Full wwPDB X-ray Structure Validation Report (i)

May 31, 2025 – 01:19 pm BST

PDB ID	:	9FHC / pdb_00009fhc
Title	:	Crystallographic structure of AcrB V612F with bound minocycline
Authors	:	Lazarova, M.; Diederichs, K.; Pos, K.M.
Deposited on	:	2024-05-27
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) 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 (i)) were used in the production of this report:

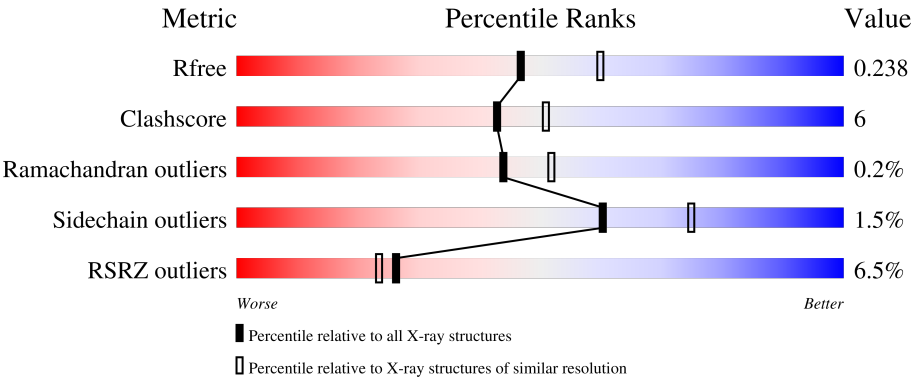
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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 <=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	1057	6% 85% 13% ••
2	B	169	7% 75% 17% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9428 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1043	Total	C	N	O	S	0	0	0
			7937	5104	1312	1477	44			

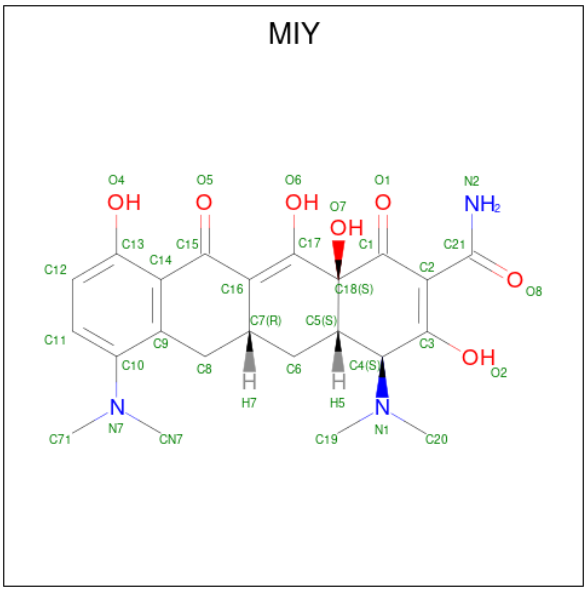
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	612	PHE	VAL	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			

- Molecule 3 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 (CCD ID: MIY) (formula: $C_{23}H_{27}N_3O_7$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

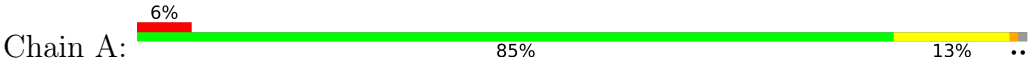
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	241	Total O 241 241	0	0
4	B	40	Total O 40 40	0	0

