



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:11 am BST

PDB ID : 6IIA
Title : MexB in complex with LMNG
Authors : Nakashima, R.; Sakurai, K.; Nakao, K.
Deposited on : 2018-10-04
Resolution : 2.91 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

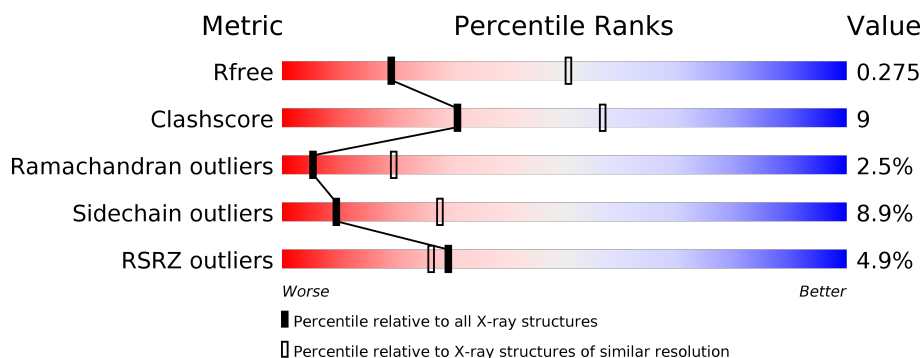
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 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	1052	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	1052	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
1	C	1052	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>• •</div> </div> </div>
1	D	1052	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	E	1052	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>• •</div> </div> </div>
1	F	1052	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46876 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 resistance protein MexB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0	0
			7718	4972	1279	1427	40			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	C	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	D	1020	Total	C	N	O	S	0	0	0
			7744	4990	1283	1431	40			
1	E	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	F	1033	Total	C	N	O	S	0	0	0
			7840	5046	1302	1452	40			

There are 36 discrepancies between the modelled and reference sequences:

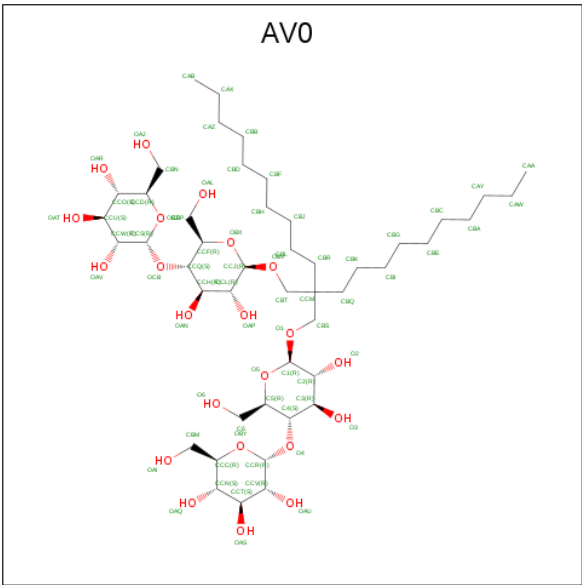
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P52002
A	1048	HIS	-	expression tag	UNP P52002
A	1049	HIS	-	expression tag	UNP P52002
A	1050	HIS	-	expression tag	UNP P52002
A	1051	HIS	-	expression tag	UNP P52002
A	1052	HIS	-	expression tag	UNP P52002
B	1047	HIS	-	expression tag	UNP P52002
B	1048	HIS	-	expression tag	UNP P52002
B	1049	HIS	-	expression tag	UNP P52002
B	1050	HIS	-	expression tag	UNP P52002
B	1051	HIS	-	expression tag	UNP P52002
B	1052	HIS	-	expression tag	UNP P52002
C	1047	HIS	-	expression tag	UNP P52002
C	1048	HIS	-	expression tag	UNP P52002
C	1049	HIS	-	expression tag	UNP P52002
C	1050	HIS	-	expression tag	UNP P52002
C	1051	HIS	-	expression tag	UNP P52002

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1052	HIS	-	expression tag	UNP P52002
D	1047	HIS	-	expression tag	UNP P52002
D	1048	HIS	-	expression tag	UNP P52002
D	1049	HIS	-	expression tag	UNP P52002
D	1050	HIS	-	expression tag	UNP P52002
D	1051	HIS	-	expression tag	UNP P52002
D	1052	HIS	-	expression tag	UNP P52002
E	1047	HIS	-	expression tag	UNP P52002
E	1048	HIS	-	expression tag	UNP P52002
E	1049	HIS	-	expression tag	UNP P52002
E	1050	HIS	-	expression tag	UNP P52002
E	1051	HIS	-	expression tag	UNP P52002
E	1052	HIS	-	expression tag	UNP P52002
F	1047	HIS	-	expression tag	UNP P52002
F	1048	HIS	-	expression tag	UNP P52002
F	1049	HIS	-	expression tag	UNP P52002
F	1050	HIS	-	expression tag	UNP P52002
F	1051	HIS	-	expression tag	UNP P52002
F	1052	HIS	-	expression tag	UNP P52002

- Molecule 2 is 2-decyl-2-[[[(4-O-alpha-D-glucopyranosyl-beta-D-glucopyranosyl)oxy]methyl]dodecyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: AV0) (formula: C₄₇H₈₈O₂₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			69	47	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			69	47	22		

