

# Full wwPDB X-ray Structure Validation Report (i)

#### May 17, 2020 - 02:47 pm BST

PDB ID	:	$6\mathrm{E}12$
$\operatorname{Title}$	:	Crystal Structure of the Alr8543 protein in complex with Oleic Acid and mag-
		nesium ion from Nostoc sp. PCC 7120, Northeast Structural Genomics Con-
		sortium Target NsR141
Authors	:	Forouhar, F.; Neely, H.; Seetharaman, J.; Xiao, R.; Ciccosanti, C.; Patel, D.;
		Belote, R.L.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.;
		Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2018-07-09
Resolution	:	2.40  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 following versions of software and data (see references (1)) were used in the production of this report:

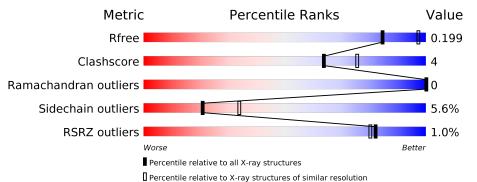
MolProbity Mogul Xtriage (Phenix) EDS	:	1.8.5 (274361), CSD as541be (2020)
buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	::	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)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

# 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 2.40 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	А	225	80%	12%	• 7%
1	В	225	% 	12%	• 6%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3618 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	210	Total 1675	C 1083	÷ ,	O 310		20	0	0	0
1	В	212	Total 1689	C 1091	N 276	0 313	S 2	Se 7	0	0	0

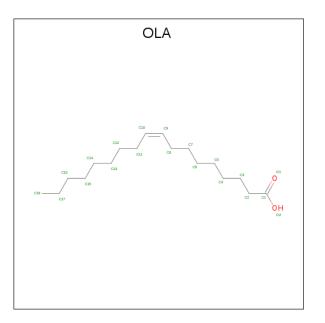
• Molecule 1 is a protein called Alr8543 protein.

Chain	Residue	Modelled	Actual	$\mathbf{Comment}$	Reference
A	218	LEU	-	expression tag	UNP Q8YJY7
A	219	GLU	-	expression tag	UNP Q8YJY7
A	220	HIS	-	expression tag	UNP Q8YJY7
A	221	HIS	-	expression tag	UNP Q8YJY7
A	222	HIS	-	expression tag	UNP Q8YJY7
A	223	HIS	-	expression tag	UNP Q8YJY7
A	224	HIS	-	expression tag	UNP Q8YJY7
A	225	HIS	-	expression tag	UNP Q8YJY7
В	218	LEU	-	expression tag	UNP Q8YJY7
В	219	GLU	-	expression tag	UNP Q8YJY7
В	220	HIS	-	expression tag	UNP Q8YJY7
В	221	HIS	-	expression tag	UNP Q8YJY7
В	222	HIS	-	expression tag	UNP Q8YJY7
В	223	HIS	-	expression tag	UNP Q8YJY7
В	224	HIS	-	expression tag	UNP Q8YJY7
В	225	HIS	-	expression tag	UNP Q8YJY7

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is OLEIC ACID (three-letter code: OLA) (formula:  $C_{18}H_{34}O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total         C         O           20         18         2	0	0
2	В	1	Total         C         O           20         18         2	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	2	Total Mg 2 2	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total Cl 1 1	0	0

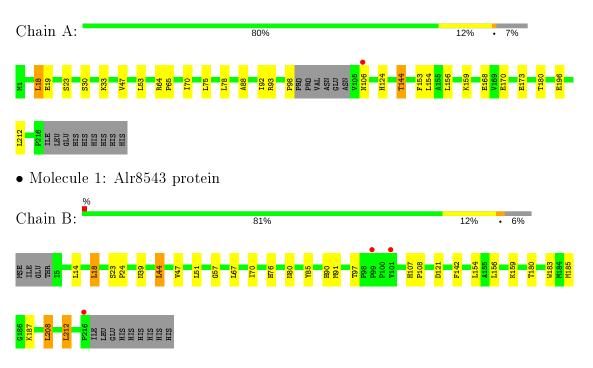
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	85	Total O 85 85	0	0
5	В	126	Total         O           126         126	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Alr8543 protein