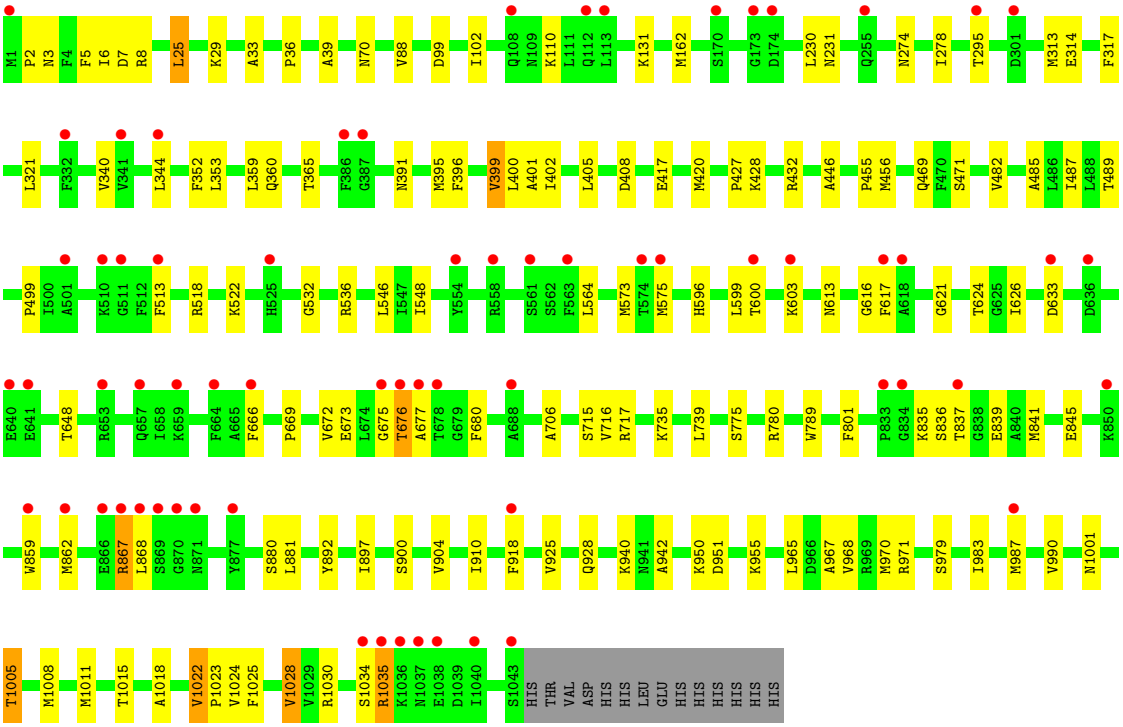
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Multidrug efflux pump subunit AcrB

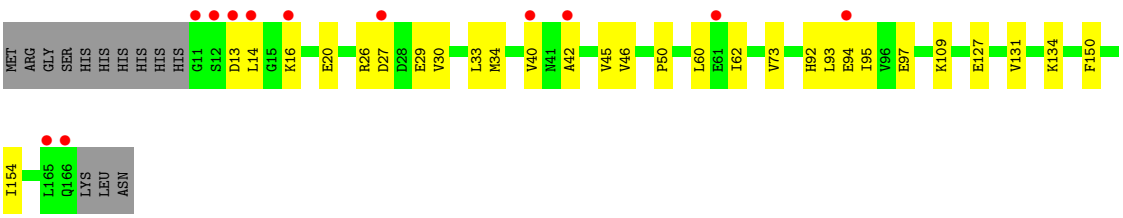
Chain A:





• Molecule 2: DARPIN

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	227.46Å 227.46Å 227.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.20 29.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.87-2.20) 94.5 (29.87-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.31 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.208 , 0.238 0.208 , 0.238	Depositor DCC
R_{free} test set	10010 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9428	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.38	0/8089	0.60	0/10982
2	B	0.36	0/1196	0.62	2/1626 (0.1%)
All	All	0.38	0/9285	0.60	2/12608 (0.0%)

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	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	14	LEU	N-CA-C	-7.56	104.06	113.28
2	B	73	VAL	N-CA-C	-5.63	104.78	113.16

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	ARG	Sidechain
1	A	780	ARG	Sidechain
1	A	867	ARG	Sidechain

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	7937	0	8077	94	0
2	B	1177	0	1159	19	0
3	A	33	0	25	1	0
4	A	241	0	0	1	0
4	B	40	0	0	1	0
All	All	9428	0	9261	113	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 6.