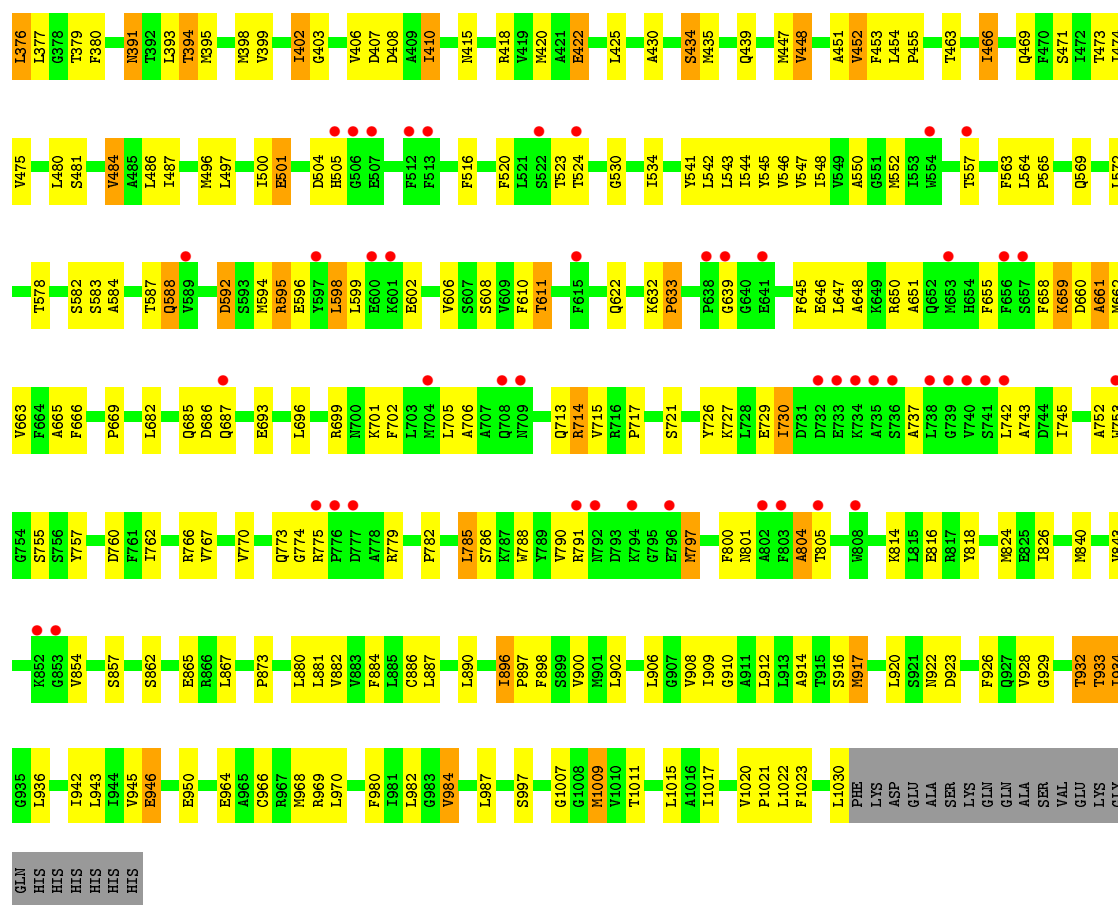
Chain B:

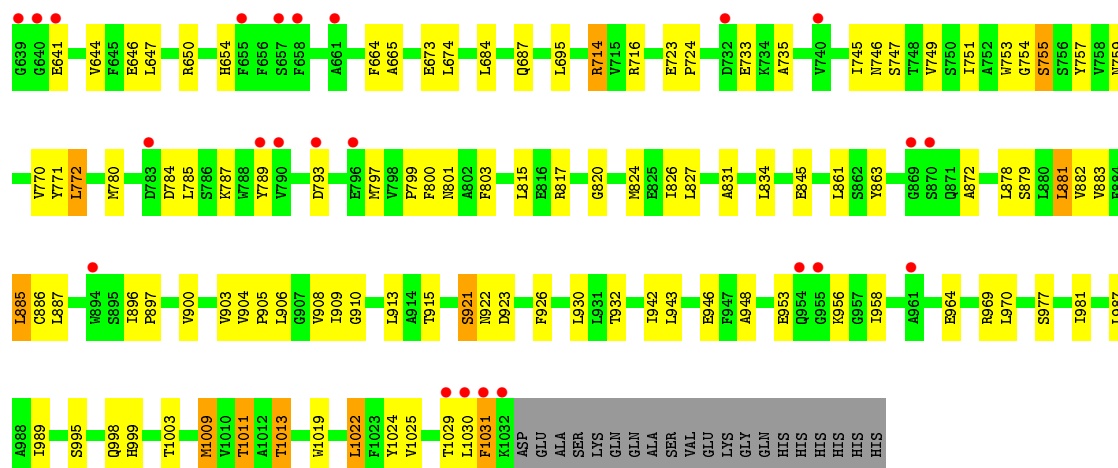
Amino Acid	Percentage
GLN	3%
ALA	3%
VAL	3%
LEU	3%
ILE	3%
LYS	3%
GLN	3%
HIS	3%
SER	3%
ASP	3%
GLU	3%
ASN	3%
PRO	3%
THR	3%
TYR	3%
PHE	3%
MET	3%
CYS	3%
TRP	3%