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	113.31Å $112.92$ Å $167.77$ Å	Deperitor
$\mathrm{a,b,c,}\alpha,\beta,\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	37.54 - 2.40	Depositor
Resolution (A)	37.54 - 2.40	EDS
% Data completeness	92.8(37.54-2.40)	Depositor
(in resolution range)	$92.8 \ (37.54 - 2.40)$	EDS
R <sub>merge</sub>	0.06	Depositor
$\mathrm{R}_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.58 (at 2.39 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
D D	0.172 , $0.199$	Depositor
$R, R_{free}$	0.172 , $0.199$	DCC
$R_{free}$ test set	3931  reflections  (10.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	39.6	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $49.7$	EDS
L-test for $twinning^2$	$<  L  > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	$\begin{array}{c} 0.010 \ {\rm for} \ -1/2^{*}{\rm h-1}/2^{*}{\rm k-1}/2^{*}{\rm l,-1}/2^{*}{\rm h-1}/2^{*}{\rm k}+\\ 1/2^{*}{\rm l,-h+k}\\ 0.010 \ {\rm for} \ -1/2^{*}{\rm h-1}/2^{*}{\rm k}+1/2^{*}{\rm l,-1}/2^{*}{\rm h-1}/2^{*}{\rm k}-\\ 1/2^{*}{\rm l,h-k}\\ 0.000 \ {\rm for} \ -1/2^{*}{\rm h}+1/2^{*}{\rm k}+1/2^{*}{\rm l,1}/2^{*}{\rm h-1}/2^{*}{\rm k}\\ +1/2^{*}{\rm l,h-k}\\ 0.013 \ {\rm for} \ -1/2^{*}{\rm h}+1/2^{*}{\rm k}-1/2^{*}{\rm l,1}/2^{*}{\rm h-1}/2^{*}{\rm k}-\\ 1/2^{*}{\rm l,-h-k}\\ 0.010 \ {\rm for} \ {\rm k,h,-l} \end{array}$	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3618	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: OLA, MG, CL

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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.37	0/1707	0.52	0/2308	
1	В	0.41	0/1724	0.54	0/2336	
All	All	0.39	0/3431	0.53	0/4644	

There are no bond length outliers.

There are no bond angle outliers.

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	А	1675	0	1683	13	0
1	В	1689	0	1689	18	0
2	А	20	0	33	1	0
2	В	20	0	33	2	0
3	В	2	0	0	0	0
4	В	1	0	0	0	0
5	А	85	0	0	1	0
5	В	126	0	0	0	0
All	All	3618	0	3438	29	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 4.



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A 4 - 1	A.L. 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:208:LEU:HD22	1:B:212:LEU:HD22	1.78	0.65
1:B:47:VAL:HG11	2:B:301:OLA:H181	1.83	0.61
1:A:18:LEU:HD21	1:B:18:LEU:HD21	1.88	0.56
1:B:91:MSE:HA	1:B:91:MSE:HE2	1.89	0.54
1:B:183:TRP:CE2	1:B:187:LYS:HD2	2.44	0.52
1:A:47:VAL:HG11	2:A:301:OLA:H181	1.90	0.52
1:B:80:ASN:HA	1:B:85:TYR:CG	2.45	0.52
1:B:90:HIS:ND1	1:B:91:MSE:CE	2.74	0.51
1:A:64:ARG:HH11	1:A:106:ASN:HA	1.74	0.51
1:A:75:LEU:HA	1:A:78:LEU:HD23	1.93	0.51
1:B:67:LEU:HD13	1:B:70:ILE:HD11	1.94	0.50
1:B:39:ASN:HB3	1:B:44:LEU:HD13	1.94	0.49
1:A:170:GLU:H	1:A:170:GLU:CD	2.18	0.47
1:B:90:HIS:ND1	1:B:91:MSE:HE3	2.29	0.46
1:B:142:PHE:CE1	1:B:185:MSE:HG2	2.51	0.46
1:A:19:GLU:OE2	1:A:33:LYS:NZ	2.47	0.46
1:A:93:ARG:NH1	5:A:402:HOH:O	2.43	0.46
1:A:168:GLU:HG2	1:A:170:GLU:OE1	2.18	0.43
1:B:142:PHE:HE1	1:B:185:MSE:HG2	1.82	0.43
1:A:70:ILE:HD11	1:A:98:PRO:HB3	2.00	0.43
1:A:180:THR:HG23	1:B:180:THR:HG23	1.99	0.43
1:B:107:HIS:CG	1:B:108:PRO:HD2	2.54	0.43
1:B:51:LEU:O	1:B:57:GLY:HA3	2.20	0.42
1:A:88:ALA:O	1:A:92:ILE:HG12	2.20	0.42
1:B:91:MSE:CE	1:B:121:ASP:HB3	2.50	0.42
1:B:23:SER:HB2	1:B:24:PRO:HD2	2.02	0.41
1:A:65:PRO:HB2	1:A:196:GLU:HG2	2.02	0.41
1:B:47:VAL:HG11	2:B:301:OLA:C18	2.50	0.41
1:A:144:THR:HG22	1:A:153:PHE:HB3	2.04	0.40

