



# Full wwPDB X-ray Structure Validation Report i

Nov 16, 2023 – 05:26 AM JST

PDB ID : 6KWA  
Title : AtDAO1(dioxygenase for auxin oxidation 1 from *Arabidopsis thaliana*)  
Authors : Rhee, S.; Jin, S.; Lee, H.  
Deposited on : 2019-09-06  
Resolution : 2.09 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

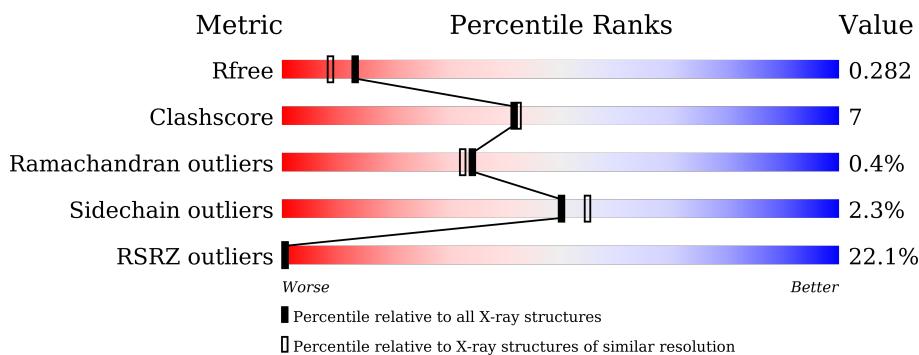
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

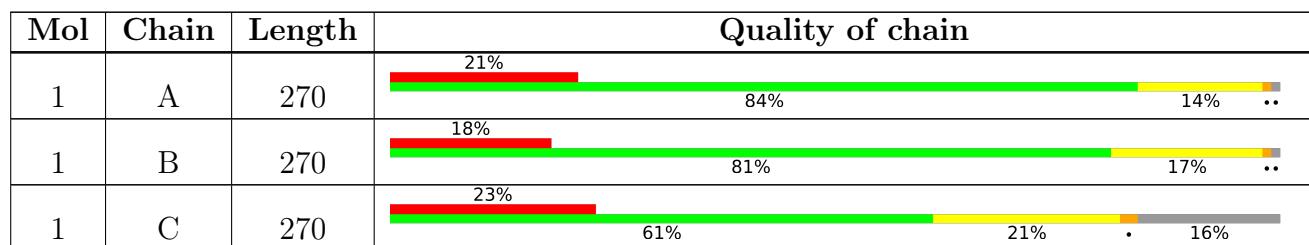
The reported resolution of this entry is 2.09 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.



## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6083 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 2-oxoglutarate (2OG) and Fe(II)-dependent oxygenase superfamily protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C 2114	N 1340	O 357	S 404	13	0	0
1	B	266	Total	C 2106	N 1334	O 356	S 403	13	0	0
1	C	226	Total	C 1805	N 1146	O 302	S 345	12	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP Q9XI75
B	8	MET	-	initiating methionine	UNP Q9XI75
C	8	MET	-	initiating methionine	UNP Q9XI75

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	28	Total O 28 28	0	0

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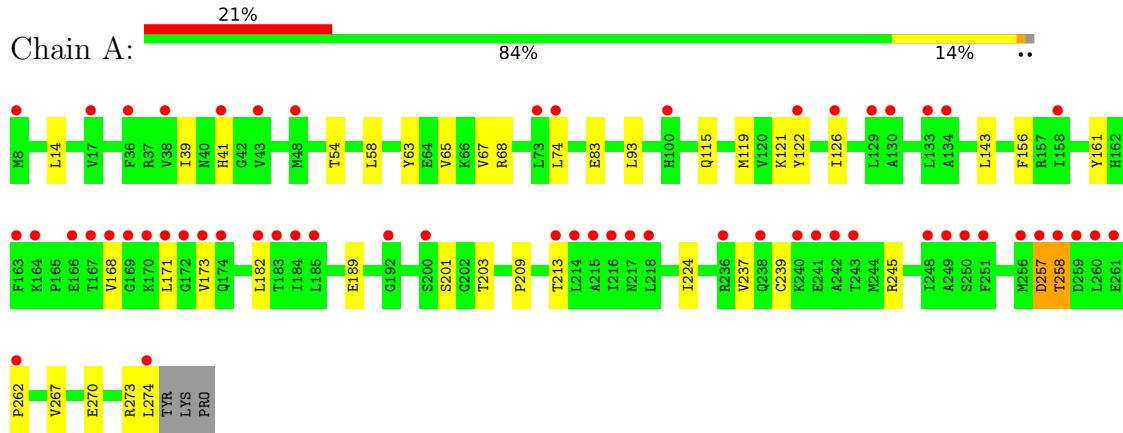
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	4	Total    O 4      4	0	0

