



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2025 – 02:27 PM JST

PDB ID : 9KPR / pdb\_00009kpr  
Title : Crystal structure of a allulose transcriptional regulator from Agrobacterium fabrum  
Authors : Wei, H.L.; Dong, Q.Z.; Liu, W.D.; Yang, J.G.; Sun, Y.X.  
Deposited on : 2024-11-24  
Resolution : 2.53 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

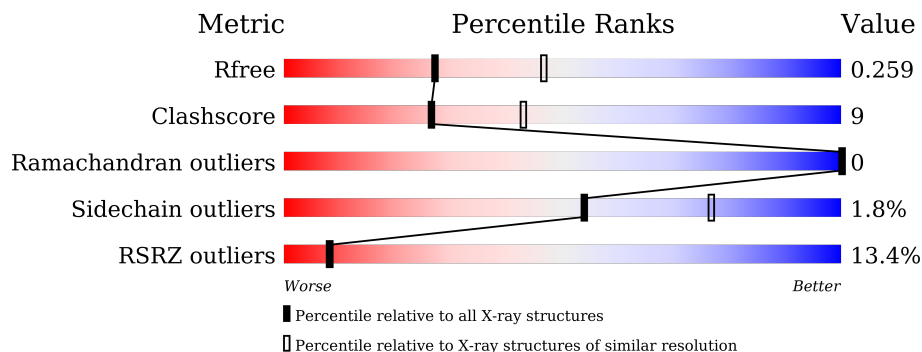
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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	6935 (2.54-2.50)
Clashscore	180529	7778 (2.54-2.50)
Ramachandran outliers	177936	7674 (2.54-2.50)
Sidechain outliers	177891	7676 (2.54-2.50)
RSRZ outliers	164620	6935 (2.54-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	359	<div> <div>11%</div> <div> <div></div> <div>63%</div> <div>15%</div> <div>•</div> <div>21%</div> </div> </div>
1	B	359	<div> <div>10%</div> <div> <div></div> <div>62%</div> <div>17%</div> <div>•</div> <div>21%</div> </div> </div>

## 2 Entry composition [i](#)

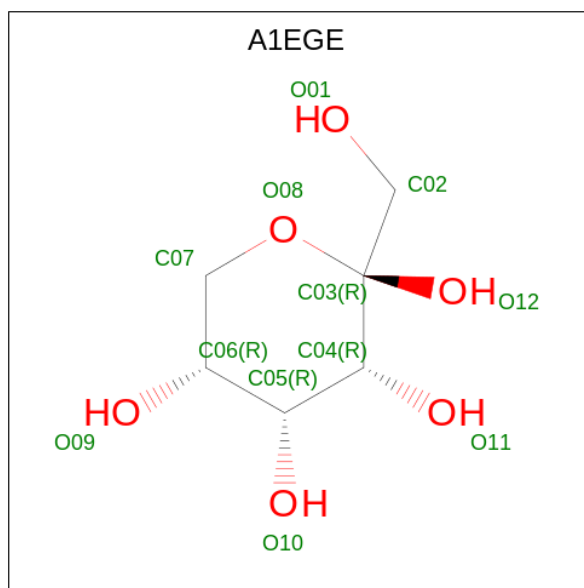
There are 3 unique types of molecules in this entry. The entry contains 4585 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transcriptional regulator, LacI family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2166	1382	364	410	10			
1	B	285	Total	C	N	O	S	0	0	0
			2201	1403	379	409	10			

- Molecule 2 is D-Allulose (CCD ID: A1EGE) (formula:  $C_6H_{12}O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