Chain C:

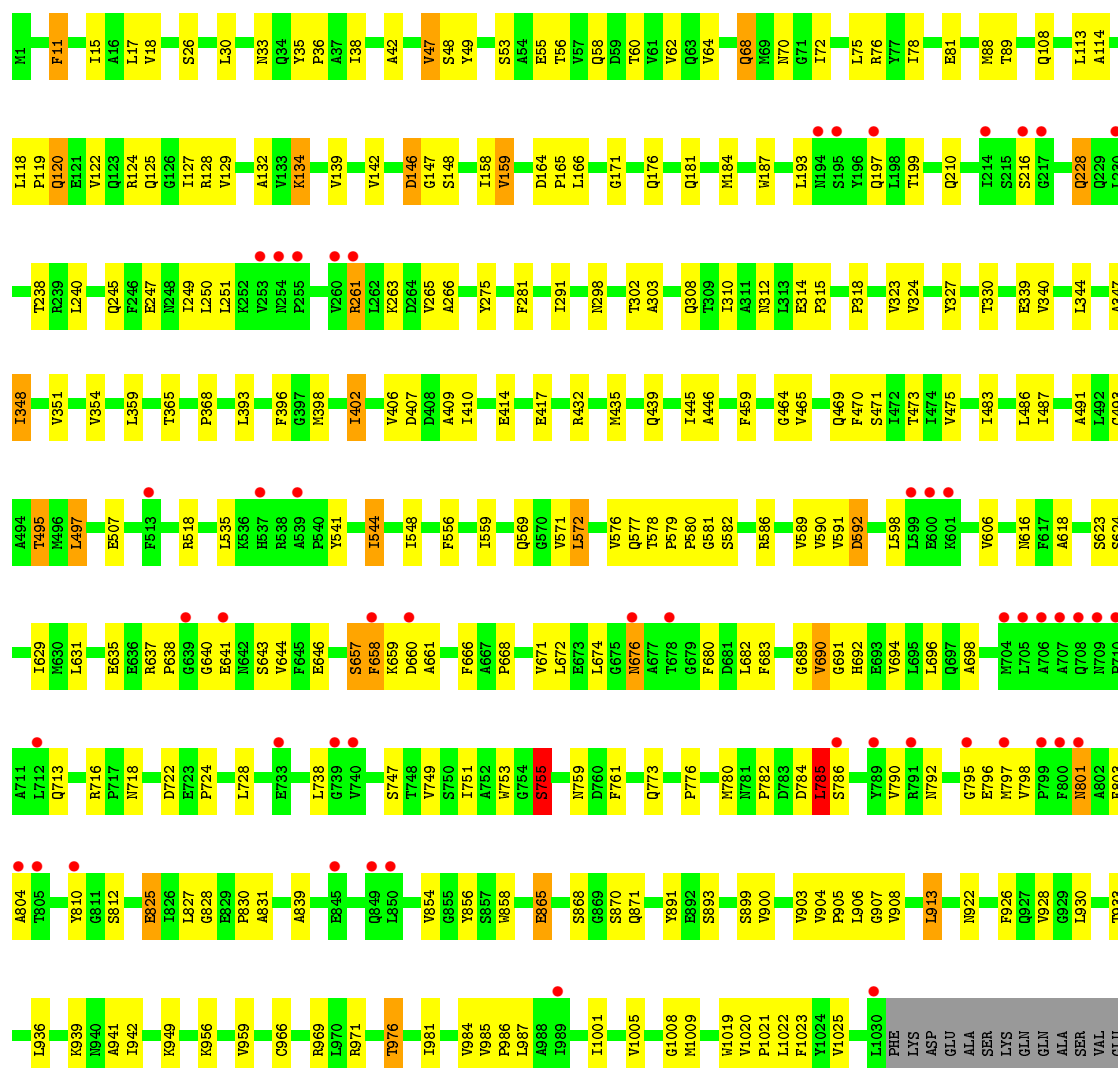
6% 67% 26%

M1 F4 F5 F11 I15 A16 L28 S29 L30 P36 A37 I38 Q46 V47 A52 T56 Q67 M88 I102 Q112 T115 P116 L117 L118 Q125 K126 I127 F136 V142 V143 S144 E152 P165 L166 T169 V172 F175 Q181 M184 W187 L188 D189 K192 L193 N194 S195 Y196 Q197 L198 T199 P200 V203 A206 Q210 Q213 S216 L219 Q220 A224 Q228 Q229 T234 T235 K237 T238 R239 L240 Q241 A243 F246 E247 N248 K252 V253 N254 P255 D256 Q257 S258 Q259 V260 P261 L262 V268 S276 Q280 F281 A286 L289 A290 T291 M298 I306 R307 E314 P315 F316 M317 P318 Q319 G320 M321 V324 Y325 P326 T330 P331 V340 T343 L348 V351 P354 M355 Y356 L357 Q360 R361 F362 L367 P368 T369 I370 V374 P375





