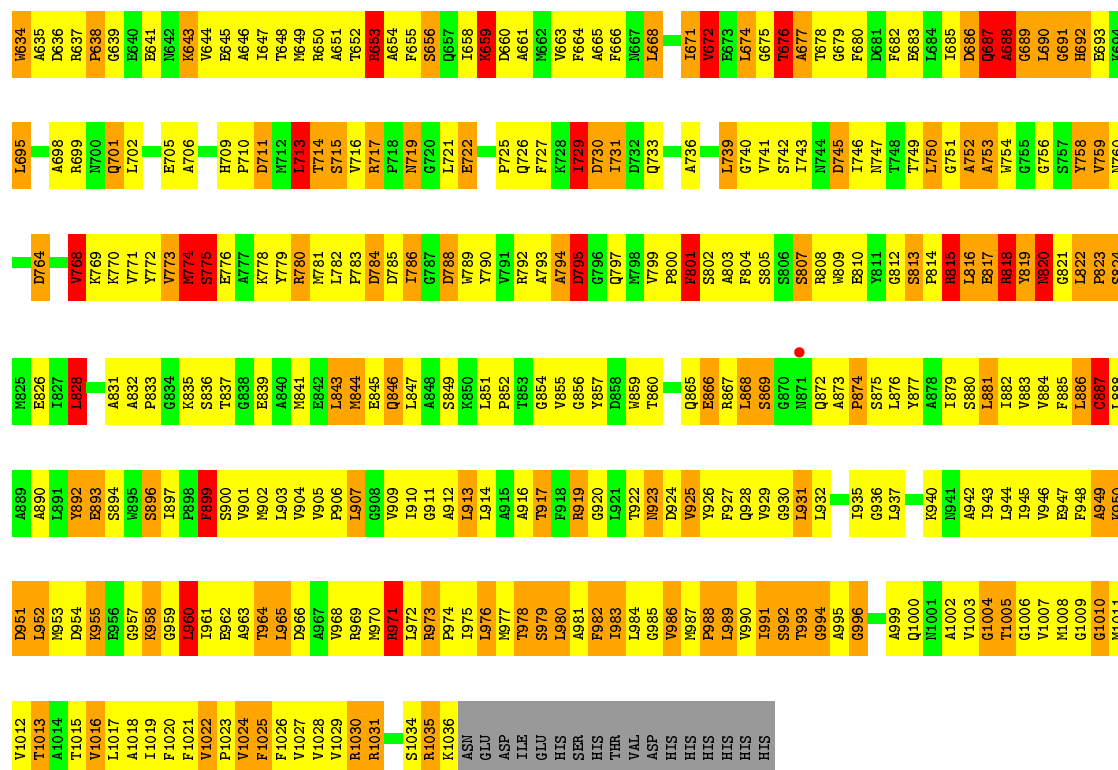
There are 12 discrepancies between the modelled and reference sequences:

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

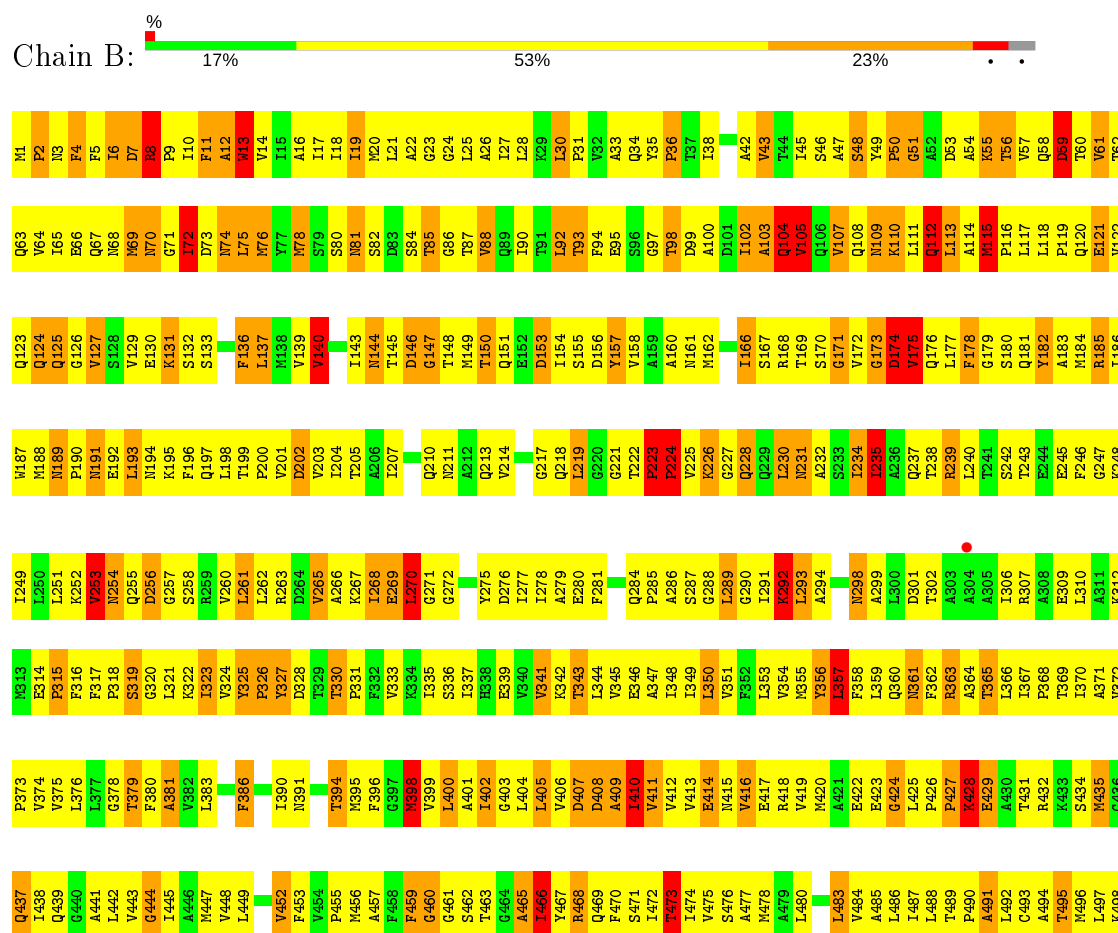
- Molecule 2 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: C₂₃H₂₇N₃O₇).