All (113) 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:575:MET:HE1	1:A:617:PHE:H	1.27	0.99
1:A:735:LYS:HE3	1:A:739:LEU:HD11	1.51	0.90
2:B:60:LEU:HD22	2:B:94:GLU:HG3	1.56	0.88
1:A:1011:MET:O	1:A:1015:THR:HG23	1.84	0.77
1:A:352:PHE:CD2	1:A:365:THR:HG21	2.22	0.75
1:A:600:THR:O	1:A:603:LYS:HG3	1.87	0.75
1:A:599:LEU:O	1:A:603:LYS:HG2	1.87	0.73
1:A:162:MET:HA	1:A:313:MET:HE1	1.68	0.73
1:A:1001:ASN:O	1:A:1005:THR:HG23	1.93	0.69
1:A:420:MET:HE2	1:A:499:PRO:HA	1.74	0.68
1:A:897:ILE:HD11	1:A:1030:ARG:NH1	2.08	0.68
2:B:27:ASP:OD1	2:B:62:ILE:CG1	2.42	0.68
1:A:706:ALA:HB1	1:A:716:VAL:HG11	1.78	0.66
2:B:150:PHE:CZ	2:B:154:ILE:HD11	2.32	0.65
1:A:274:ASN:HD21	3:A:2001:MIY:C1	2.09	0.65
2:B:27:ASP:OD1	2:B:62:ILE:HG12	1.97	0.63
1:A:990:VAL:HG13	1:A:1005:THR:HG22	1.79	0.63
1:A:575:MET:HE1	1:A:617:PHE:N	2.08	0.62
2:B:16:LYS:O	2:B:20:GLU:HG3	1.99	0.62
1:A:897:ILE:HD11	1:A:1030:ARG:HH11	1.64	0.61
1:A:352:PHE:CD2	1:A:365:THR:CG2	2.83	0.60
1:A:575:MET:CE	1:A:617:PHE:H	2.10	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ALA:CB	1:A:716:VAL:HG11	2.31	0.59
2:B:154:ILE:HG23	4:B:217:HOH:O	2.03	0.59
2:B:150:PHE:CZ	2:B:154:ILE:CD1	2.87	0.57
1:A:971:ARG:HD3	4:A:2315:HOH:O	2.05	0.57
1:A:573:MET:HE3	1:A:666:PHE:HE1	1.69	0.56
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.88	0.55
2:B:30:VAL:O	2:B:34:MET:HG2	2.06	0.55
1:A:352:PHE:HD1	1:A:353:LEU:HD12	1.72	0.55
1:A:401:ALA:O	1:A:405:LEU:HG	2.06	0.55
2:B:127:GLU:O	2:B:131:VAL:HG23	2.07	0.54
1:A:420:MET:HE3	1:A:427:PRO:HA	1.90	0.54
1:A:1018:ALA:O	1:A:1022:VAL:HG13	2.07	0.53
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.90	0.53
1:A:715:SER:O	1:A:717:ARG:NH1	2.41	0.53
1:A:360:GLN:HG2	1:A:513:PHE:CD1	2.44	0.53
1:A:573:MET:HE3	1:A:666:PHE:CE1	2.43	0.53
1:A:669:PRO:HG2	1:A:675:GLY:HA2	1.91	0.53
1:A:836:SER:O	1:A:839:GLU:HG2	2.08	0.53
1:A:965:LEU:O	1:A:968:VAL:HG22	2.09	0.52
1:A:621:GLY:O	1:A:624:THR:HG22	2.10	0.52
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.75	0.52
2:B:34:MET:HA	2:B:34:MET:HE2	1.91	0.52
1:A:518:ARG:O	1:A:522:LYS:HG3	2.10	0.51
1:A:596:HIS:CE1	1:A:600:THR:HG21	2.46	0.51
2:B:45:VAL:HG23	2:B:46:VAL:HG13	1.93	0.50
1:A:408:ASP:OD1	1:A:940:LYS:NZ	2.31	0.50
1:A:676:THR:HG23	1:A:677:ALA:H	1.77	0.50
1:A:428:LYS:HE2	1:A:432:ARG:NH2	2.26	0.49
1:A:3:ASN:OD1	1:A:432:ARG:HG2	2.11	0.49
2:B:92:HIS:HB3	2:B:95:ILE:HD12	1.94	0.49
1:A:1024:VAL:O	1:A:1028:VAL:HG13	2.12	0.49
1:A:340:VAL:O	1:A:344:LEU:HG	2.13	0.49
1:A:616:GLY:HA2	1:A:626:ILE:CG1	2.43	0.48