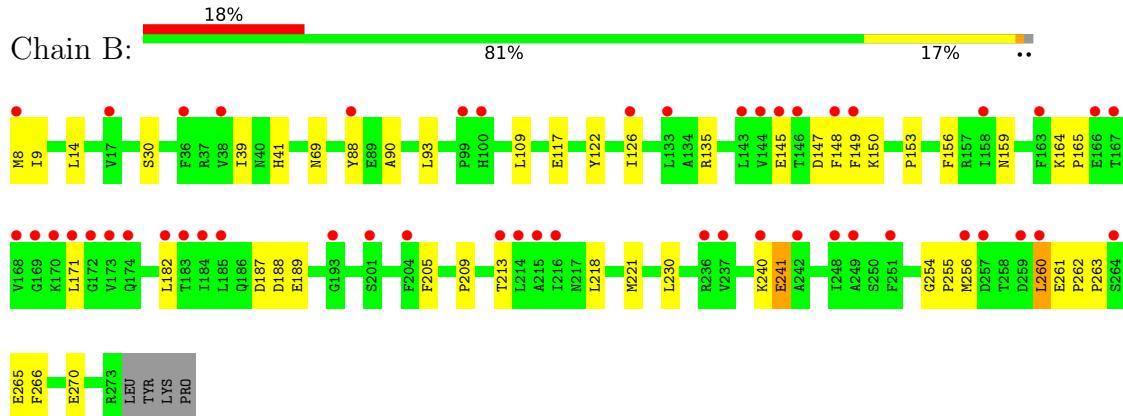
### 3 Residue-property plots [\(i\)](#)

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.

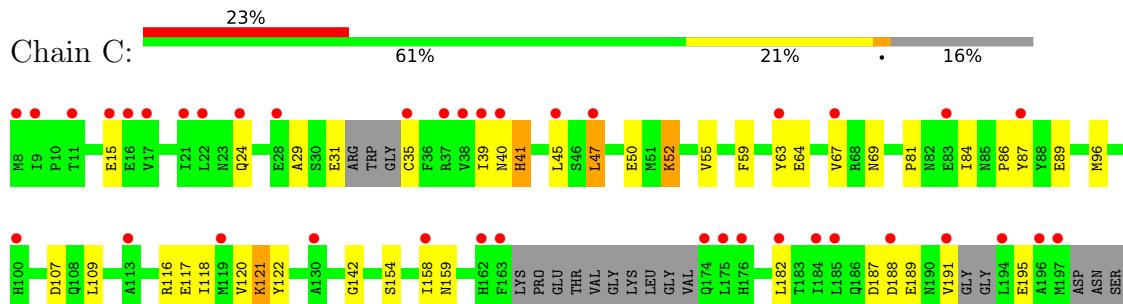
- Molecule 1: 2-oxoglutarate (2OG) and Fe(II)-dependent oxygenase superfamily protein

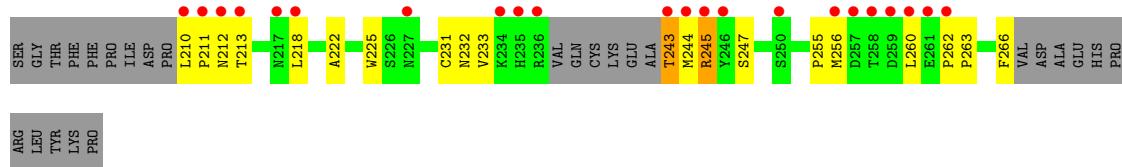


- Molecule 1: 2-oxoglutarate (2OG) and Fe(II)-dependent oxygenase superfamily protein



