



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:20 AM EDT

PDB ID : 9FE2 / pdb_00009fe2
Title : Crystallographic structure of AcrB V612W with bound minocycline
Authors : Lazarova, M.; Pos, K.M.
Deposited on : 2024-05-17
Resolution : 1.89 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 ⓘ 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)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

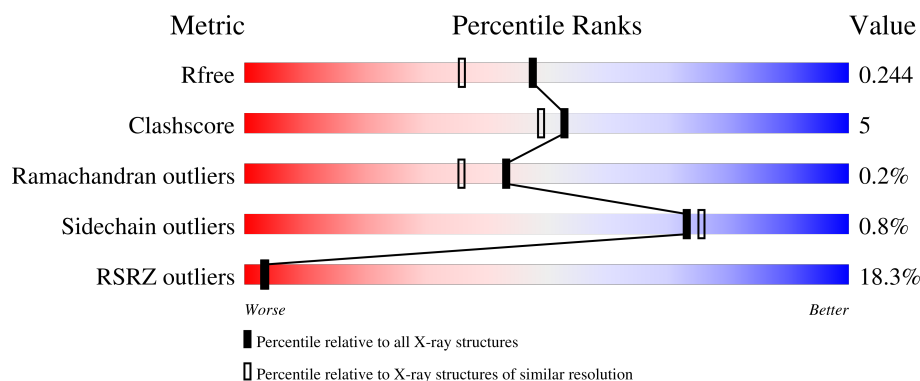
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	D	169	37% 75% 14% 11%
2	A	1057	15% 88% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9499 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 DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	151	Total	C	N	O	S	0	0	0
			1142	721	200	220	1			

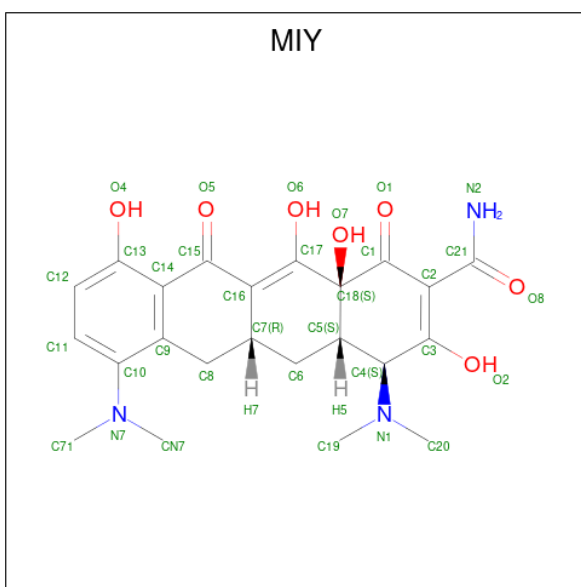
- Molecule 2 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1043	Total	C	N	O	S	0	0	0
			7940	5106	1313	1477	44			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	612	TRP	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 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: C₂₃H₂₇N₃O₇) (labeled as "Ligand of Interest" by depositor).



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

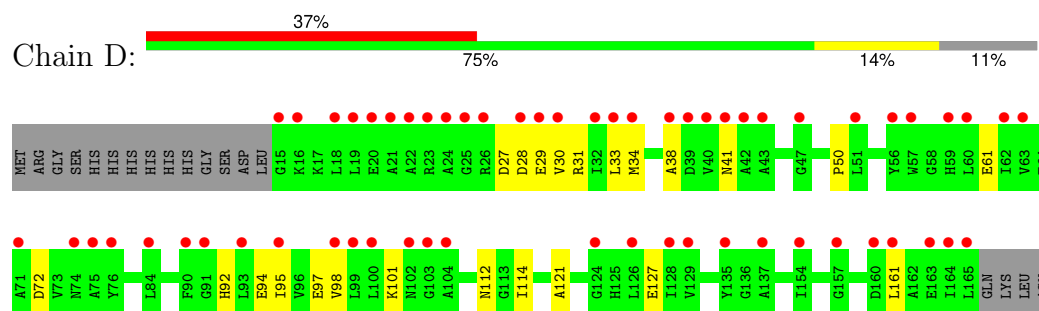
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	20	Total O 20 20	0	0
4	A	364	Total O 364 364	0	0