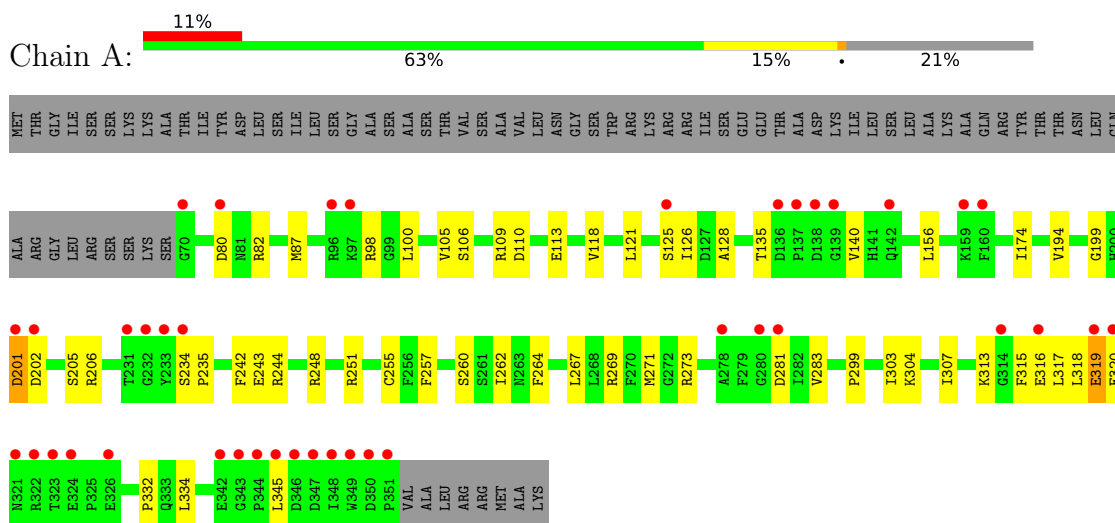
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	B	96	Total 96	O 96	0	0

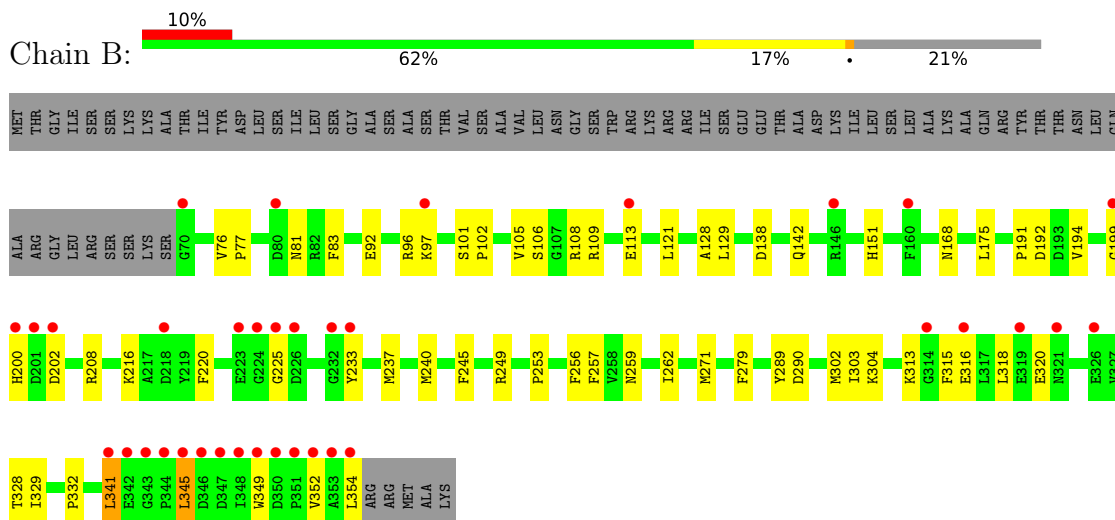
### 3 Residue-property plots

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: Transcriptional regulator, LacI family



- Molecule 1: Transcriptional regulator, LacI family



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.11Å 113.11Å 210.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.53 50.00 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.53) 99.8 (50.00-2.53)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, $R_{free}$	0.231 , 0.261 0.234 , 0.259	Depositor DCC
$R_{free}$ test set	2314 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EGE

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	0.27	0/2222	0.51	0/3016
1	B	0.32	0/2257	0.56	0/3061
All	All	0.29	0/4479	0.54	0/6077

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

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	2166	0	2066	44	0
1	B	2201	0	2125	43	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
3	A	98	0	0	4	0
3	B	96	0	0	6	0
All	All	4585	0	4191	79	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.