- Molecule 1: 2-oxoglutarate (2OG) and Fe(II)-dependent oxygenase superfamily protein





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.63 Å   75.55 Å   165.32 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	33.88 – 2.09 33.88 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.2 (33.88-2.09) 99.2 (33.88-2.09)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.32 (at 2.10 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
$R$ , $R_{free}$	0.242 , 0.282 0.245 , 0.282	Depositor DCC
$R_{free}$ test set	2001 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.0	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.50	0/2160	0.68	1/2927 (0.0%)
1	B	0.50	0/2152	0.65	1/2916 (0.0%)
1	C	0.42	1/1837 (0.1%)	0.68	3/2480 (0.1%)
All	All	0.48	1/6149 (0.0%)	0.67	5/8323 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	231	CYS	CB-SG	5.59	1.91	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	LEU	CA-CB-CG	6.46	130.17	115.30
1	C	47	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	182	LEU	CA-CB-CG	5.54	128.04	115.30
1	C	182	LEU	CA-CB-CG	5.27	127.42	115.30
1	C	231	CYS	CA-CB-SG	5.24	123.43	114.00

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	2114	0	2077	21	0
1	B	2106	0	2066	31	0
1	C	1805	0	1774	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	24	0	0	0	0
3	B	28	0	0	0	0
3	C	4	0	0	0	0
All	All	6083	0	5917	84	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 7.