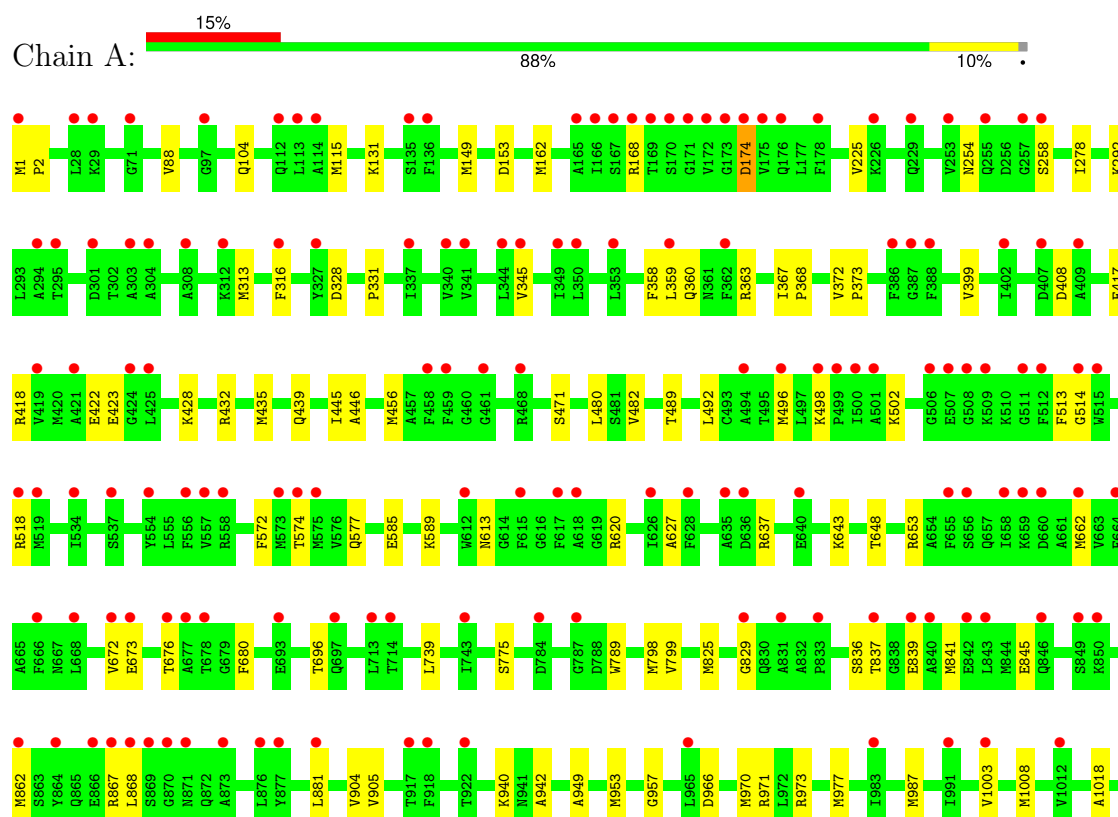
3 Residue-property plots [i](#)

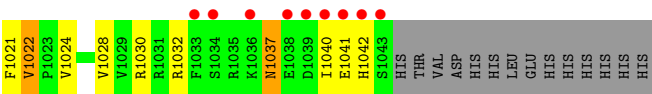
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DARPIN



• Molecule 2: Multidrug efflux pump subunit AcrB





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	227.50Å 227.50Å 227.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.44 – 1.89 46.44 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.4 (46.44-1.89) 97.0 (46.44-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.222 , 0.244 0.225 , 0.244	Depositor DCC
R_{free} test set	1998 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9499	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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 [i](#)

5.1 Standard geometry [i](#)

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	D	0.37	0/1161	0.58	0/1579
2	A	0.55	1/8093 (0.0%)	0.72	2/10989 (0.0%)
All	All	0.53	1/9254 (0.0%)	0.70	2/12568 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	905	VAL	CA-CB	-5.04	1.51	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1021	PHE	CA-C-N	-5.13	112.65	122.13
2	A	1021	PHE	C-N-CA	-5.13	112.65	122.13

There are no chirality outliers.

There are no planarity outliers.

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	D	1142	0	1128	20	0
2	A	7940	0	8078	71	0
3	A	33	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	364	0	0	5	0
4	D	20	0	0	0	0
All	All	9499	0	9233	91	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 5.