1:A:735:LYS:HE3	1:A:739:LEU:CD1	2.34	0.48
1:A:835:LYS:HD2	1:A:839:GLU:OE2	2.13	0.48
1:A:2:PRO:O	1:A:6:ILE:HG13	2.13	0.48
2:B:34:MET:HE1	2:B:40:VAL:HG12	1.96	0.48
1:A:485:ALA:HA	1:A:489:THR:OG1	2.14	0.48
1:A:867:ARG:O	1:A:867:ARG:HG2	2.14	0.48
1:A:396:PHE:HA	1:A:399:VAL:HG13	1.97	0.47
2:B:27:ASP:OD1	2:B:62:ILE:HG13	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ALA:HB2	1:A:673:GLU:HG3	1.97	0.46
1:A:1022:VAL:HA	1:A:1025:PHE:CD2	2.50	0.46
2:B:42:ALA:O	2:B:50:PRO:HD3	2.16	0.46
2:B:93:LEU:O	2:B:97:GLU:HG3	2.15	0.46
1:A:548:ILE:HG23	1:A:910:ILE:HD13	1.98	0.46
1:A:5:PHE:CE2	1:A:487:ILE:HG12	2.51	0.45
1:A:278:ILE:HB	1:A:613:ASN:HB3	1.97	0.45
1:A:359:LEU:HD13	1:A:417:GLU:HG3	1.98	0.45
1:A:775:SER:HB2	1:A:789:TRP:CZ2	2.51	0.45
1:A:841:MET:O	1:A:845:GLU:HG3	2.16	0.44
1:A:951:ASP:O	1:A:955:LYS:HG2	2.18	0.44
1:A:33:ALA:O	1:A:391:ASN:HA	2.18	0.44
1:A:983:ILE:O	1:A:987:MET:HG3	2.18	0.44
2:B:26:ARG:O	2:B:30:VAL:HG23	2.17	0.44
1:A:616:GLY:HA2	1:A:626:ILE:HG12	1.99	0.44
1:A:230:LEU:HD12	1:A:231:ASN:N	2.33	0.44
1:A:70:ASN:O	1:A:110:LYS:HE3	2.18	0.43
1:A:456:MET:HE3	1:A:471:SER:HB2	2.00	0.43
1:A:314:GLU:HG3	1:A:317:PHE:CE2	2.53	0.43
2:B:134:LYS:HB2	2:B:134:LYS:HE3	1.62	0.43
1:A:352:PHE:CD1	1:A:352:PHE:C	2.97	0.43
1:A:317:PHE:HB3	1:A:321:LEU:HB3	2.01	0.43
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.33	0.43
1:A:925:VAL:HA	1:A:928:GLN:OE1	2.19	0.42
1:A:340:VAL:HG21	1:A:395:MET:HB3	2.01	0.42
1:A:352:PHE:CE2	1:A:365:THR:HG21	2.54	0.42
1:A:564:LEU:HD23	1:A:925:VAL:HG22	2.01	0.42
1:A:7:ASP:HB2	1:A:8:ARG:NH1	2.34	0.42
1:A:36:PRO:HG3	1:A:469:GLN:HG3	2.01	0.42
1:A:967:ALA:HA	1:A:970:MET:HE3	2.00	0.42
1:A:400:LEU:HD23	1:A:400:LEU:HA	1.88	0.42
1:A:99:ASP:CG	1:A:102:ILE:HG12	2.45	0.42
1:A:131:LYS:HE2	1:A:131:LYS:HB2	1.90	0.42
1:A:979:SER:CB	1:A:1015:THR:HG21	2.50	0.42
1:A:881:LEU:HD12	1:A:881:LEU:HA	1.92	0.42
1:A:892:TYR:O	1:A:950:LYS:HE3	2.20	0.42
1:A:25:LEU:O	1:A:29:LYS:HG3	2.20	0.41
1:A:352:PHE:CD1	1:A:353:LEU:HD12	2.53	0.41
1:A:455:PRO:HG2	1:A:880:SER:HB2	2.02	0.41
1:A:1008:MET:HE2	1:A:1008:MET:HB3	1.91	0.41
1:A:532:GLY:O	1:A:536:ARG:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.84	0.41
1:A:564:LEU:HD21	1:A:925:VAL:CG2	2.51	0.41
2:B:29:GLU:O	2:B:33:LEU:HD12	2.21	0.41
1:A:900:SER:HA	1:A:1025:PHE:HB3	2.02	0.40
1:A:676:THR:OG1	1:A:677:ALA:N	2.54	0.40
1:A:904:VAL:HG11	1:A:942:ALA:HB2	2.03	0.40
1:A:918:PHE:CD1	1:A:918:PHE:C	2.99	0.40
1:A:1034:SER:OG	1:A:1035:ARG:N	2.55	0.40
1:A:352:PHE:HA	1:A:365:THR:HG23	2.02	0.40