All (84) 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:270:GLU:OE2	1:B:88:TYR:OH	2.04	0.74
1:B:39:ILE:HG22	1:B:213:THR:HG22	1.72	0.70
1:C:210:LEU:HD12	1:C:211:PRO:HD2	1.75	0.69
1:C:187:ASP:OD1	1:C:188:ASP:N	2.25	0.66
1:C:69:ASN:HB2	1:C:109:LEU:HD11	1.78	0.65
1:A:201:SER:OG	1:A:203:THR:HG22	1.97	0.65
1:B:8:MET:SD	1:B:8:MET:N	2.71	0.64
1:C:81:PRO:HD3	1:C:89:GLU:HB3	1.77	0.63
1:A:267:VAL:HG21	1:A:273:ARG:HD3	1.82	0.61
1:C:45:LEU:HG	1:C:212:ASN:HD21	1.66	0.60
1:B:153:PRO:HD3	1:B:256:MET:HG2	1.85	0.58
1:B:221:MET:SD	1:B:260:LEU:HD11	2.44	0.58
1:B:69:ASN:HB2	1:B:109:LEU:HD11	1.87	0.57
1:A:189:GLU:OE1	1:A:189:GLU:N	2.34	0.56
1:A:39:ILE:HG22	1:A:213:THR:HG22	1.88	0.56
1:B:88:TYR:HE2	1:B:159:ASN:HB3	1.71	0.55
1:B:263:PRO:HG2	1:B:266:PHE:CD2	2.41	0.55
1:C:255:PRO:HG3	1:C:260:LEU:HB2	1.88	0.54
1:A:63:TYR:O	1:A:67:VAL:HG23	2.07	0.54
1:C:189:GLU:OE1	1:C:189:GLU:N	2.33	0.53
1:C:50:GLU:HB3	1:C:118:ILE:HD13	1.88	0.53
1:A:54:THR:HG23	1:A:115:GLN:HG2	1.90	0.53
1:B:164:LYS:HB3	1:B:165:PRO:HD2	1.92	0.52
1:B:189:GLU:OE1	1:B:189:GLU:N	2.37	0.52
1:C:52:LYS:NZ	1:C:188:ASP:OD1	2.38	0.51
1:C:232:ASN:OD1	1:C:232:ASN:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ARG:HG3	1:B:149:PHE:CZ	2.46	0.50
1:B:189:GLU:HA	1:B:209:PRO:HB2	1.94	0.50
1:B:135:ARG:HG3	1:B:149:PHE:CE2	2.48	0.49
1:B:93:LEU:HG	1:B:156:PHE:HB3	1.93	0.49
1:C:225:TRP:O	1:C:262:PRO:HB3	2.13	0.48
1:A:65:VAL:O	1:A:68:ARG:HB2	2.13	0.48
1:C:86:PRO:HG2	1:C:87:TYR:CE2	2.48	0.48
1:A:189:GLU:HA	1:A:209:PRO:HB2	1.96	0.48
1:C:243:THR:HG22	1:C:244:MET:H	1.77	0.48
1:A:224:ILE:O	1:A:262:PRO:HG3	2.12	0.48
1:C:47:LEU:HD11	1:C:122:TYR:HA	1.95	0.48
1:B:147:ASP:HB3	1:B:150:LYS:HD3	1.96	0.48
1:B:14:LEU:HD12	1:B:41:HIS:HA	1.95	0.47
1:C:255:PRO:CG	1:C:260:LEU:HB2	2.44	0.47
1:C:263:PRO:HG2	1:C:266:PHE:CD2	2.50	0.47
1:B:263:PRO:HG2	1:B:266:PHE:HD2	1.80	0.46
1:A:93:LEU:HG	1:A:156:PHE:HB3	1.97	0.46
1:B:30:SER:HB3	1:B:218:LEU:HD11	1.98	0.46
1:B:122:TYR:CE2	1:B:126:ILE:HG13	2.50	0.46
1:A:14:LEU:HD12	1:A:41:HIS:HA	1.96	0.46
1:C:35:CYS:HB3	1:C:233:VAL:HG11	1.97	0.46
1:A:83:GLU:HB2	1:C:142:GLY:HA3	1.99	0.45