All (91) 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:D:50:PRO:HB2	1:D:66:LEU:HD21	1.26	1.12
1:D:92:HIS:HB3	1:D:95:ILE:HD13	1.36	1.06
2:A:676:THR:HB	2:A:862:MET:HE2	1.62	0.80
2:A:456:MET:HE3	2:A:471:SER:HB2	1.68	0.75
2:A:360:GLN:HG2	2:A:513:PHE:CD2	2.23	0.73
2:A:574:THR:CG2	2:A:627:ALA:HB3	2.17	0.73
2:A:574:THR:HG23	2:A:627:ALA:HB3	1.73	0.71
1:D:50:PRO:HB2	1:D:66:LEU:CD2	2.14	0.69
1:D:95:ILE:HD12	1:D:95:ILE:H	1.58	0.68
2:A:971:ARG:HD3	4:A:1414:HOH:O	1.95	0.66
2:A:637:ARG:O	2:A:643:LYS:NZ	2.28	0.65
1:D:30:VAL:HG12	1:D:34:MET:HE1	1.80	0.64
2:A:363:ARG:HD2	2:A:498:LYS:HE2	1.82	0.62
1:D:94:GLU:H	1:D:94:GLU:CD	2.08	0.61
2:A:973:ARG:O	2:A:977:MET:HG3	1.99	0.61
1:D:61:GLU:CD	1:D:61:GLU:H	2.08	0.61
2:A:168:ARG:HA	4:A:1299:HOH:O	2.01	0.61
1:D:112:ASN:HB2	1:D:114:ILE:HD12	1.83	0.60
2:A:162:MET:HA	2:A:313:MET:HE1	1.83	0.60
2:A:966:ASP:O	2:A:970:MET:HG3	2.02	0.59
2:A:408:ASP:OD1	2:A:940:LYS:NZ	2.28	0.59
2:A:577:GLN:HG2	2:A:662:MET:HE3	1.83	0.59
2:A:841:MET:O	2:A:845:GLU:HG3	2.04	0.58
1:D:50:PRO:CB	1:D:66:LEU:HD21	2.17	0.57
2:A:867:ARG:HH21	2:A:868:LEU:HD11	1.71	0.55
2:A:949:ALA:O	2:A:953:MET:HG3	2.07	0.54
2:A:1018:ALA:O	2:A:1022:VAL:HG13	2.09	0.53
1:D:28:ASP:HA	1:D:31:ARG:HD2	1.91	0.53
1:D:94:GLU:O	1:D:98:VAL:HG23	2.09	0.53
2:A:363:ARG:HD3	2:A:498:LYS:HG3	1.91	0.52
2:A:676:THR:HB	2:A:862:MET:CE	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:MET:HB3	2:A:2:PRO:HD3	1.93	0.51
2:A:696:THR:OG1	2:A:825:MET:HE1	2.11	0.50
1:D:121:ALA:HA	1:D:161:LEU:HD21	1.93	0.49
2:A:418:ARG:O	2:A:422:GLU:HG3	2.13	0.48
1:D:29:GLU:O	1:D:33:LEU:HD23	2.14	0.48
1:D:41:ASN:HD21	1:D:72:ASP:HB2	1.78	0.48
2:A:514:GLY:O	2:A:518:ARG:HG3	2.14	0.48
2:A:435:MET:O	2:A:439:GLN:HG2	2.14	0.47
2:A:278:ILE:HB	2:A:613:ASN:HB3	1.96	0.47
1:D:33:LEU:O	1:D:38:ALA:N	2.40	0.47
1:D:97:GLU:O	1:D:101:LYS:HG3	2.14	0.47
2:A:359:LEU:HD22	2:A:417:GLU:HG3	1.96	0.47
2:A:653:ARG:HG3	2:A:653:ARG:HH11	1.79	0.47
2:A:316:PHE:CD1	2:A:316:PHE:N	2.83	0.46
2:A:1032:ARG:O	2:A:1032:ARG:NH1	2.44	0.46
2:A:489:THR:HG21	4:A:1381:HOH:O	2.15	0.46
2:A:1037:ASN:HA	4:A:1377:HOH:O	2.16	0.46
2:A:585:GLU:O	2:A:589:LYS:HE2	2.16	0.46
1:D:41:ASN:ND2	1:D:72:ASP:HB2	2.31	0.45
2:A:492:LEU:O	2:A:496:MET:HB2	2.17	0.45
2:A:358:PHE:HB2	2:A:977:MET:HE3	1.98	0.45
2:A:456:MET:HG3	4:A:1309:HOH:O	2.16	0.45
2:A:775:SER:HB2	2:A:789:TRP:CZ2	2.52	0.45