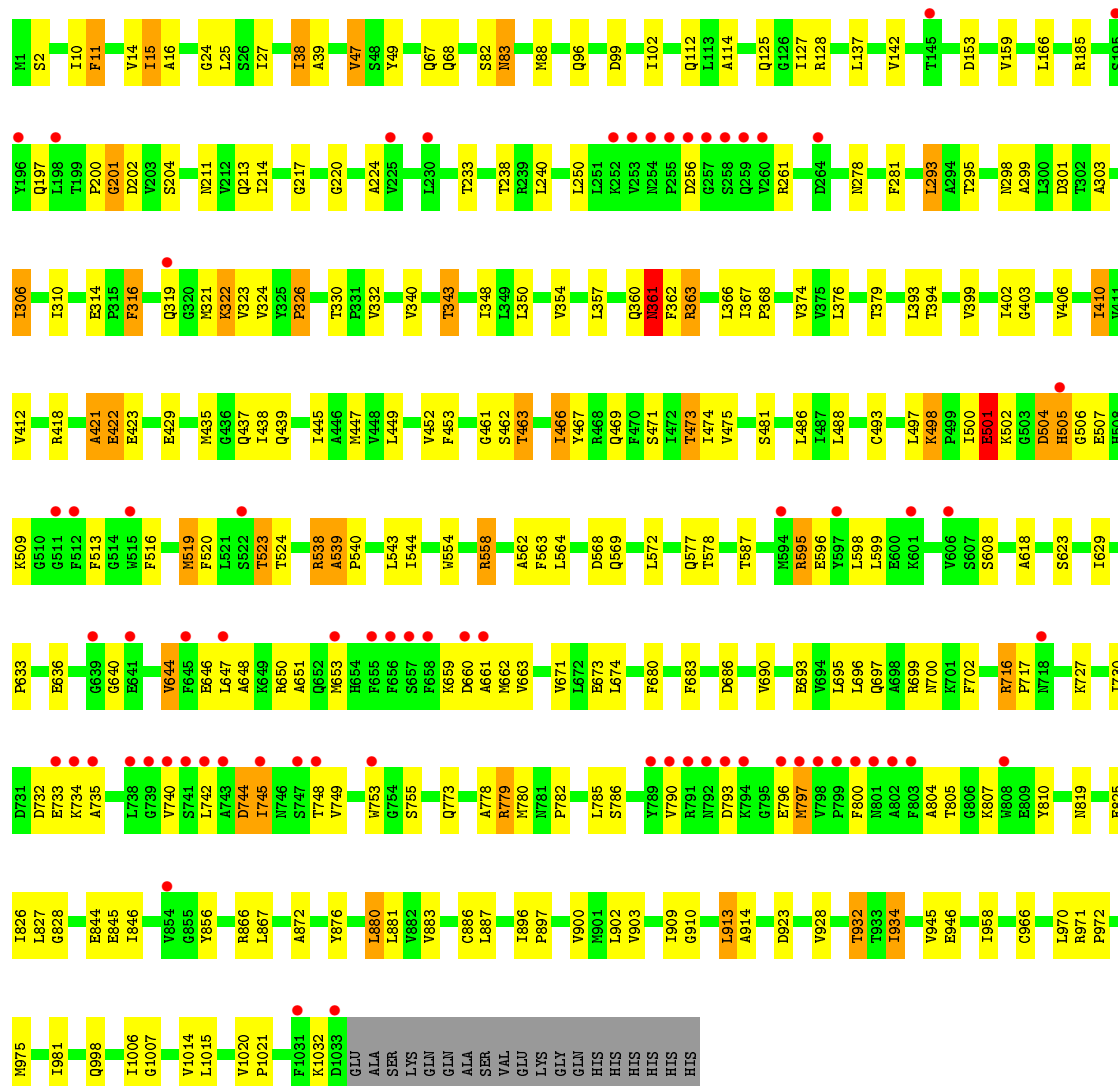
• Molecule 1: Multidrug resistance protein MexB



LYS
GLY
GLN
HIS
HIS
HIS
HIS
HIS
HIS

● Molecule 1: Multidrug resistance protein MexB

Chain F:  7% 73% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.95Å 134.34Å 149.69Å 87.53° 70.20° 89.02°	Depositor
Resolution (Å)	140.73 – 2.91 50.05 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.7 (140.73-2.91) 92.8 (50.05-2.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.234 , 0.278 0.234 , 0.275	Depositor DCC
R_{free} test set	9196 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	46876	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: AV0

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	0.66	1/7873 (0.0%)	0.84	3/10701 (0.0%)
1	B	0.68	0/7971	0.86	0/10833
1	C	0.61	0/7971	0.81	0/10833
1	D	0.62	0/7901	0.80	0/10739
1	E	0.61	0/7971	0.79	1/10833 (0.0%)
1	F	0.61	0/8000	0.80	1/10871 (0.0%)
All	All	0.63	1/47687 (0.0%)	0.82	5/64810 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	808	TRP	CB-CG	-5.43	1.40	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	791	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	E	971	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	F	293	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	674	LEU	CA-CB-CG	5.01	126.83	115.30

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	A	7718	0	7858	167	0
1	B	7812	0	7944	131	0
1	C	7812	0	7944	183	0
1	D	7744	0	7886	129	0
1	E	7812	0	7944	147	0
1	F	7840	0	7970	136	0
2	B	69	0	0	1	0
2	E	69	0	0	0	0
All	All	46876	0	47546	858	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 9.