1:C:63:TYR:O	1:C:67:VAL:HG13	2.16	0.45
1:C:45:LEU:HA	1:C:45:LEU:HD13	1.69	0.45
1:A:74:LEU:HD12	1:A:74:LEU:HA	1.76	0.45
1:A:257:ASP:HB2	1:A:258:THR:H	1.58	0.44
1:C:29:ALA:C	1:C:31:GLU:H	2.21	0.44
1:C:117:GLU:HA	1:C:120:VAL:HG22	2.00	0.44
1:C:55:VAL:HG13	1:C:158:ILE:HD12	1.99	0.44
1:C:96:MET:HG2	1:C:154:SER:HB2	2.00	0.44
1:B:187:ASP:OD1	1:B:188:ASP:N	2.47	0.43
1:B:255:PRO:HG3	1:B:260:LEU:HB3	2.00	0.43
1:C:15:GLU:HG3	1:C:40:ASN:HB3	1.99	0.43
1:A:168:VAL:HA	1:A:239:CYS:SG	2.59	0.43
1:C:191:VAL:CG1	1:C:245:ARG:HE	2.32	0.43
1:A:58:LEU:HD11	1:A:119:MET:HE1	2.01	0.43
1:A:122:TYR:CE2	1:A:126:ILE:HG13	2.53	0.43
1:C:41:HIS:NE2	1:C:213:THR:HA	2.34	0.43
1:A:173:VAL:HG12	1:A:237:VAL:HG12	2.01	0.42
1:C:107:ASP:OD2	1:C:116:ARG:NH1	2.41	0.42
1:B:240:LYS:C	1:B:241:GLU:HG3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLU:HB3	1:C:84:ILE:HD12	2.01	0.42
1:B:153:PRO:HB3	1:B:256:MET:HE3	2.02	0.42
1:C:263:PRO:HG2	1:C:266:PHE:HD2	1.84	0.42
1:C:59:PHE:CE1	1:C:89:GLU:HG3	2.55	0.42
1:A:121:LYS:HD3	1:A:121:LYS:HA	1.76	0.41
1:C:39:ILE:HG12	1:C:40:ASN:N	2.36	0.41
1:B:153:PRO:HD2	1:B:254:GLY:O	2.20	0.41
1:C:64:GLU:HA	1:C:67:VAL:HG22	2.02	0.41
1:A:161:TYR:HB2	1:A:245:ARG:HB3	2.02	0.41
1:B:30:SER:HB3	1:B:230:LEU:HD22	2.02	0.41
1:B:270:GLU:OE2	1:C:159:ASN:ND2	2.48	0.41
1:C:218:LEU:HD23	1:C:222:ALA:HB1	2.03	0.41
1:C:121:LYS:HB2	1:C:121:LYS:HE3	1.91	0.41
1:B:145:GLU:OE2	1:B:148:PHE:HA	2.21	0.41
1:B:88:TYR:CZ	1:B:90:ALA:HB2	2.57	0.40
1:B:261:GLU:HG3	1:B:262:PRO:O	2.20	0.40
1:B:9:ILE:HG23	1:B:205:PHE:CE1	2.56	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	265/270 (98%)	253 (96%)	10 (4%)	2 (1%)	19 15
1	B	264/270 (98%)	254 (96%)	10 (4%)	0	100 100
1	C	214/270 (79%)	205 (96%)	8 (4%)	1 (0%)	29 26
All	All	743/810 (92%)	712 (96%)	28 (4%)	3 (0%)	34 32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	THR
1	C	256	MET
1	A	257	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	232/235 (99%)	229 (99%)	3 (1%)	69   75
1	B	231/235 (98%)	227 (98%)	4 (2%)	60   67
1	C	199/235 (85%)	191 (96%)	8 (4%)	31   32
All	All	662/705 (94%)	647 (98%)	15 (2%)	50   55