All (79) 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:251:ARG:HH22	1:A:281:ASP:HB3	1.43	0.82
1:B:315:PHE:O	1:B:316:GLU:HG2	1.90	0.71
1:A:248:ARG:NH1	3:A:501:HOH:O	2.24	0.69
1:A:80:ASP:HB3	1:B:345:LEU:HD21	1.73	0.69
1:A:82:ARG:NH2	1:B:290:ASP:OD1	2.25	0.68
1:A:110:ASP:HB3	1:A:113:GLU:HB2	1.76	0.67
1:A:135:THR:HB	1:B:352:VAL:HG21	1.78	0.66
1:A:319:GLU:HG2	1:A:320:GLU:N	2.11	0.64
1:A:243:GLU:HB2	1:A:273:ARG:HH22	1.60	0.64
1:A:244:ARG:HG2	1:A:248:ARG:HH12	1.64	0.62
1:A:244:ARG:NH2	3:A:504:HOH:O	2.31	0.62
1:B:97:LYS:NZ	3:B:507:HOH:O	2.32	0.61
1:B:225:GLY:N	3:B:502:HOH:O	2.26	0.61
1:B:194:VAL:HB	1:B:216:LYS:HD2	1.84	0.60
1:B:108:ARG:HG3	1:B:113:GLU:OE1	2.01	0.60
1:A:315:PHE:O	1:A:316:GLU:HG2	2.02	0.59
1:B:192:ASP:O	1:B:249:ARG:NH2	2.36	0.59
1:A:125:SER:O	1:A:125:SER:OG	2.21	0.58
1:B:245:PHE:CE1	1:B:249:ARG:HG3	2.39	0.58
1:B:199:GLY:H	1:B:259:ASN:HD22	1.53	0.57
1:A:109:ARG:HD2	1:B:349:TRP:CE3	2.39	0.56
1:B:77:PRO:HB3	1:B:109:ARG:HG2	1.88	0.55
1:A:118:VAL:HG21	1:A:140:VAL:HG13	1.88	0.55
1:B:105:VAL:HG21	1:B:121:LEU:HD11	1.88	0.54
1:A:267:LEU:HD11	1:A:271:MET:HE3	1.89	0.54
1:A:80:ASP:CB	1:B:345:LEU:HD21	2.36	0.54
1:A:260:SER:OG	1:A:262:ILE:HG13	2.08	0.54
1:B:138:ASP:O	1:B:142:GLN:HG2	2.10	0.52
1:A:109:ARG:HD2	1:B:349:TRP:CZ3	2.45	0.51
1:B:316:GLU:O	1:B:320:GLU:HG3	2.11	0.50
1:A:98:ARG:HB2	1:A:100:LEU:HG	1.94	0.50
1:A:243:GLU:HB2	1:A:273:ARG:NH2	2.25	0.50
1:A:135:THR:HG21	1:B:352:VAL:HG11	1.94	0.49
1:A:304:LYS:NZ	3:A:512:HOH:O	2.39	0.49
1:A:235:PRO:HB2	1:A:269:ARG:NH1	2.27	0.49
1:A:174:ILE:HD12	1:A:334:LEU:HB2	1.93	0.49
1:A:313:LYS:O	1:A:317:LEU:HB2	2.13	0.48
1:B:76:VAL:O	1:B:106:SER:HA	2.14	0.48
1:B:313:LYS:HG2	1:B:328:THR:HG21	1.96	0.47
1:B:96:ARG:HH11	1:B:96:ARG:HA	1.79	0.47
1:B:109:ARG:HH12	1:B:200:HIS:CE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:MET:HA	1:B:240:MET:HE2	1.97	0.47
1:B:245:PHE:CE1	1:B:253:PRO:HD3	2.50	0.47
1:B:302:MET:HG3	3:B:508:HOH:O	2.15	0.47
1:A:307:ILE:HD12	3:A:512:HOH:O	2.14	0.47
1:B:253:PRO:HG2	1:B:256:PHE:CD1	2.49	0.47
1:A:128:ALA:HB1	1:A:318:LEU:HD13	1.97	0.46
1:A:251:ARG:NH2	1:A:281:ASP:HB3	2.22	0.45
1:B:233:TYR:O	1:B:262:ILE:HG23	2.16	0.45
1:A:201:ASP:N	1:A:201:ASP:OD1	2.42	0.45
1:A:202:ASP:O	1:A:206:ARG:HG3	2.16	0.45
1:A:194:VAL:HA	1:A:255:CYS:O	2.17	0.45
1:A:234:SER:HA	1:A:235:PRO:HD3	1.78	0.45
1:B:271:MET:HG2	1:B:279:PHE:CE2	2.52	0.45
1:B:225:GLY:CA	3:B:502:HOH:O	2.62	0.45
1:B:341:LEU:HD13	1:B:341:LEU:HA	1.89	0.44
1:A:303:ILE:HG23	1:A:332:PRO:HB2	2.00	0.44
1:B:289:TYR:CZ	1:B:341:LEU:HD23	2.53	0.44
1:A:199:GLY:O	1:A:205:SER:HB3	2.17	0.44
1:B:303:ILE:HG23	1:B:332:PRO:HB2	2.00	0.44
1:A:87:MET:HA	1:A:307:ILE:HG21	2.00	0.43
1:B:304:LYS:NZ	3:B:512:HOH:O	2.46	0.43
1:B:129:LEU:O	1:B:151:HIS:HA	2.19	0.43
1:B:168:ASN:HB3	1:B:208:ARG:HG3	2.01	0.43
1:A:98:ARG:NH1	1:A:315:PHE:HB3	2.33	0.42
1:B:225:GLY:HA3	3:B:502:HOH:O	2.20	0.42
1:A:121:LEU:HD13	1:A:126:ILE:HD13	2.02	0.42
1:B:101:SER:HA	1:B:102:PRO:HD3	1.93	0.41
1:B:81:ASN:OD1	1:B:83:PHE:N	2.53	0.41
1:B:128:ALA:HB1	1:B:318:LEU:HD13	2.02	0.41
1:A:264:PHE:CE1	1:A:267:LEU:HD23	2.55	0.41
1:B:175:LEU:HD23	1:B:257:PHE:CE2	2.55	0.41
1:A:106:SER:HB3	1:B:92:GLU:CD	2.46	0.41
1:B:191:PRO:HA	1:B:220:PHE:CE2	2.55	0.41
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.84	0.40
1:A:257:PHE:CD1	1:A:257:PHE:C	2.99	0.40
1:A:105:VAL:HG11	1:A:121:LEU:HD21	2.04	0.40
1:A:242:PHE:CE2	1:A:267:LEU:HB2	2.57	0.40
1:A:283:VAL:HG22	1:A:299:PRO:HG2	2.04	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	A	280/359 (78%)	273 (98%)	7 (2%)	0	100	100
1	B	283/359 (79%)	273 (96%)	10 (4%)	0	100	100
All	All	563/718 (78%)	546 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	225/293 (77%)	222 (99%)	3 (1%)	65	83
1	B	229/293 (78%)	224 (98%)	5 (2%)	47	71
All	All	454/586 (78%)	446 (98%)	8 (2%)	54	77