The worst 5 of 858 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:219:LEU:HG	1:C:234:ILE:HD11	1.52	0.92
1:E:782:PRO:O	1:E:785:LEU:HG	1.75	0.86
1:E:142:VAL:HG21	1:E:158:ILE:HD11	1.57	0.84
1:B:56:THR:O	1:B:60:THR:HB	1.81	0.81
1:F:524:THR:HG22	1:F:970:LEU:HD12	1.61	0.81

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	1011/1052 (96%)	909 (90%)	82 (8%)	20 (2%)	7	26
1	B	1028/1052 (98%)	918 (89%)	91 (9%)	19 (2%)	8	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1028/1052 (98%)	885 (86%)	114 (11%)	29 (3%)	5	17
1	D	1016/1052 (97%)	889 (88%)	105 (10%)	22 (2%)	6	23
1	E	1028/1052 (98%)	907 (88%)	100 (10%)	21 (2%)	7	26
1	F	1031/1052 (98%)	876 (85%)	114 (11%)	41 (4%)	3	10
All	All	6142/6312 (97%)	5384 (88%)	606 (10%)	152 (2%)	5	20

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	PRO
1	A	714	ARG
1	A	715	VAL
1	A	740	VAL
1	A	872	ALA

5.3.2 Protein sidechains ⓘ

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	832/860 (97%)	757 (91%)	75 (9%)	9	27
1	B	841/860 (98%)	749 (89%)	92 (11%)	6	18
1	C	841/860 (98%)	766 (91%)	75 (9%)	9	28
1	D	835/860 (97%)	768 (92%)	67 (8%)	12	32
1	E	841/860 (98%)	775 (92%)	66 (8%)	12	33
1	F	844/860 (98%)	772 (92%)	72 (8%)	10	30
All	All	5034/5160 (98%)	4587 (91%)	447 (9%)	9	28

5 of 447 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	481	SER
1	D	121	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	488	LEU
1	C	592	ASP
1	C	898	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	849	GLN
1	E	58	GLN
1	F	176	GLN
1	D	33	ASN
1	D	213	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	AV0	E	1101	-	72,72,72	0.48	0	96,98,98	1.19	11 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AV0	B	1101	-	72,72,72	0.51	0	96,98,98	1.13	9 (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
2	AV0	E	1101	-	-	22/50/130/130	0/4/4/4
2	AV0	B	1101	-	-	15/50/130/130	0/4/4/4

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1101	AV0	CBR-CCM-CBQ	3.43	116.39	109.97
2	B	1101	AV0	CCR-O4-C4	-2.86	110.88	117.96
2	E	1101	AV0	CCJ-OBX-CCF	-2.65	108.49	113.69
2	B	1101	AV0	CCU-CCO-CCD	-2.63	105.55	110.24
2	E	1101	AV0	CCV-CCT-CCN	-2.61	106.26	110.82

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1101	AV0	CBL-CBR-CCM-CBQ
2	E	1101	AV0	CBL-CBR-CCM-CBS
2	E	1101	AV0	CBL-CBR-CCM-CBT
2	B	1101	AV0	OBV-CBT-CCM-CBQ
2	B	1101	AV0	OBV-CBT-CCM-CBR