2:A:620:ARG:HH11	2:A:620:ARG:HG3	1.82	0.45
2:A:653:ARG:HG3	2:A:653:ARG:NH1	2.32	0.44
2:A:739:LEU:HD13	2:A:799:VAL:HG11	1.99	0.44
2:A:446:ALA:HB2	2:A:482:VAL:HG21	2.00	0.44
2:A:836:SER:O	2:A:839:GLU:HG2	2.17	0.44
2:A:987:MET:HG3	2:A:1008:MET:HE2	1.98	0.44
2:A:620:ARG:HG3	2:A:620:ARG:NH1	2.32	0.44
2:A:363:ARG:CD	2:A:498:LYS:HG3	2.47	0.44
2:A:904:VAL:HG11	2:A:942:ALA:HB2	1.99	0.43
1:D:27:ASP:O	1:D:31:ARG:HG3	2.19	0.43
2:A:676:THR:CB	2:A:862:MET:HE2	2.43	0.43
2:A:798:MET:HB3	2:A:798:MET:HE3	1.62	0.43
1:D:95:ILE:H	1:D:95:ILE:CD1	2.29	0.43
1:D:127:GLU:H	1:D:127:GLU:CD	2.27	0.43
2:A:572:PHE:CD2	2:A:648:THR:HG22	2.54	0.43
2:A:149:MET:HB3	2:A:153:ASP:HB2	1.99	0.43
2:A:881:LEU:HD23	2:A:881:LEU:HA	1.75	0.42
2:A:836:SER:HB3	2:A:839:GLU:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:957:GLY:HA2	2:A:1042:HIS:CE1	2.54	0.42
2:A:174:ASP:HB3	2:A:292:LYS:HB2	2.02	0.41
2:A:445:ILE:HD13	2:A:940:LYS:HG3	2.01	0.41
2:A:1030:ARG:HA	2:A:1030:ARG:HD2	1.70	0.41
2:A:254:ASN:HB2	2:A:258:SER:OG	2.20	0.41
2:A:115:MET:HE3	2:A:115:MET:HB3	1.90	0.41
2:A:360:GLN:HG2	2:A:513:PHE:CE2	2.56	0.41
2:A:328:ASP:O	2:A:331:PRO:HD2	2.21	0.41
2:A:367:ILE:HB	2:A:368:PRO:HD3	2.03	0.41
2:A:680:PHE:CZ	2:A:829:GLY:HA3	2.56	0.41
2:A:837:THR:O	2:A:841:MET:HG3	2.20	0.41
2:A:428:LYS:HE2	2:A:432:ARG:NH2	2.36	0.41
2:A:423:GLU:HA	2:A:502:LYS:HD2	2.03	0.40
2:A:480:LEU:HD12	2:A:480:LEU:HA	1.90	0.40
2:A:987:MET:HG3	2:A:1008:MET:CE	2.51	0.40
2:A:104:GLN:OE1	2:A:131:LYS:HE3	2.21	0.40
2:A:372:VAL:HB	2:A:373:PRO:HD3	2.03	0.40
2:A:1024:VAL:O	2:A:1028:VAL:HG13	2.21	0.40
2:A:1040:ILE:HG22	2:A:1041:GLU:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	D	149/169 (88%)	141 (95%)	8 (5%)	0	100	100
2	A	1041/1057 (98%)	1008 (97%)	31 (3%)	2 (0%)	43	36
All	All	1190/1226 (97%)	1149 (97%)	39 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	174	ASP
2	A	1037	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	D	116/132 (88%)	116 (100%)	0	100	100
2	A	849/863 (98%)	841 (99%)	8 (1%)	70	73
All	All	965/995 (97%)	957 (99%)	8 (1%)	73	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	88	VAL
2	A	225	VAL
2	A	345	VAL
2	A	399	VAL
2	A	672	VAL
2	A	673	GLU
2	A	1003	VAL
2	A	1022	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	59	HIS
2	A	89	GLN
2	A	120	GLN
2	A	439	GLN
2	A	505	HIS
2	A	577	GLN
2	A	846	GLN
2	A	1000	GLN