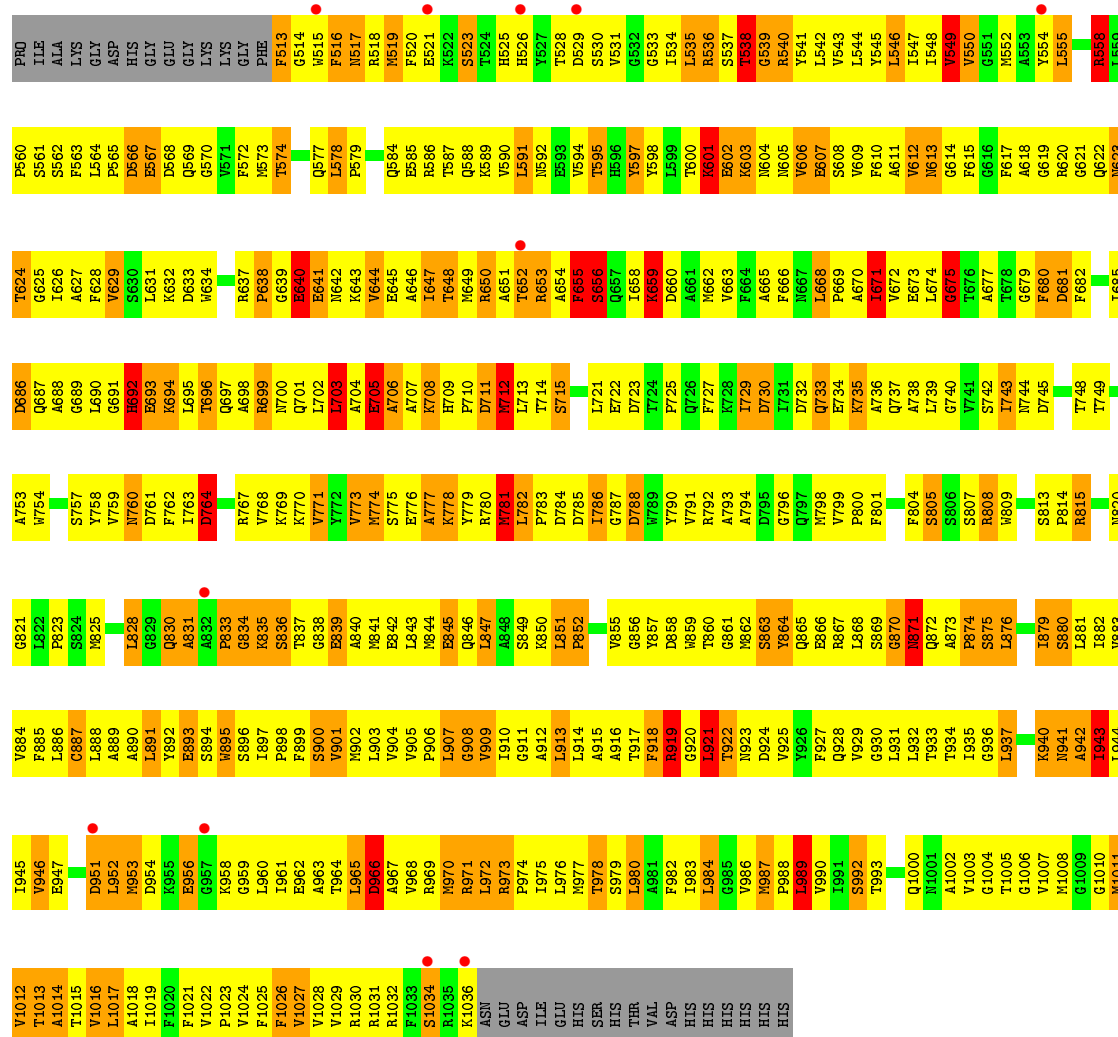


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	23	3	7		



• Molecule 1: ACRB





T1005	M941	1879	R818	G751	D886	G625	P660	IIE	L488	L376	K312
G1006	A942	S880	Y819	A752	Q887	I626	S861	ALA	Q439	L377	K313
V1007	I943		M820	A753	A888	A627	S662	LYS		G378	E314
M1008	L944	V883		W754	G689	F628	F563	GLY	L442	T379	P315
G1009	I945	V884	P823	G755	L690	V629	L564	ASP	F628	F380	F316
G1010	V946	F885	S824		H692	S630	P565	HIS	G443	A381	F317
M1011	E947	L886	M825	Y758	H692	L631	D666	GLY	G444	V382	P318
V1012	F948	C887	E826	Y759	H692	D632	E567	GLY	G445	I383	S319
T1013	A949	L888	I827	W760	K694	D633	D568	GLU	A446	L384	G320
A1014	K950	A889	L828	W761	K694	H634	Q569	LYS	M447	A385	
T1015	D951	A890	G829	F762	T696	H635	Q570	LYS	V448		K321
V1016	L952	L891	Q830	W763	Q697	D636	V571	LYS	L449		K322
L1017	M953	L892	Q831	F764	A698	H637	P572	PHE	S450		K323
A1018	D954	E893	A832	R765	R699	P638	M673		A451	S389	K324
I1019		S894	P833	G766	Q701	G639	M674	F513	V452	I390	
F1020	K958	S894	G834	G766	Q701	G639	M674	G514	I391		K325
F1021	G959	W896	K835	G768	W707	E641	M675	M515	F453	I392	
V1022	L960	S896	K836	W768	L702	E641	M675	F516	V454	T393	
P1023	I961	L897	S836	W768	L703	N642	Q577	N517	P455	T394	
V1024	E962	P898	T837	K770	A704	H643	L578	R518	M456	T329	
F1025	A963	S899	G838	W771	E705	V644	P579	M519	A457	T330	
V1026	T964	V901	E839	Y772	A706	V645		F520	F458	F396	
F1027	L965		A840	Y773	A707	A646		F521	F459	G397	
V1028	D966	V904	M841	W774	K708	L647	A582	E522	G460	I398	
A1029	A967	Q905	E842	W775	H709	T648	D584	S523	G461	V399	
R1030	V968	P906	L843	E776	P710	H649	E585	T524	G462	L400	
R1031	R969	L907	M844	A777	D711	R650	R586	H525	T463	A401	
R1032	M970	G908	Q846	W778	L713	R653	Q588		S462	I402	
F1033	R971	L910	L847	Y779	L714	A654	K589		T464	L403	
S1034	L972	I910	A848	W781	S715	F655	V590	D529	Y467	V406	
R1035	R973	G911	S849	L782	V716	S656	L591	S530	R468	D407	
V1036	P974	A912	K850	F783	R717	Q657	N592	V531	Q469	P408	
ASN	I975	L913	L851	D784	R718	L658	E593	G533	F470	A409	
GLU	L976	A915	P852	W785	N719	D660	V594	I534	S471	I410	
ASP	M977	L915	T853	L786	K720	L660				V411	
IIE	T978	A916	G854	G787	L721	D661				V412	
GLU	S979	T917	V855	D788	L722	A661	V597	L535	V475	V413	