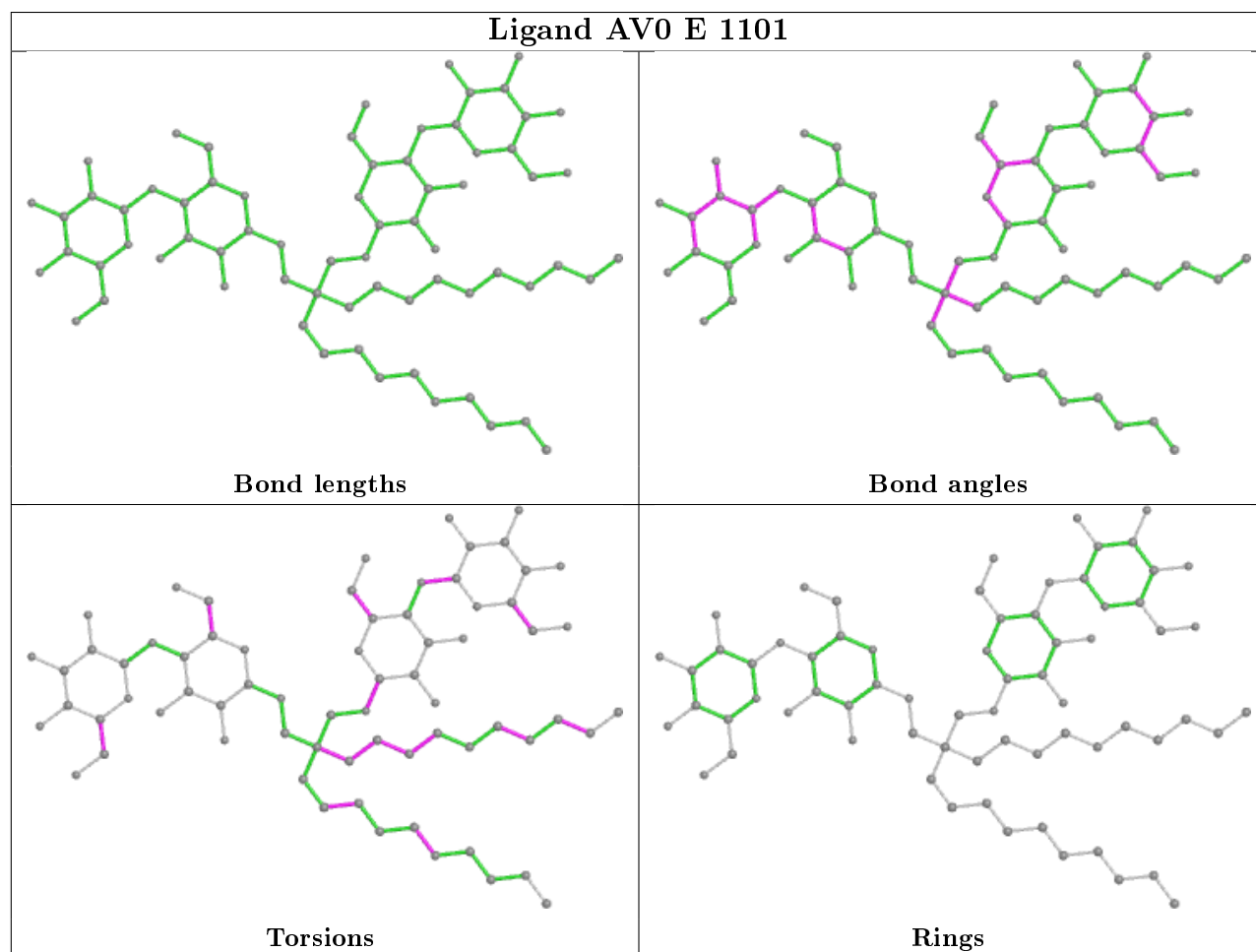
There are no ring outliers.

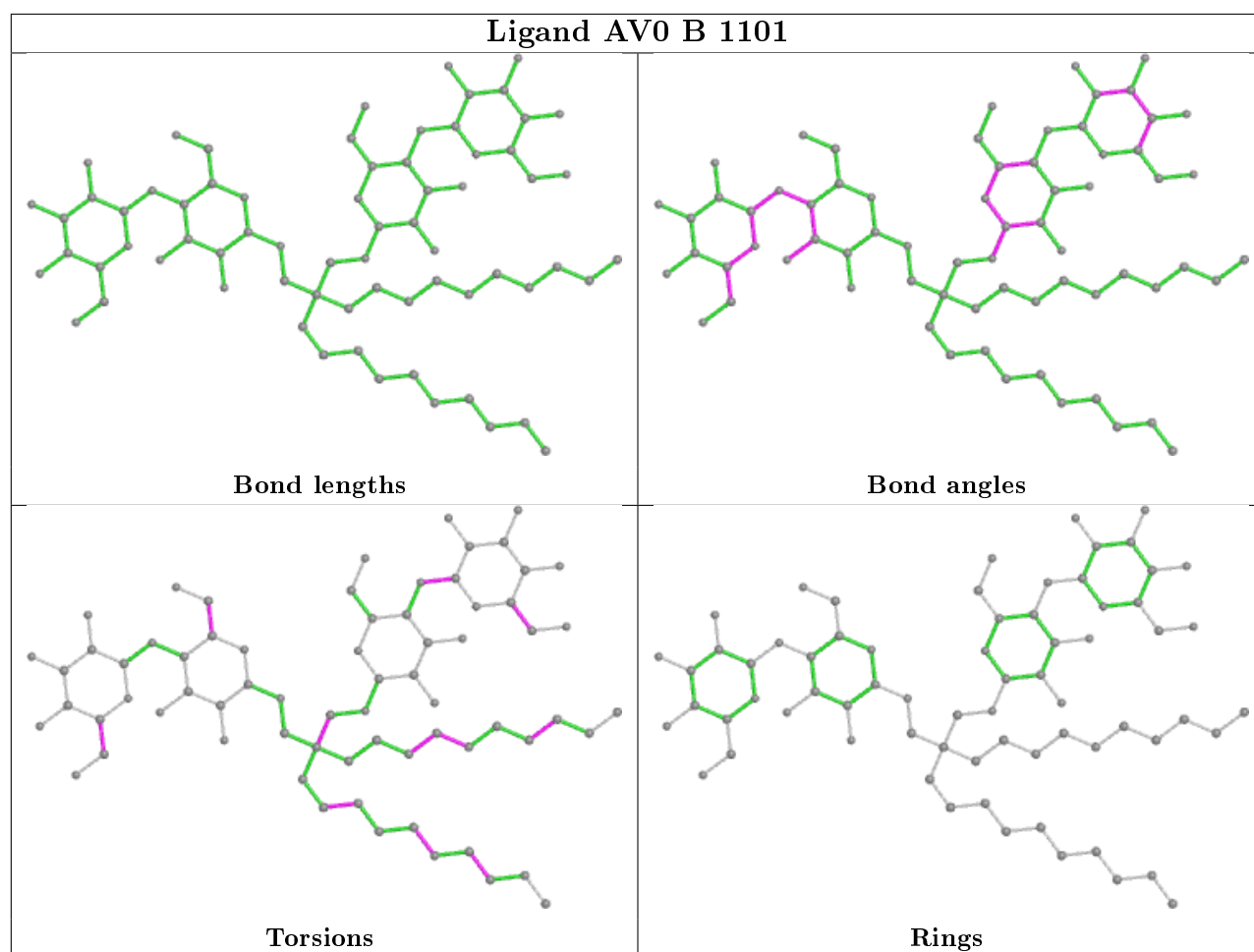
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	AV0	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 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 [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	1017/1052 (96%)	0.00	36 (3%) 44 40	13, 47, 94, 148	0
1	B	1030/1052 (97%)	-0.04	33 (3%) 47 44	12, 40, 79, 117	0
1	C	1030/1052 (97%)	0.29	63 (6%) 21 18	15, 55, 110, 162	0
1	D	1020/1052 (96%)	0.10	52 (5%) 28 24	17, 53, 97, 144	0
1	E	1030/1052 (97%)	0.11	51 (4%) 28 25	18, 52, 99, 137	0
1	F	1033/1052 (98%)	0.17	69 (6%) 17 14	21, 52, 111, 166	0
All	All	6160/6312 (97%)	0.11	304 (4%) 29 26	12, 50, 99, 166	0