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

Mol	Chain	Res	Type
1	A	201	ASP
1	A	319	GLU
1	A	345	LEU
1	B	202	ASP
1	B	329	ILE
1	B	341	LEU
1	B	345	LEU
1	B	354	LEU

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	153	ASN
1	B	94	GLN
1	B	153	ASN
1	B	236	HIS
1	B	259	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 oligosaccharides 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	A1EGE	B	401	-	12,12,12	1.97	4 (33%)	18,18,18	2.88	8 (44%)
2	A1EGE	A	401	-	12,12,12	2.06	5 (41%)	18,18,18	1.52	6 (33%)

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	A1EGE	B	401	-	-	2/3/23/23	0/1/1/1
2	A1EGE	A	401	-	-	3/3/23/23	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A1EGE	O08-C03	3.63	1.45	1.42
2	B	401	A1EGE	O08-C03	3.63	1.45	1.42
2	A	401	A1EGE	C06-C05	-3.35	1.47	1.52
2	B	401	A1EGE	C06-C05	-3.03	1.48	1.52
2	A	401	A1EGE	C05-C04	-2.92	1.48	1.53
2	B	401	A1EGE	C05-C04	-2.87	1.48	1.53
2	B	401	A1EGE	O12-C03	-2.71	1.36	1.40
2	A	401	A1EGE	O08-C07	2.39	1.47	1.43
2	A	401	A1EGE	O12-C03	-2.38	1.36	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	A1EGE	O08-C03-C04	6.63	116.39	109.76
2	B	401	A1EGE	C06-C05-C04	6.08	117.28	110.48
2	B	401	A1EGE	C03-C04-C05	4.63	116.92	110.70
2	B	401	A1EGE	C07-O08-C03	-2.93	110.77	114.09
2	B	401	A1EGE	O01-C02-C03	-2.83	105.84	111.86
2	B	401	A1EGE	C07-C06-C05	2.81	113.12	109.67
2	A	401	A1EGE	C07-O08-C03	-2.61	111.14	114.09
2	A	401	A1EGE	C07-C06-C05	2.42	112.64	109.67
2	A	401	A1EGE	O08-C03-C02	2.36	108.51	105.58
2	B	401	A1EGE	O12-C03-C02	-2.30	107.55	111.12
2	A	401	A1EGE	O12-C03-O08	-2.27	106.99	110.69
2	B	401	A1EGE	O10-C05-C04	-2.21	105.24	109.73
2	A	401	A1EGE	C06-C05-C04	2.12	112.85	110.48
2	A	401	A1EGE	O08-C03-C04	2.04	111.80	109.76