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

Mol	Chain	Res	Type
1	A	143	LEU
1	A	171	LEU
1	A	274	LEU
1	B	117	GLU
1	B	171	LEU
1	B	241	GLU
1	B	260	LEU
1	C	24	GLN
1	C	41	HIS
1	C	52	LYS
1	C	121	LYS
1	C	195	GLU
1	C	243	THR
1	C	245	ARG
1	C	247	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	HIS
1	C	212	ASN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	267/270 (98%)	1.17	58 (21%) 0   0	36, 54, 87, 101	0
1	B	266/270 (98%)	1.06	49 (18%) 1   1	39, 57, 91, 104	0
1	C	226/270 (83%)	1.46	61 (26%) 0   0	51, 76, 98, 108	0
All	All	759/810 (93%)	1.22	168 (22%) 0   0	36, 62, 94, 108	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	163	PHE	11.4
1	A	172	GLY	10.3
1	B	144	VAL	7.3
1	B	173	VAL	7.0
1	A	258	THR	6.7
1	A	173	VAL	6.7
1	C	28	GLU	6.4
1	A	259	ASP	6.1
1	C	191	VAL	5.9
1	C	257	ASP	5.8
1	C	8	MET	5.5
1	A	169	GLY	5.5
1	B	172	GLY	5.3
1	B	169	GLY	5.3
1	A	168	VAL	5.1
1	A	256	MET	5.1
1	C	227	ASN	5.0
1	C	261	GLU	5.0
1	B	257	ASP	4.8
1	A	216	ILE	4.8
1	C	87	TYR	4.7
1	A	261	GLU	4.7
1	C	17	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	184	ILE	4.6
1	C	174	GLN	4.4
1	B	149	PHE	4.4
1	A	171	LEU	4.4
1	C	256	MET	4.4
1	C	11	THR	4.3
1	C	243	THR	4.3
1	A	260	LEU	4.3
1	B	256	MET	4.1
1	A	249	ALA	4.1
1	C	37	ARG	4.0
1	A	164	LYS	4.0
1	C	210	LEU	4.0
1	B	184	ILE	3.9
1	B	259	ASP	3.8
1	B	166	GLU	3.8
1	C	250	SER	3.7
1	A	185	LEU	3.7
1	C	236	ARG	3.7
1	A	214	LEU	3.6
1	C	47	LEU	3.6
1	A	250	SER	3.5
1	A	241	GLU	3.5
1	C	244	MET	3.5
1	B	148	PHE	3.5
1	C	9	ILE	3.5
1	B	260	LEU	3.4
1	C	83	GLU	3.4
1	C	245	ARG	3.4
1	C	246	TYR	3.4
1	A	182	LEU	3.4
1	C	39	ILE	3.4
1	B	214	LEU	3.4
1	A	183	THR	3.3
1	B	171	LEU	3.3
1	A	129	LEU	3.3
1	C	196	ALA	3.3
1	B	183	THR	3.3
1	A	38	VAL	3.3
1	C	197	MET	3.3
1	A	238	GLN	3.2
1	B	193	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	134	ALA	3.2
1	B	204	PHE	3.2
1	C	176	HIS	3.1
1	B	99	PRO	3.1
1	C	63	TYR	3.1
1	C	258	THR	3.1
1	C	259	ASP	3.1
1	A	192	GLY	3.1
1	A	218	LEU	3.0
1	C	182	LEU	3.0
1	B	185	LEU	3.0
1	B	174	GLN	3.0
1	A	200	SER	3.0
1	A	240	LYS	3.0
1	B	170	LYS	3.0
1	A	215	ALA	3.0
1	C	260	LEU	3.0
1	C	184	ILE	2.9
1	C	234	LYS	2.9
1	C	113	ALA	2.9
1	B	145	GLU	2.9
1	B	213	THR	2.9
1	C	35	CYS	2.9
1	B	143	LEU	2.9
1	B	168	VAL	2.8
1	B	100	HIS	2.8
1	A	166	GLU	2.8
1	A	257	ASP	2.8
1	B	17	VAL	2.8
1	B	38	VAL	2.8
1	C	21	ILE	2.8
1	C	158	ILE	2.8
1	B	251	PHE	2.8
1	C	211	PRO	2.8
1	A	242	ALA	2.8
1	A	248	ILE	2.8
1	A	174	GLN	2.7
1	A	133	LEU	2.7
1	A	163	PHE	2.7
1	B	146	THR	2.7
1	C	162	HIS	2.7
1	A	170	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	48	MET	2.6
1	A	100	HIS	2.6
1	C	262	PRO	2.6
1	B	36	PHE	2.6
1	A	43	VAL	2.6
1	B	237	VAL	2.6
1	C	130	ALA	2.6
1	A	74	LEU	2.6
1	B	182	LEU	2.6
1	C	45	LEU	2.6
1	A	213	THR	2.5
1	C	175	LEU	2.5
1	B	133	LEU	2.5
1	A	17	VAL	2.5
1	A	126	ILE	2.5
1	A	251	PHE	2.5
1	A	41	HIS	2.5
1	A	130	ALA	2.4
1	A	8	MET	2.4
1	A	236	ARG	2.4
1	A	217	ASN	2.4
1	B	216	ILE	2.4
1	C	188	ASP	2.4
1	A	262	PRO	2.4
1	A	243	THR	2.4
1	B	167	THR	2.4
1	B	163	PHE	2.4
1	C	185	LEU	2.4
1	C	213	THR	2.4
1	A	274	LEU	2.3
1	C	40	ASN	2.3
1	C	38	VAL	2.3
1	B	126	ILE	2.3
1	C	15	GLU	2.3
1	A	73	LEU	2.3
1	B	88	TYR	2.3
1	A	122	TYR	2.2
1	B	249	ALA	2.2
1	C	235	HIS	2.2
1	C	16	GLU	2.2
1	C	212	ASN	2.2
1	B	8	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	119	MET	2.2
1	C	22	LEU	2.2
1	C	218	LEU	2.2
1	B	215	ALA	2.2
1	B	248	ILE	2.2
1	C	194	LEU	2.2
1	C	217	ASN	2.1
1	B	158	ILE	2.1
1	A	158	ILE	2.1
1	B	264	SER	2.1
1	A	36	PHE	2.1
1	C	24	GLN	2.1
1	C	100	HIS	2.1
1	B	240	LYS	2.0
1	C	67	VAL	2.0
1	B	201	SER	2.0
1	B	236	ARG	2.0
1	B	242	ALA	2.0
1	A	167	THR	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.