The worst 5 of 304 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	742	LEU	12.3
1	F	742	LEU	9.2
1	A	955	GLY	8.9
1	C	657	SER	8.1
1	C	259	GLN	7.4

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](#)

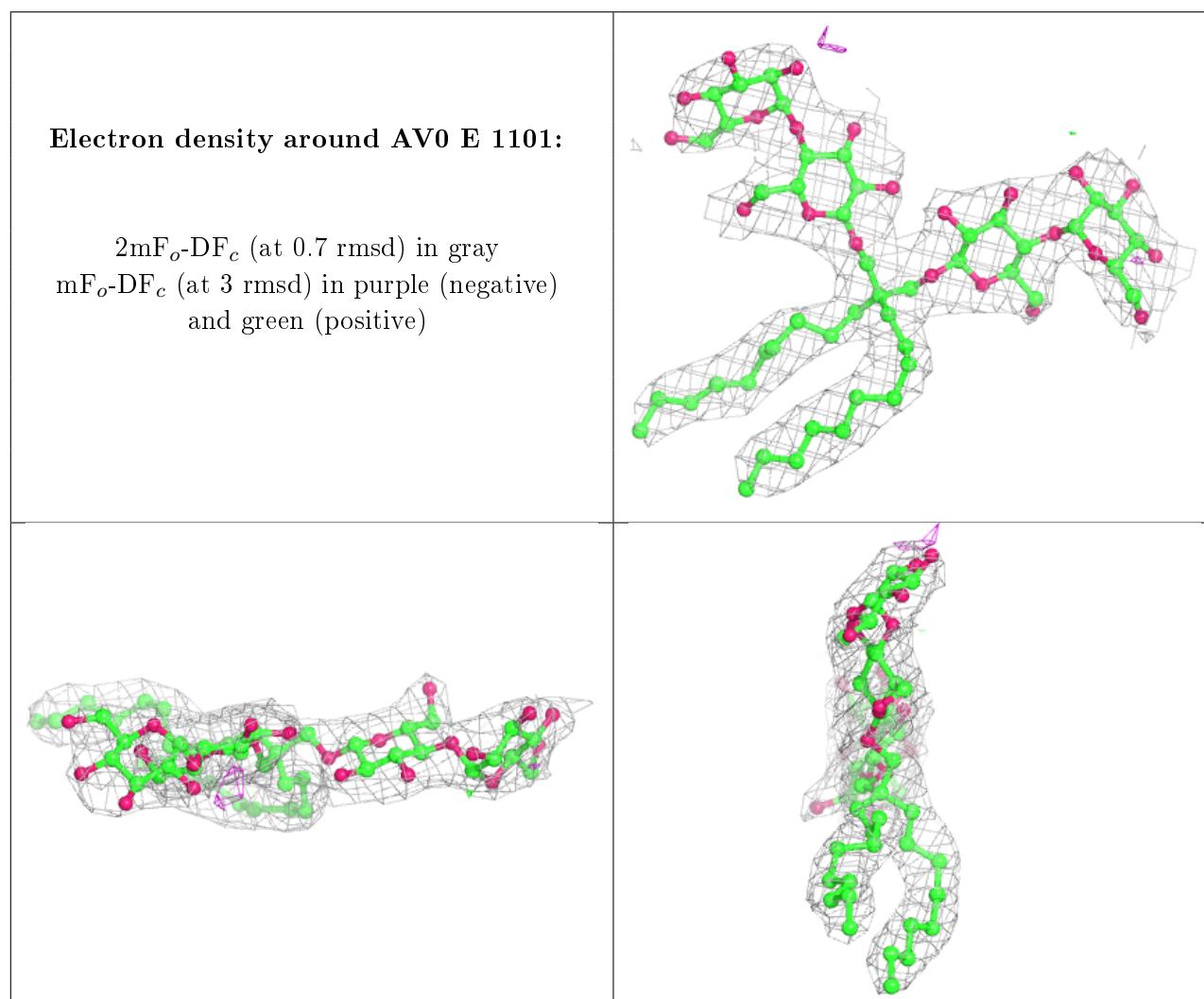
There are no carbohydrates in this entry.