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1EGE	O01-C02-C03-C04
2	A	401	A1EGE	O01-C02-C03-O08
2	A	401	A1EGE	O01-C02-C03-O12
2	B	401	A1EGE	O01-C02-C03-C04

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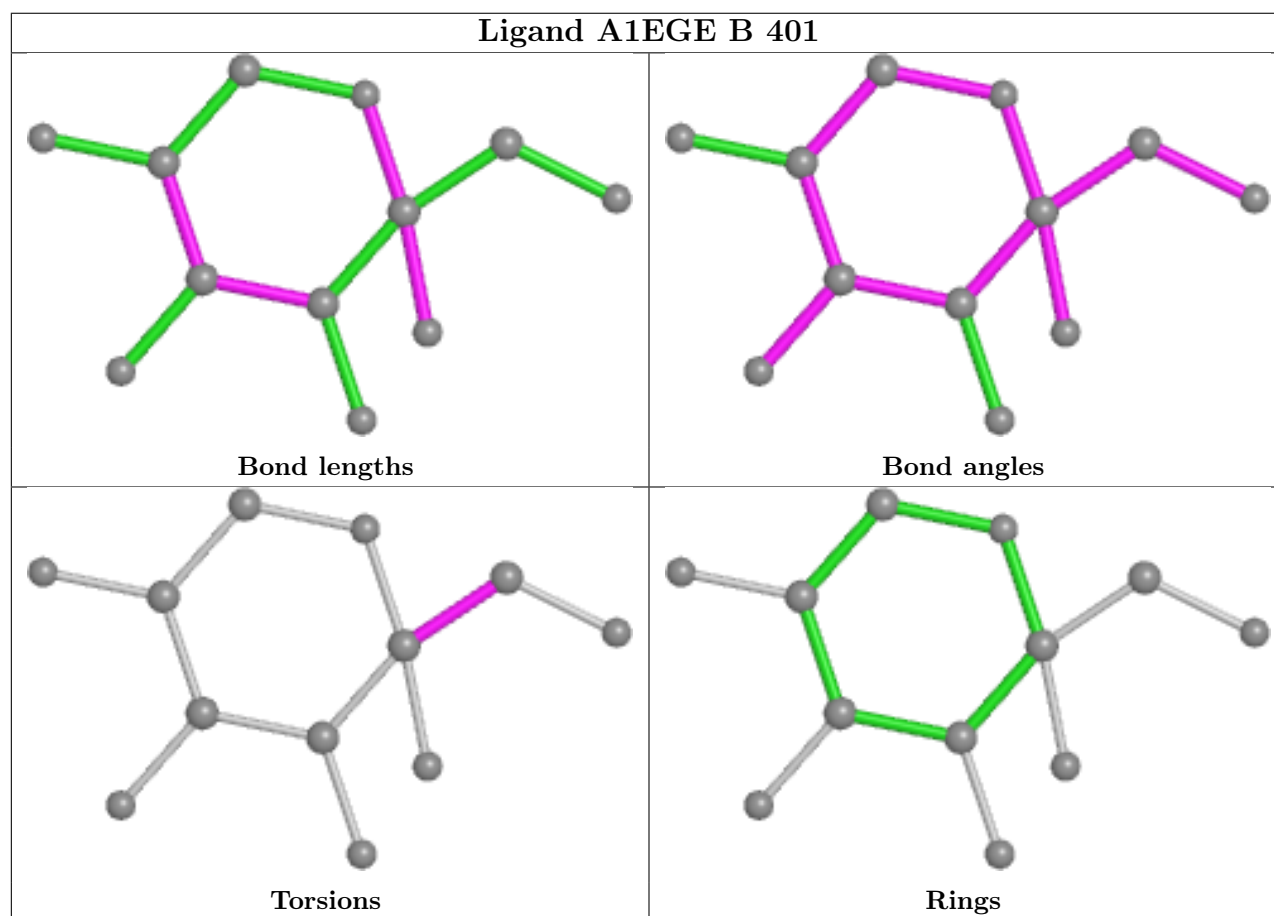
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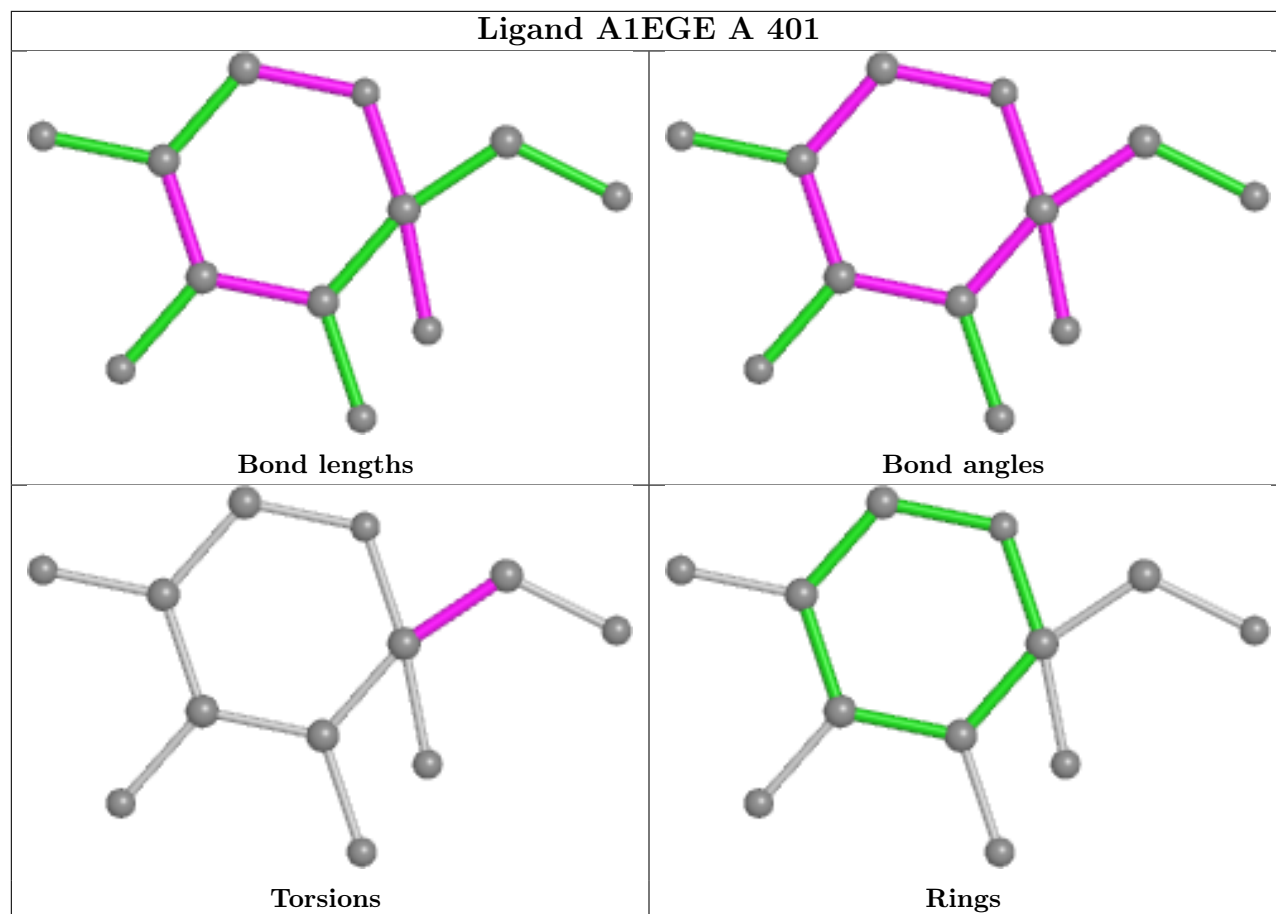
Mol	Chain	Res	Type	Atoms
2	B	401	A1EGE	O01-C02-C03-O12