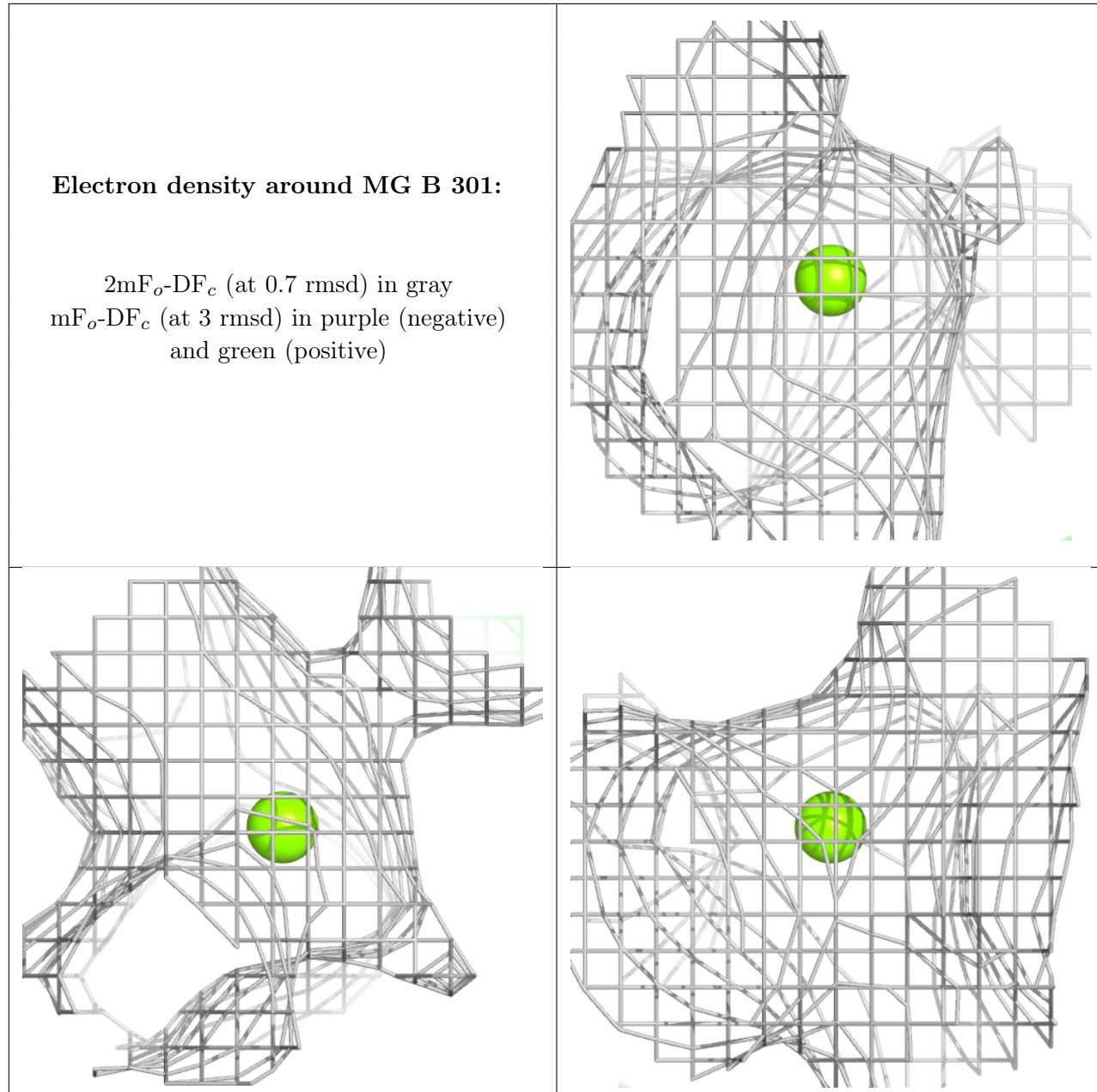
## 6.4 Ligands [\(i\)](#)