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 oligosaccharides 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	$\# Z > 2$
3	MIY	A	1101	-	36,36,36	2.21	12 (33%)	42,58,58	2.08	17 (40%)

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	1101	-	-	5/12/70/70	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	MIY	C18-C5	7.00	1.59	1.53
3	A	1101	MIY	O7-C18	3.95	1.48	1.42
3	A	1101	MIY	C4-N1	3.92	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	MIY	C4-C3	3.92	1.59	1.51
3	A	1101	MIY	C71-N7	3.16	1.52	1.45
3	A	1101	MIY	C18-C17	3.05	1.54	1.52
3	A	1101	MIY	CN7-N7	3.01	1.52	1.45
3	A	1101	MIY	C2-C21	2.90	1.53	1.47
3	A	1101	MIY	C5-C4	2.79	1.57	1.54
3	A	1101	MIY	C18-C1	2.47	1.58	1.55
3	A	1101	MIY	C7-C16	-2.47	1.49	1.51
3	A	1101	MIY	C21-N2	2.15	1.39	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	MIY	C15-C16-C17	4.19	122.11	118.80
3	A	1101	MIY	C11-C12-C13	-3.82	116.67	120.50
3	A	1101	MIY	C1-C18-C17	3.68	114.19	109.88
3	A	1101	MIY	C19-N1-C4	3.47	122.01	114.10
3	A	1101	MIY	C11-C10-N7	-3.38	117.00	121.65
3	A	1101	MIY	C21-C2-C1	-3.29	117.07	120.97
3	A	1101	MIY	O6-C17-C18	3.11	117.87	113.37
3	A	1101	MIY	C9-C8-C7	-3.04	109.10	113.12
3	A	1101	MIY	O6-C17-C16	-2.71	118.25	123.52
3	A	1101	MIY	O7-C18-C17	-2.64	105.92	110.14
3	A	1101	MIY	C71-N7-CN7	2.54	124.35	116.18
3	A	1101	MIY	C7-C6-C5	2.47	114.59	110.38
3	A	1101	MIY	C20-N1-C4	2.39	119.55	114.10
3	A	1101	MIY	C6-C5-C4	-2.31	110.39	113.73
3	A	1101	MIY	C12-C13-C14	2.20	122.96	120.15
3	A	1101	MIY	O8-C21-N2	-2.09	118.21	122.89
3	A	1101	MIY	C6-C7-C16	2.02	114.66	110.28

There are no chirality outliers.

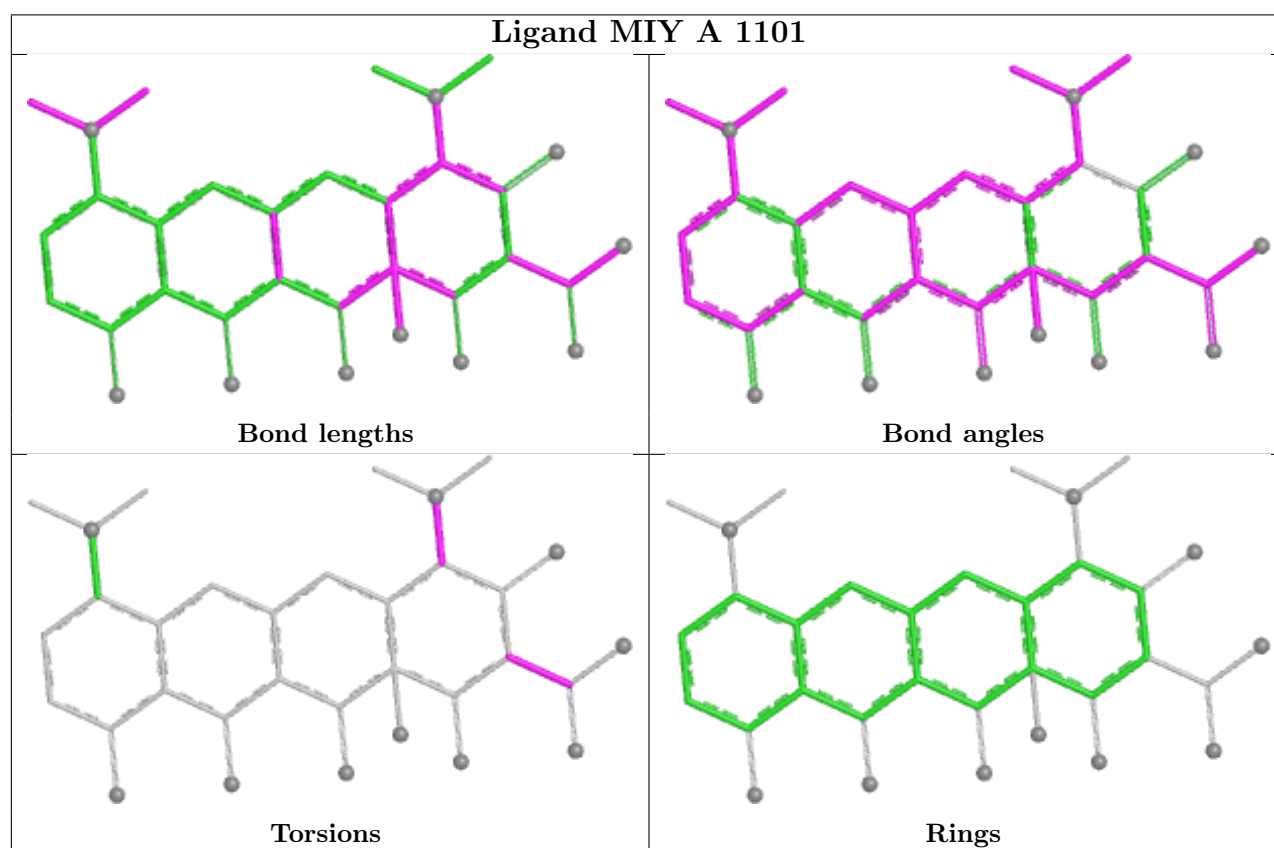
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	MIY	C1-C2-C21-O8
3	A	1101	MIY	C1-C2-C21-N2
3	A	1101	MIY	C5-C4-N1-C19
3	A	1101	MIY	C3-C2-C21-N2
3	A	1101	MIY	C3-C2-C21-O8