HIS	L980	F918	G856	W789	E722	V662	L599	R536	S476	F352	
SER	A981	R919	T857	W790	Q726	V663	T600	S537	A477	E414	
HIS	F982	G920	D858	Y791	F727	A665	R601	T538	A479	E417	
THR	I983	L921	W859	R792	K728	F666	E602	R540	L480	R418	
VAL	L984	T922	T860	A793	I729	N667	K603	Y541	S481	V419	
ASP	G985	N923	G861		D730	L668		L542	V482	M420	
HIS	V986	D924	M862	W798	L731	P669	V606	V543	L483	A421	
HIS	M987	V925	S863	W799	D732	A670	E607	L544	V484	E422	
HIS	P988	V926	Y864	P900	Q733	L671	S608	Y545	A485	E423	
HIS	L989	F927	Q865	F801	E734	V672		L546	L486	G424	
HIS	V990	Q928	E866	F804	K735	E673	V612	I547	I487	I425	
HIS	I991	V929	R867	S805	A736	L674	N613	I548	I488	P426	
	S992	G930	L868		Q737	G675	G614	V549	T489	P427	
	T993	L931	S869			T676	P615	V550	P490	K428	
	G994	L932	G870	R808	S742	A677	G616	G551	A491	E429	
		T933	M871	W809	I743	T678	F617	N552	L492	P368	
	S997	T934	Q872		I744	G679	A618	Y546	Q493	T369	
G998	A999	R873	A873	G812	D745	G680	G619	Y554	A494	I370	
A999	Q1000	P874	S875	S813	I746	D681	R620	L565	T495	A432	
M1001		L937	P814	P814	I747	F682	G621	F566	M496	K433	
		S998	R815	R815	T748	E683	Q622	V557	S434	V372	
		A939	L877	L816	T749	E683	Q622	R558	M495	V373	
		K940	A878	E817	L750	I685	T624	L498	G436	V374	
								PRU	Q437	V375	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	78.1	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 97.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	5
1	B	833/859 (97%)	665 (80%)	168 (20%)	1	5
1	C	833/859 (97%)	665 (80%)	168 (20%)	1	5
All	All	2499/2577 (97%)	1991 (80%)	508 (20%)	1	5

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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1.27	3 (8%)	41,58,58	2.61	17 (41%)

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	-	-	5/12/70/70	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-N1	4.03	1.56	1.47
2	A	2001	MIY	C18-C17	3.08	1.54	1.52
2	A	2001	MIY	C4-C3	2.33	1.56	1.51

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	MIY	C1-C18-C17	8.44	119.78	109.88
2	A	2001	MIY	O6-C17-C16	-5.94	115.77	123.90
2	A	2001	MIY	O7-C18-C17	-4.52	102.92	110.14
2	A	2001	MIY	C18-C17-C16	4.14	127.27	123.06
2	A	2001	MIY	CN7-N7-C10	-3.93	102.99	115.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