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	1041/1057 (98%)	1009 (97%)	31 (3%)	1 (0%)	48 57
2	B	154/169 (91%)	147 (96%)	6 (4%)	1 (1%)	22 23
All	All	1195/1226 (98%)	1156 (97%)	37 (3%)	2 (0%)	44 52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	676	THR
2	B	13	ASP

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	849/863 (98%)	835 (98%)	14 (2%)	58 73
2	B	120/132 (91%)	119 (99%)	1 (1%)	79 88
All	All	969/995 (97%)	954 (98%)	15 (2%)	60 75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	88	VAL
1	A	295	THR
1	A	399	VAL
1	A	633	ASP
1	A	648	THR
1	A	672	VAL
1	A	801	PHE
1	A	837	THR
1	A	862	MET
1	A	868	LEU
1	A	1005	THR
1	A	1022	VAL
1	A	1028	VAL
2	B	109	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	274	ASN
1	A	284	GLN
1	A	657	GLN
2	B	92	HIS

5.3.3 RNA

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	$\#\|Z\| > 2$
3	MIY	A	2001	-	35,36,36	1.19	2 (5%)	41,58,58	1.13	4 (9%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	MIY	C21-N2	5.39	1.47	1.33
3	A	2001	MIY	O5-C15	2.15	1.27	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001	MIY	O7-C18-C17	-2.81	105.65	110.14
3	A	2001	MIY	C15-C16-C17	2.69	120.93	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001	MIY	C5-C18-C1	-2.69	107.97	111.05
3	A	2001	MIY	O6-C17-C16	-2.68	120.24	123.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	MIY	C1-C2-C21-O8
3	A	2001	MIY	C3-C2-C21-O8
3	A	2001	MIY	C1-C2-C21-N2
3	A	2001	MIY	C3-C2-C21-N2

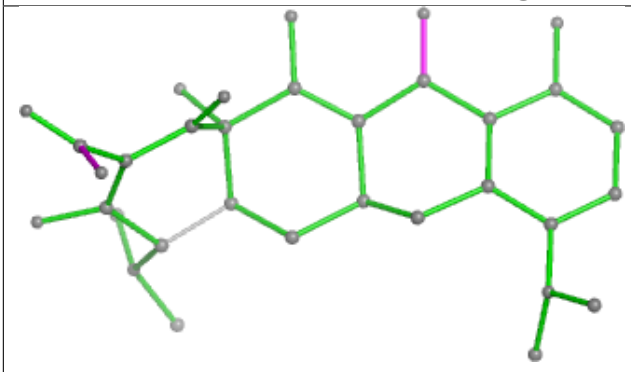
There are no ring outliers.

1 monomer is involved in 1 short contact:

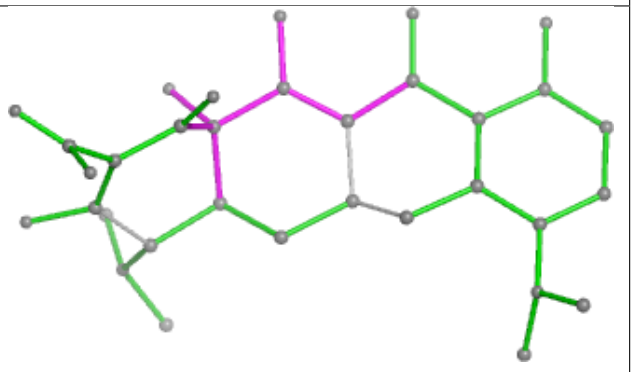
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	MIY	1	0

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 then 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.