There are no ring outliers.

No monomer is involved in short contacts.

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

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	D	151/169 (89%)	1.86	62 (41%) 0 0	43, 68, 109, 122	0
2	A	1043/1057 (98%)	1.04	157 (15%) 5 5	33, 53, 77, 108	0
All	All	1194/1226 (97%)	1.15	219 (18%) 3 3	33, 54, 84, 122	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	170	SER	9.5
2	A	617	PHE	7.2
2	A	868	LEU	7.1
2	A	664	PHE	6.3
2	A	113	LEU	6.0
2	A	136	PHE	5.7
1	D	66	LEU	5.6
2	A	301	ASP	5.3
2	A	918	PHE	5.2
2	A	693	GLU	5.1
1	D	15	GLY	4.9
1	D	40	VAL	4.7
2	A	341	VAL	4.7
1	D	164	ILE	4.7
2	A	169	THR	4.6
2	A	877	TYR	4.5
1	D	76	TYR	4.5
1	D	63	VAL	4.4
1	D	18	LEU	4.3
2	A	837	THR	4.2
2	A	575	MET	4.2
2	A	1034	SER	4.2
1	D	60	LEU	4.2
1	D	65	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	42	ALA	4.2
2	A	257	GLY	4.1
2	A	508	GLY	4.1
2	A	635	ALA	4.1
1	D	30	VAL	4.0
2	A	344	LEU	4.0
2	A	615	PHE	4.0
2	A	869	SER	4.0
2	A	327	TYR	3.8
2	A	1033	PHE	3.8
2	A	1038	GLU	3.8
1	D	24	ALA	3.8
1	D	22	ALA	3.8
1	D	98	VAL	3.8
2	A	255	GLN	3.7
2	A	666	PHE	3.7
1	D	20	GLU	3.7
1	D	32	ILE	3.7
2	A	112	GLN	3.6
2	A	662	MET	3.6
2	A	1040	ILE	3.6
2	A	850	LYS	3.6
1	D	62	ILE	3.6
2	A	419	VAL	3.6
2	A	676	THR	3.6
1	D	16	LYS	3.6
1	D	23	ARG	3.6
2	A	172	VAL	3.5
2	A	316	PHE	3.5
2	A	171	GLY	3.5
2	A	312	LYS	3.5
2	A	556	PHE	3.5
2	A	173	GLY	3.5
2	A	295	THR	3.4
2	A	512	PHE	3.4
2	A	554	TYR	3.4
2	A	655	PHE	3.4
2	A	677	ALA	3.4
1	D	128	ILE	3.3
2	A	165	ALA	3.3
2	A	229	GLN	3.3
2	A	518	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	557	VAL	3.2
2	A	386	PHE	3.2
1	D	163	GLU	3.2
1	D	95	ILE	3.2
1	D	57	TRP	3.1
2	A	866	GLU	3.1
2	A	135	SER	3.1
1	D	75	ALA	3.1
1	D	29	GLU	3.1
2	A	174	ASP	3.1
2	A	846	GLN	3.1
2	A	842	GLU	3.1
2	A	345	VAL	3.0
1	D	33	LEU	3.0
2	A	362	PHE	3.0
1	D	137	ALA	3.0
1	D	154	ILE	3.0
2	A	166	ILE	3.0
2	A	509	LYS	2.9
2	A	97	GLY	2.9
1	D	43	ALA	2.9
2	A	658	ILE	2.9
2	A	784	ASP	2.9
1	D	126	LEU	2.9
2	A	353	LEU	2.9
2	A	881	LEU	2.9
2	A	304	ALA	2.8
2	A	501	ALA	2.8
2	A	1043	SER	2.8
2	A	506	GLY	2.8
1	D	100	LEU	2.8
2	A	253	VAL	2.8
2	A	496	MET	2.8
1	D	165	LEU	2.8
2	A	507	GLU	2.8