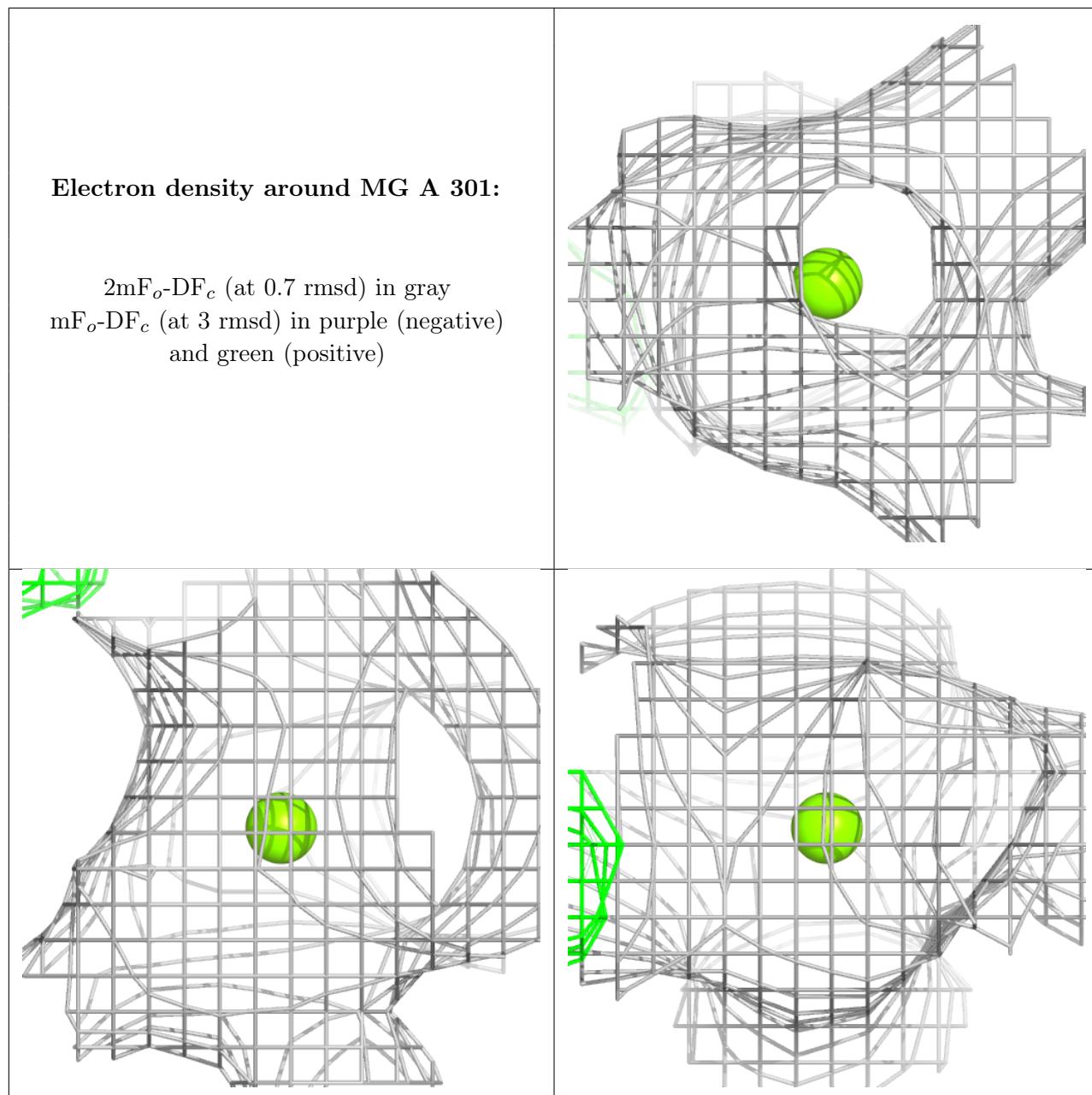
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	301	1/1	0.90	0.09	61,61,61,61	0
2	MG	A	301	1/1	0.91	0.32	65,65,65,65	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.