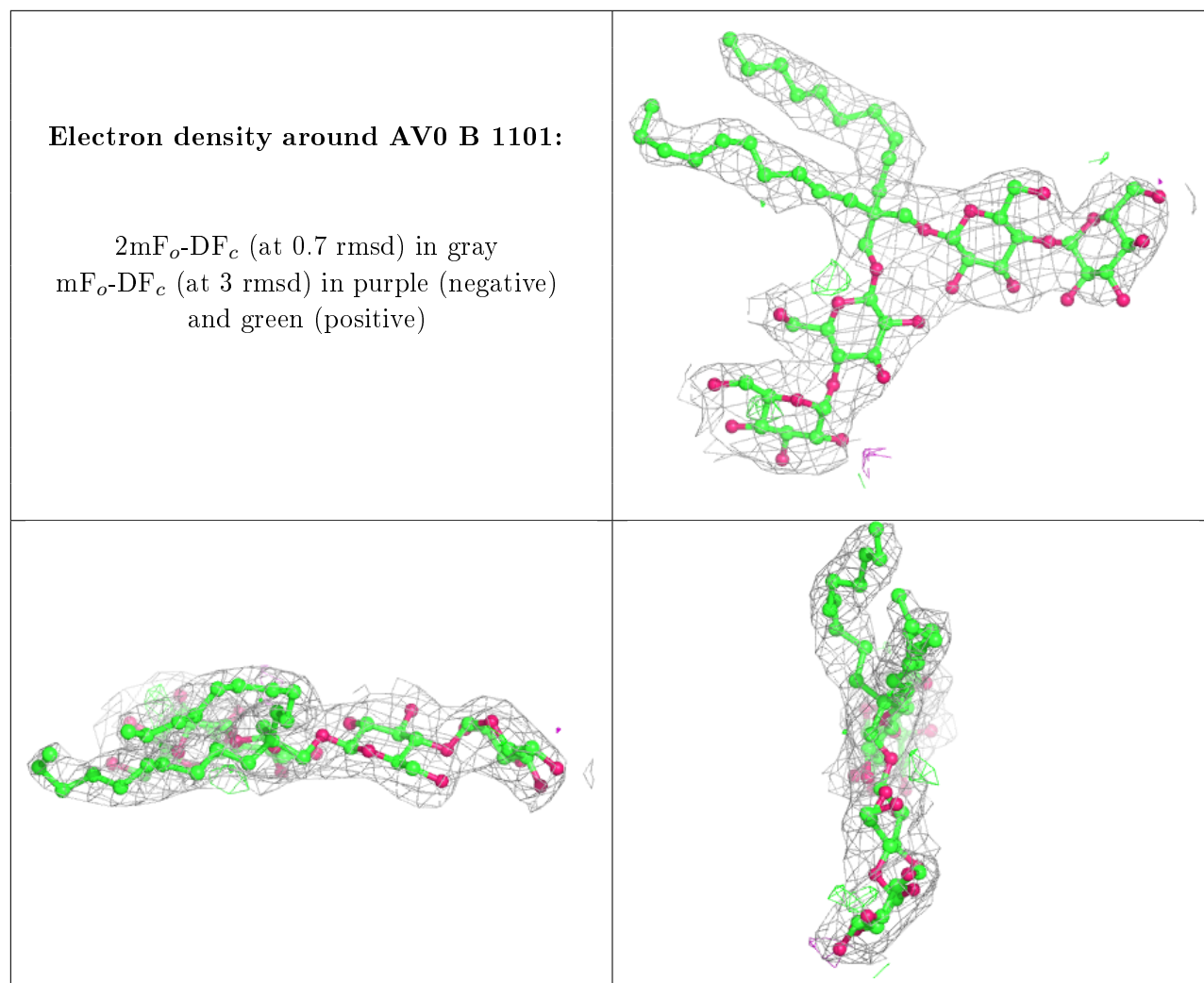
6.4 Ligands [i](#)

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	AV0	E	1101	69/69	0.93	0.18	30,49,65,69	0
2	AV0	B	1101	69/69	0.93	0.19	29,46,63,70	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 [i](#)

There are no such residues in this entry.