2	A	833	PRO	2.8
2	A	308	ALA	2.7
2	A	573	MET	2.7
2	A	537	SER	2.7
2	A	558	ARG	2.7
2	A	409	ALA	2.7
2	A	873	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	388	PHE	2.7
2	A	714	THR	2.7
1	D	102	ASN	2.7
2	A	1036	LYS	2.7
2	A	840	ALA	2.7
1	D	135	TYR	2.7
2	A	628	PHE	2.7
1	D	93	LEU	2.7
1	D	41	ASN	2.7
2	A	29	LYS	2.7
2	A	1012	VAL	2.7
1	D	26	ARG	2.6
2	A	697	GLN	2.6
1	D	67	LEU	2.6
2	A	876	LEU	2.6
1	D	21	ALA	2.6
1	D	38	ALA	2.6
2	A	612	TRP	2.6
1	D	91	GLY	2.6
2	A	71	GLY	2.6
2	A	494	ALA	2.6
2	A	425	LEU	2.6
2	A	337	ILE	2.6
2	A	1041	GLU	2.6
1	D	129	VAL	2.6
2	A	421	ALA	2.6
2	A	668	LEU	2.5
1	D	103	GLY	2.5
2	A	226	LYS	2.5
2	A	983	ILE	2.5
2	A	458	PHE	2.5
2	A	787	GLY	2.5
2	A	402	ILE	2.5
2	A	849	SER	2.5
2	A	340	VAL	2.5
1	D	51	LEU	2.5
2	A	991	ILE	2.5
2	A	640	GLU	2.5
2	A	862	MET	2.5
1	D	28	ASP	2.5
2	A	424	GLY	2.4
2	A	743	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	659	LYS	2.4
1	D	74	ASN	2.4
2	A	461	GLY	2.4
2	A	500	ILE	2.4
2	A	626	ILE	2.4
2	A	660	ASP	2.4
2	A	831	ALA	2.4
2	A	168	ARG	2.4
1	D	19	LEU	2.4
1	D	124	GLY	2.4
2	A	870	GLY	2.4
2	A	1039	ASP	2.3
2	A	359	LEU	2.3
2	A	498	LYS	2.3
1	D	84	LEU	2.3
2	A	574	THR	2.3
2	A	1042	HIS	2.3
2	A	618	ALA	2.3
2	A	349	ILE	2.3
1	D	157	GLY	2.3
2	A	511	GLY	2.3
2	A	175	VAL	2.3
2	A	636	ASP	2.3
2	A	673	GLU	2.3
2	A	350	LEU	2.3
2	A	459	PHE	2.3
2	A	678	THR	2.3
2	A	713	LEU	2.3
2	A	515	TRP	2.2
2	A	867	ARG	2.2
1	D	25	GLY	2.2
2	A	499	PRO	2.2
2	A	839	GLU	2.2
2	A	656	SER	2.2
1	D	160	ASP	2.2
1	D	34	MET	2.2
1	D	161	LEU	2.2
2	A	176	GLN	2.2
2	A	672	VAL	2.2
2	A	1003	VAL	2.2
1	D	39	ASP	2.2
2	A	387	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	178	PHE	2.2
1	D	59	HIS	2.2
2	A	519	MET	2.2
1	D	71	ALA	2.2
2	A	468	ARG	2.2
2	A	922	THR	2.1
2	A	28	LEU	2.1
1	D	104	ALA	2.1
2	A	114	ALA	2.1
2	A	534	ILE	2.1
1	D	99	LEU	2.1
2	A	843	LEU	2.1
2	A	294	ALA	2.1
2	A	303	ALA	2.1
2	A	258	SER	2.1
2	A	917	THR	2.1
1	D	47	GLY	2.1
2	A	829	GLY	2.1
2	A	871	ASN	2.0
2	A	965	LEU	2.0
2	A	407	ASP	2.0
2	A	167	SER	2.0
2	A	1	MET	2.0
1	D	90	PHE	2.0
2	A	514	GLY	2.0
1	D	56	TYR	2.0
2	A	864	TYR	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 oligosaccharides in this entry.