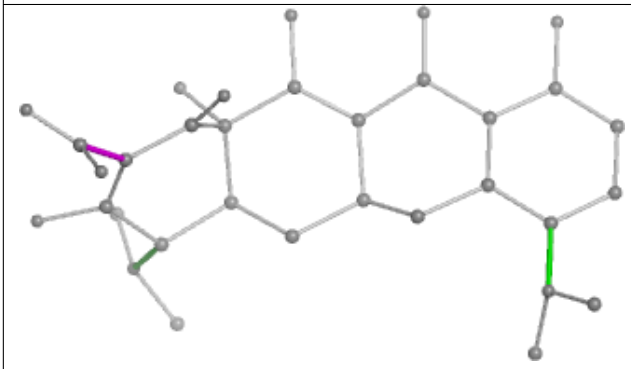
Ligand MIY A 2001



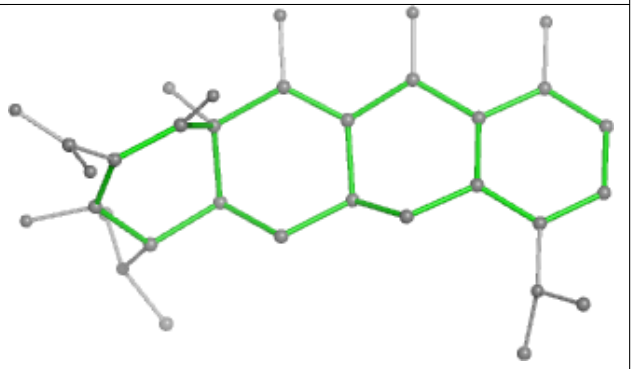
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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^{th} 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	1043/1057 (98%)	0.21	66 (6%)	27	24	16, 40, 63, 88	0
2	B	156/169 (92%)	0.36	12 (7%)	21	18	23, 39, 69, 90	0
All	All	1199/1226 (97%)	0.22	78 (6%)	26	23	16, 40, 64, 90	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	617	PHE	6.9
1	A	676	THR	5.6
1	A	868	LEU	5.6
2	B	11	GLY	5.5
1	A	1038	GLU	5.3
1	A	173	GLY	4.7
1	A	869	SER	4.7
1	A	113	LEU	4.6
1	A	301	ASP	4.2
1	A	866	GLU	4.0
1	A	1034	SER	4.0
2	B	166	GLN	3.9
1	A	867	ARG	3.9
2	B	12	SER	3.9
1	A	859	TRP	3.7
1	A	1036	LYS	3.7
1	A	108	GLN	3.5
1	A	653	ARG	3.5
2	B	13	ASP	3.5
1	A	918	PHE	3.4
1	A	170	SER	3.4
2	B	27	ASP	3.4
1	A	870	GLY	3.3
1	A	633	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	666	PHE	3.3
1	A	344	LEU	3.3
1	A	664	PHE	3.3
1	A	837	THR	3.2
1	A	675	GLY	3.1
1	A	1040	ILE	3.1
1	A	603	LYS	3.1
1	A	332	PHE	3.1
1	A	688	ALA	3.1
1	A	1035	ARG	3.0
1	A	987	MET	3.0
1	A	1043	SER	3.0
1	A	174	ASP	3.0
1	A	510	LYS	2.9
1	A	575	MET	2.9
1	A	1037	ASN	2.9
1	A	677	ALA	2.9
1	A	563	PHE	2.8
2	B	94	GLU	2.8
1	A	511	GLY	2.7
1	A	600	THR	2.7
1	A	871	ASN	2.7
1	A	834	GLY	2.6
1	A	877	TYR	2.6
1	A	678	THR	2.6
1	A	554	TYR	2.4
1	A	659	LYS	2.4
1	A	862	MET	2.4
1	A	386	PHE	2.4
1	A	513	PHE	2.4
1	A	636	ASP	2.4
2	B	14	LEU	2.3
1	A	574	THR	2.3
1	A	387	GLY	2.3
1	A	501	ALA	2.2
1	A	561	SER	2.2
1	A	618	ALA	2.2
1	A	833	PRO	2.2
1	A	295	THR	2.2
1	A	525	HIS	2.2
1	A	640	GLU	2.2
1	A	112	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	16	LYS	2.2
1	A	1	MET	2.2
2	B	40	VAL	2.2
1	A	341	VAL	2.1
2	B	165	LEU	2.1
1	A	255	GLN	2.1
1	A	850	LYS	2.1
1	A	657	GLN	2.1
2	B	42	ALA	2.1
1	A	558	ARG	2.0
1	A	641	GLU	2.0
2	B	61	GLU	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