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, 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	282/359 (78%)	0.73	40 (14%) <b>7</b> <b>7</b>	12, 35, 74, 110	0
1	B	285/359 (79%)	0.63	36 (12%) <b>9</b> <b>9</b>	16, 30, 70, 98	0
All	All	567/718 (78%)	0.68	76 (13%) <b>8</b> <b>8</b>	12, 33, 74, 110	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	LEU	7.5
1	A	322	ARG	7.5
1	A	323	THR	7.4
1	B	353	ALA	7.2
1	B	201	ASP	6.8
1	B	224	GLY	6.4
1	A	344	PRO	6.3
1	B	345	LEU	6.2
1	B	347	ASP	6.0
1	B	342	GLU	5.9
1	A	321	ASN	5.8
1	B	352	VAL	5.8
1	A	351	PRO	5.4
1	B	344	PRO	5.4
1	A	324	GLU	5.2
1	A	234	SER	5.1
1	A	343	GLY	4.8
1	A	349	TRP	4.8
1	B	202	ASP	4.8
1	A	202	ASP	4.7
1	B	343	GLY	4.6
1	B	200	HIS	4.5
1	B	346	ASP	4.4
1	A	326	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	223	GLU	4.3
1	B	326	GLU	4.2
1	A	231	THR	4.1
1	A	232	GLY	4.1
1	B	199	GLY	4.1
1	A	316	GLU	3.9
1	B	354	LEU	3.9
1	B	349	TRP	3.8
1	A	350	ASP	3.7
1	B	70	GLY	3.7
1	A	70	GLY	3.7
1	B	80	ASP	3.6
1	A	233	TYR	3.6
1	B	232	GLY	3.5
1	B	341	LEU	3.4
1	A	346	ASP	3.4
1	B	225	GLY	3.2
1	A	319	GLU	3.1
1	A	160	PHE	3.1
1	B	226	ASP	3.1
1	B	350	ASP	3.0
1	B	351	PRO	3.0
1	A	314	GLY	3.0
1	A	348	ILE	3.0
1	A	320	GLU	3.0
1	A	80	ASP	2.9
1	A	347	ASP	2.9
1	A	138	ASP	2.8
1	A	159	LYS	2.7
1	A	96	ARG	2.6
1	A	137	PRO	2.6
1	A	281	ASP	2.6
1	B	113	GLU	2.6
1	B	314	GLY	2.6
1	A	125	SER	2.5
1	A	342	GLU	2.5
1	A	139	GLY	2.5
1	A	278	ALA	2.5
1	A	280	GLY	2.5
1	B	321	ASN	2.5
1	B	97	LYS	2.4
1	B	319	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	201	ASP	2.4
1	B	233	TYR	2.3
1	B	348	ILE	2.2
1	A	97	LYS	2.2
1	A	142	GLN	2.2
1	A	136	ASP	2.1
1	B	146	ARG	2.1
1	B	218	ASP	2.1
1	B	160	PHE	2.1
1	B	316	GLU	2.1

## 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](#)

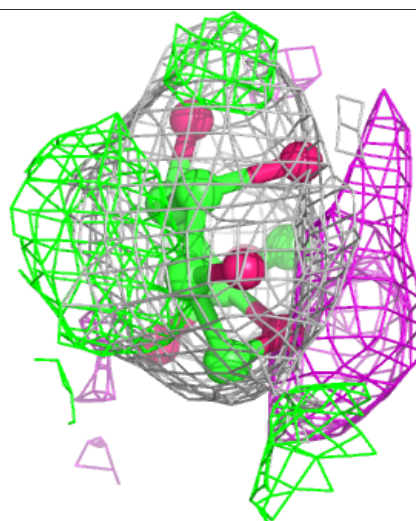
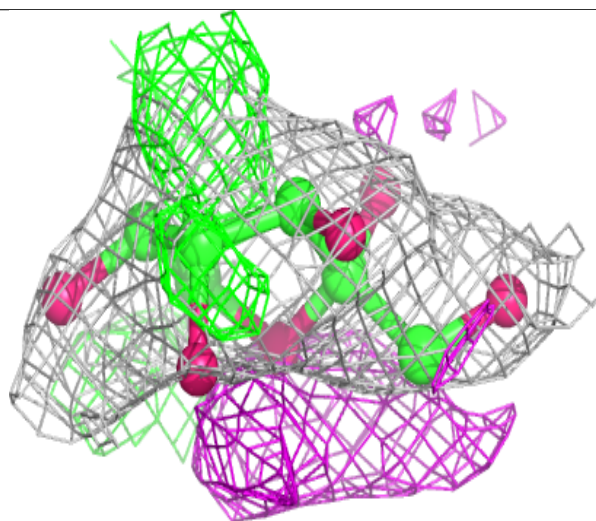
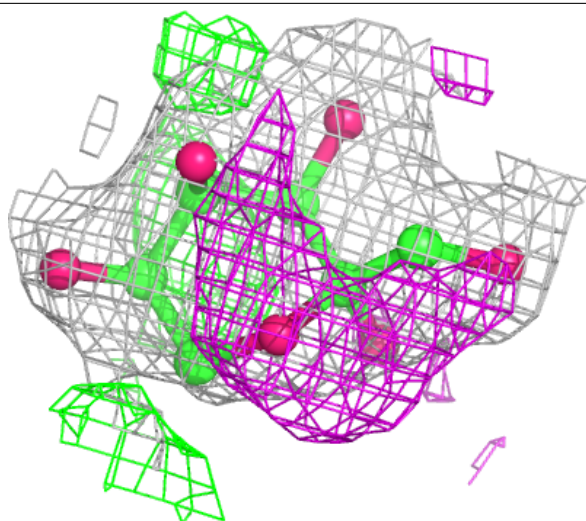
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1EGE	A	401	12/12	0.80	0.23	38,47,55,73	0
2	A1EGE	B	401	12/12	0.87	0.20	41,50,56,71	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.