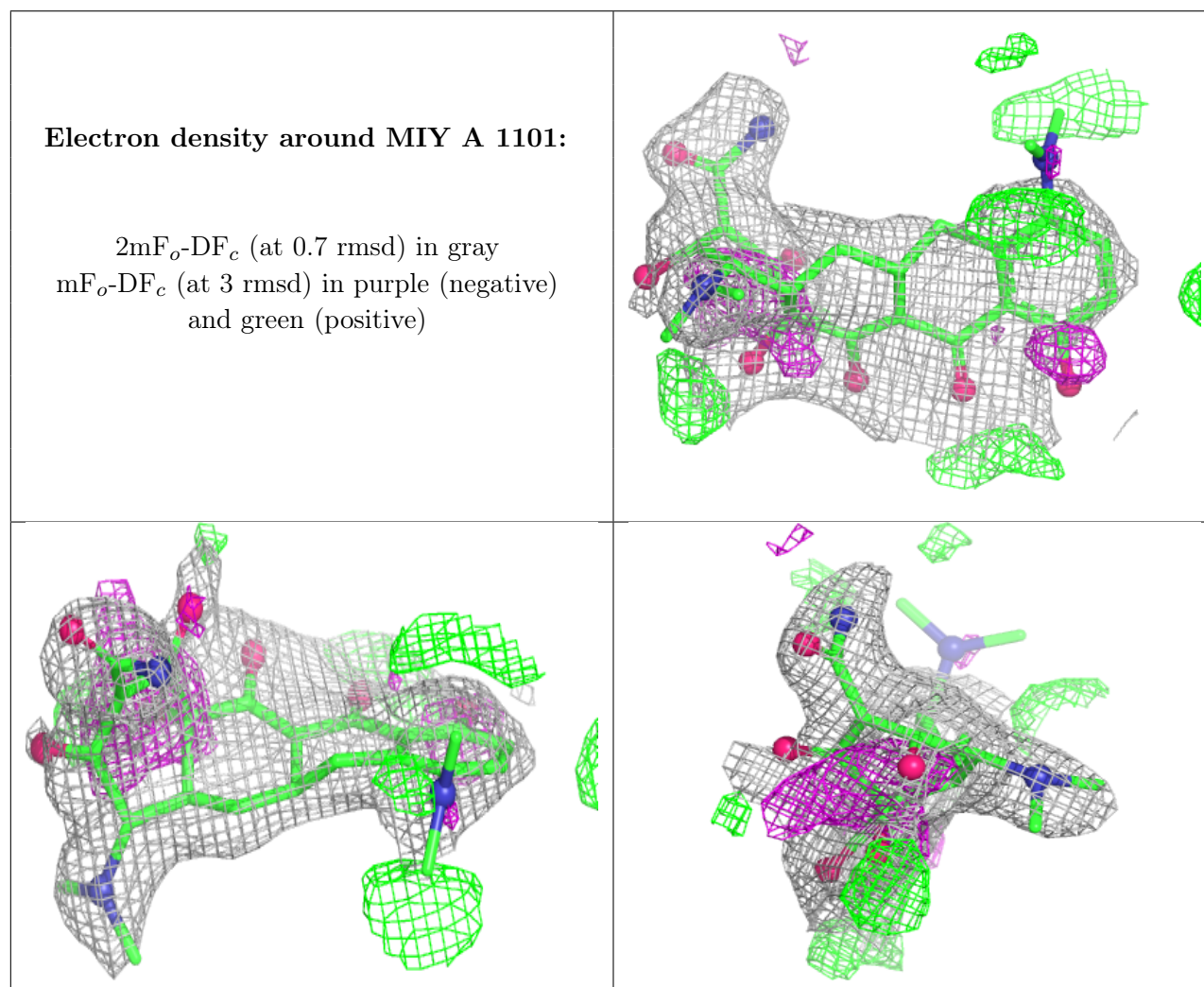
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	MIY	A	1101	33/33	0.63	0.26	69,83,91,100	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.