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentil	es
1	А	206/225~(92%)	204~(99%)	2(1%)	0	100 100	0
1	В	210/225~(93%)	207~(99%)	3 (1%)	0	100 100	0
All	All	416/450 (92%)	411 (99%)	5 (1%)	0	100 100	0

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

There are no Ramachandran outliers to report.

#### 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	А	185/192~(96%)	174~(94%)	11 (6%)	19 32
1	В	187/192~(97%)	177~(95%)	10~(5%)	22 37
All	All	372/384~(97%)	351 (94%)	21~(6%)	21 34

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	18	LEU
1	А	23	SER
1	А	30	SER
1	А	53	LEU
1	А	124	HIS
1	А	144	THR
1	А	154	LEU
1	А	156	LEU
1	А	159	LYS
1	А	173	GLU
1	А	212	LEU
1	В	14	LEU
1	В	18	LEU
1	В	44	LEU
1	В	76	HIS

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Mol	Chain	Res	Type
1	В	97	THR
1	В	154	LEU
1	В	156	LEU
1	В	159	LYS
1	В	208	LEU
1	В	212	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	Trees	Chain	Dec	Link	Bo	ond leng	ths	В	ond ang	les
INIOI	Type	Chain	$\mathbf{Res}$		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLA	А	301	-	16, 19, 19	0.95	1(6%)	$15,\!19,\!19$	0.75	0
2	OLA	В	301	-	16, 19, 19	0.91	1(6%)	$15,\!19,\!19$	0.97	1(6%)

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	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
2	OLA	А	301	-	-	10/15/17/17	-
2	OLA	В	301	-	-	7/15/17/17	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	301	OLA	C10-C9	3.65	1.52	1.31
2	В	301	OLA	C10-C9	3.55	1.52	1.31

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	301	OLA	C8-C9-C10	-2.07	108.81	124.73

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	301	OLA	C1-C2-C3-C4
2	А	301	OLA	С11-С10-С9-С8
2	В	301	OLA	C1-C2-C3-C4
2	В	301	OLA	С11-С10-С9-С8
2	В	301	OLA	C11-C12-C13-C14
2	А	301	OLA	C4-C5-C6-C7
2	А	301	OLA	C2-C3-C4-C5
2	В	301	OLA	C5-C6-C7-C8
2	А	301	OLA	C13-C14-C15-C16
2	В	301	OLA	C4-C5-C6-C7
2	А	301	OLA	C6-C7-C8-C9
2	В	301	OLA	C14-C15-C16-C17
2	А	301	OLA	C5-C6-C7-C8
2	А	301	OLA	C9-C10-C11-C12
2	А	301	OLA	C14-C15-C16-C17
2	А	301	OLA	C7-C8-C9-C10
2	В	301	OLA	C10-C11-C12-C13