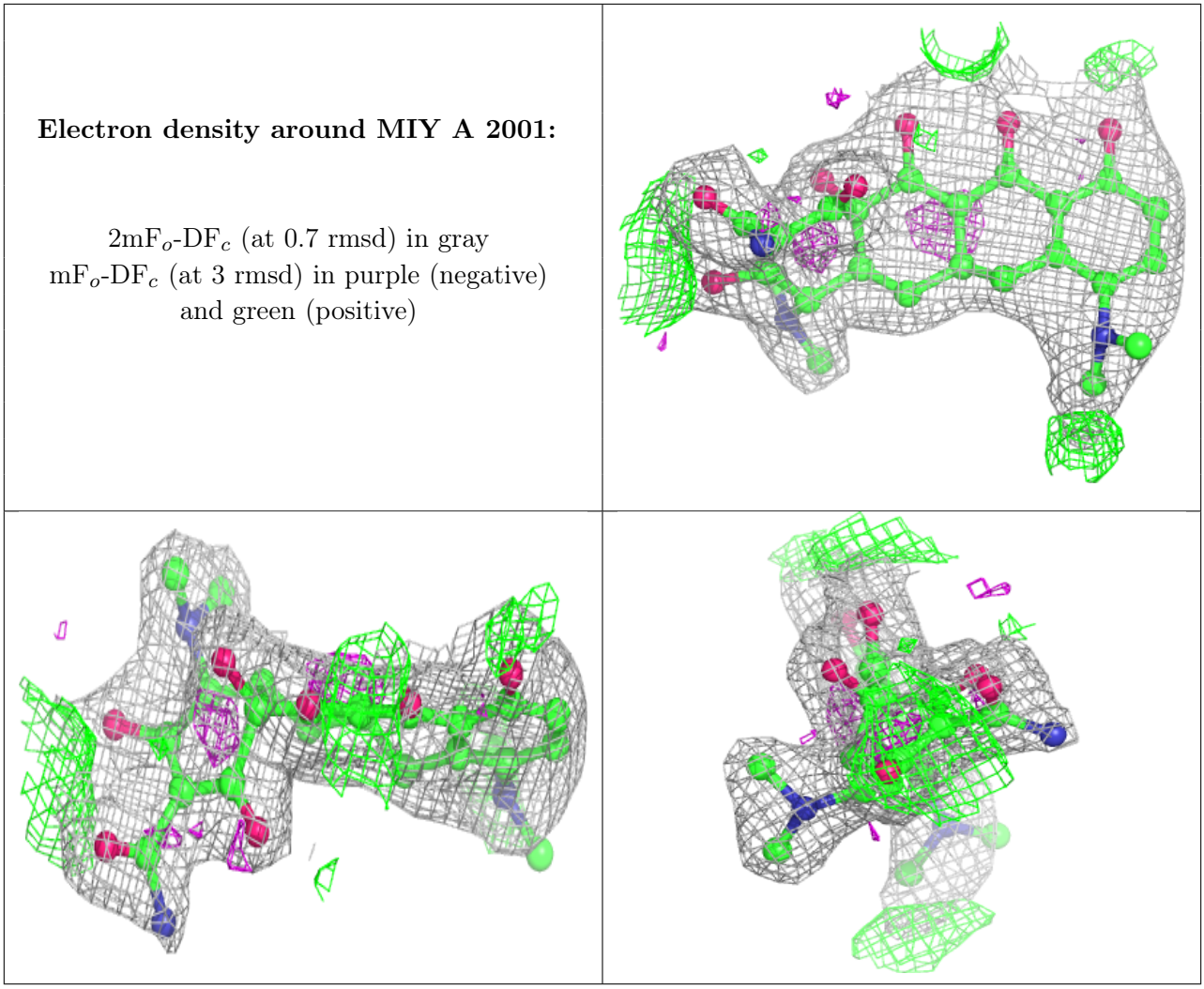
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MIY	A	2001	33/33	0.85	0.13	29,38,47,52	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.

Electron density around MIY A 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.