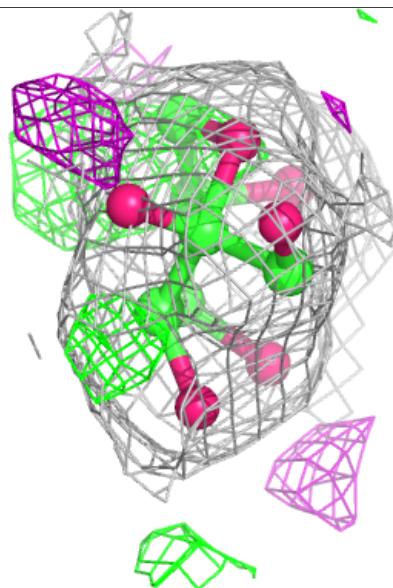
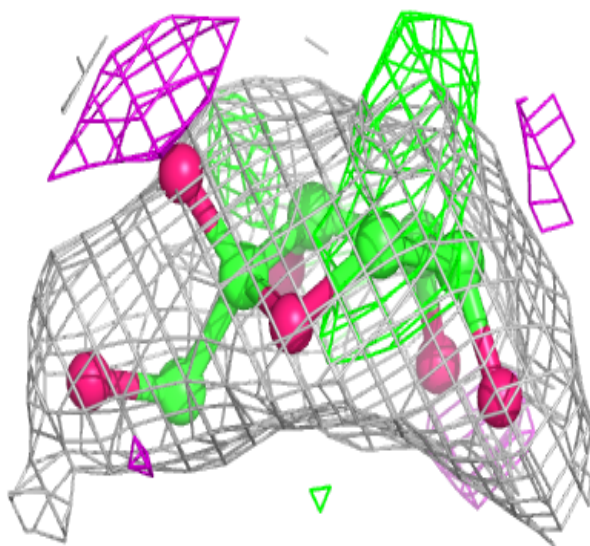
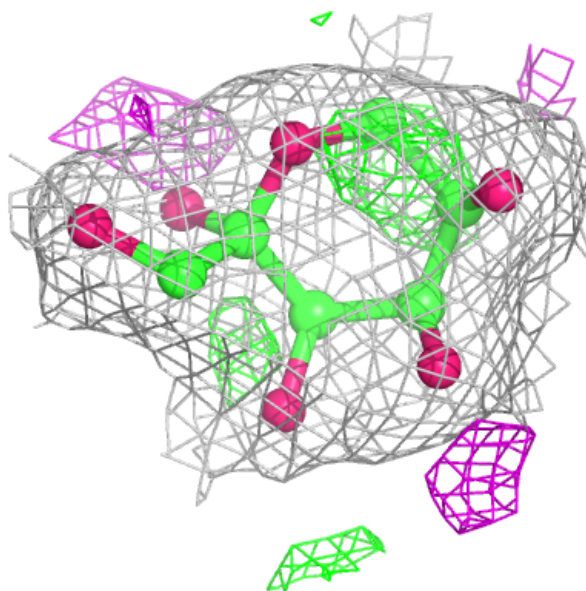
**Electron density around A1EGE A 401:**

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



**Electron density around A1EGE B 401:**

$2mF_o-DF_c$  (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.