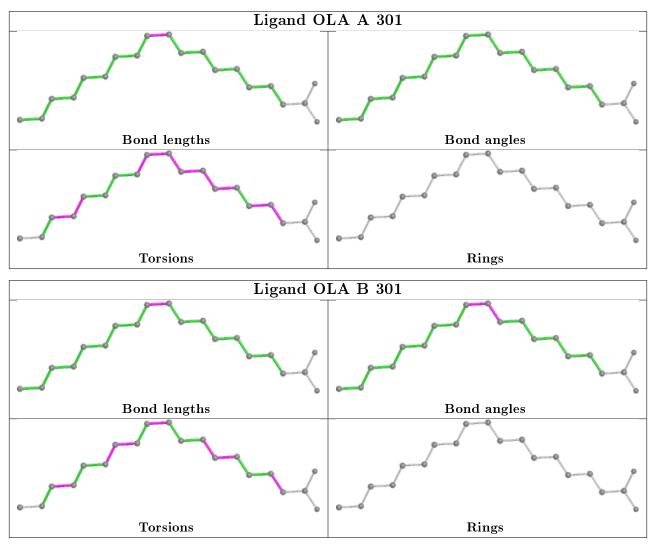
There are no ring outliers.

2 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	301	OLA	1	0
2	В	301	OLA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.





## 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		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	202/225 (89%)	-0.41	1 (0%) 9	91 89	27,  46,  85,  135	0
1	В	205/225 (91%)	-0.43	3 (1%) 7	73 72	26,  39,  76,  106	0
All	All	407/450 (90%)	-0.42	4 (0%) 8	82 80	26,  42,  83,  135	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	106	ASN	3.6
1	В	101	VAL	2.5
1	В	216	PRO	2.5
1	В	99	PRO	2.2

### 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$Q{<}0.9$
4	CL	В	304	1/1	0.93	0.15	$69,\!69,\!69,\!69$	0

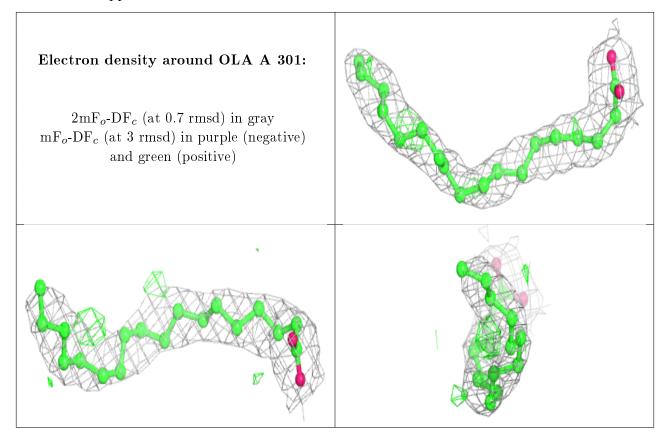
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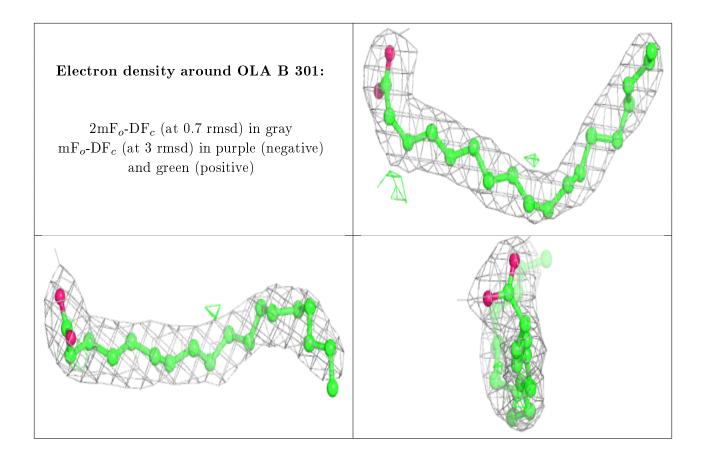
Mol	Type	Chain	$\mathbf{Res}$	Atoms	RSCC	RSR	${f B} ext{-factors}({f A}^2)$	$Q{<}0.9$	
3	MG	В	302	1/1	0.93	0.18	$48,\!48,\!48,\!48$	0	
2	OLA	А	301	20/20	0.94	0.22	53,72,84,84	0	
2	OLA	В	301	20/20	0.94	0.25	$35,\!55,\!66,\!72$	0	
3	MG	В	303	1/1	0.98	0.12	$54,\!54,\!54,\!54$	0	

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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.