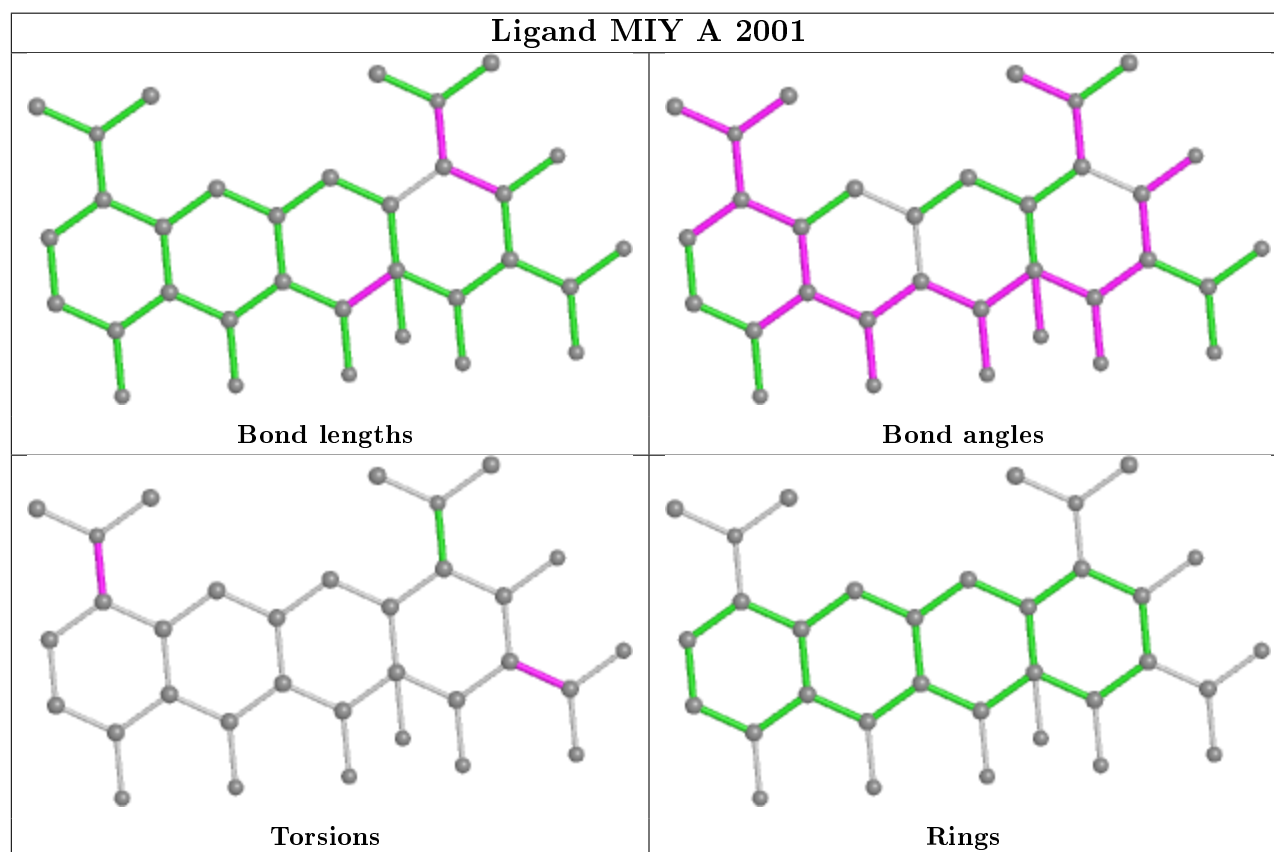
Mol	Chain	Res	Type	Atoms
2	A	2001	MIY	C1-C2-C21-O8
2	A	2001	MIY	C1-C2-C21-N2
2	A	2001	MIY	C3-C2-C21-N2
2	A	2001	MIY	C3-C2-C21-O8
2	A	2001	MIY	C9-C10-N7-CN7

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

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 ⓘ

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, 95th 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 ²)	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 47	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](#)

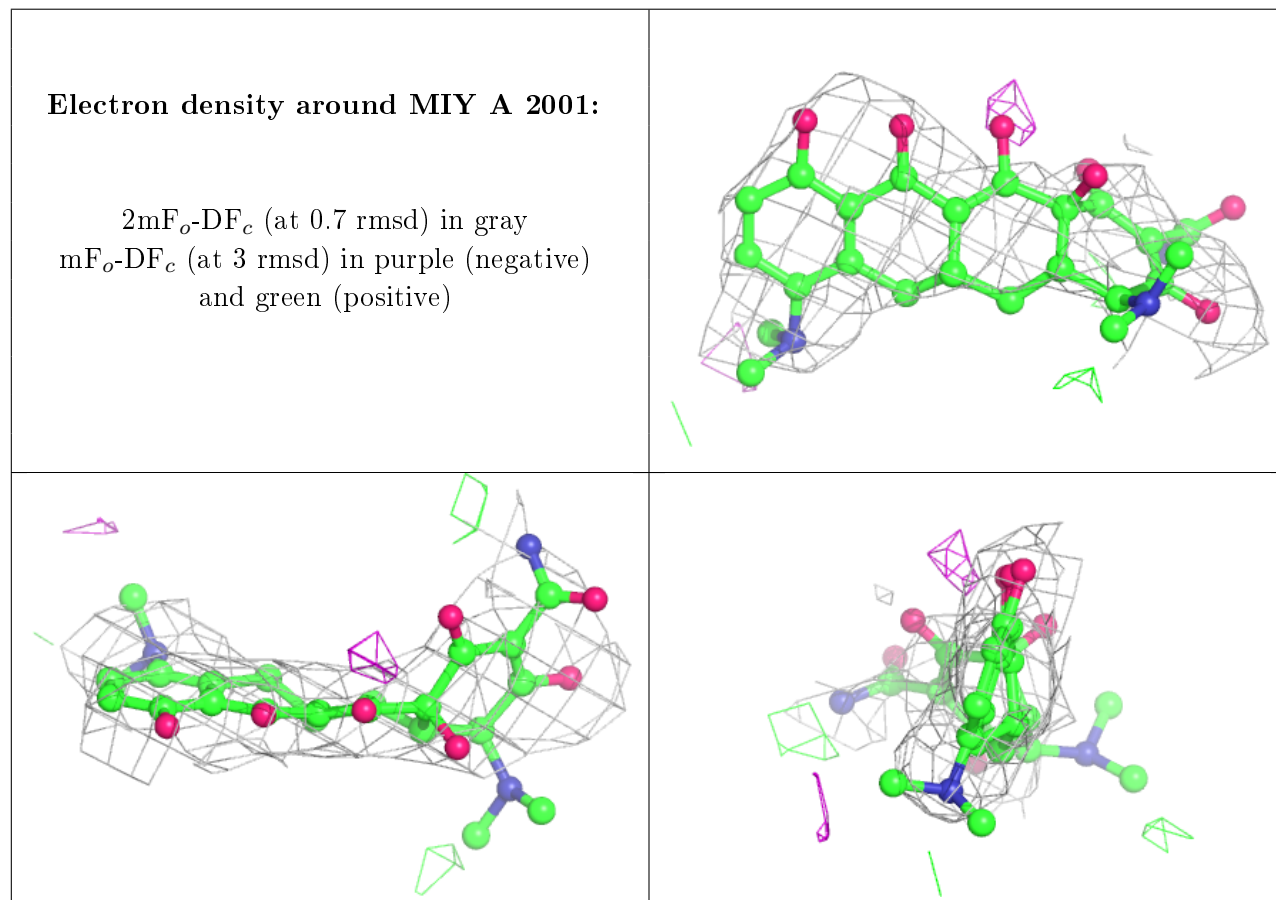
There are no carbohydrates in this entry.

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, 95th 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(\AA^2)	Q<0.9
2	MIY	A	2001	33/33	0.82	0.32	112,122,129,131	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.