



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 7, 2017 – 02:05 AM EDT

PDB ID : 2Q4D  
Title : Ensemble refinement of the crystal structure of a lysine decarboxylase-like protein from Arabidopsis thaliana gene At5g11950  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : unknown  
Resolution : 2.15 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

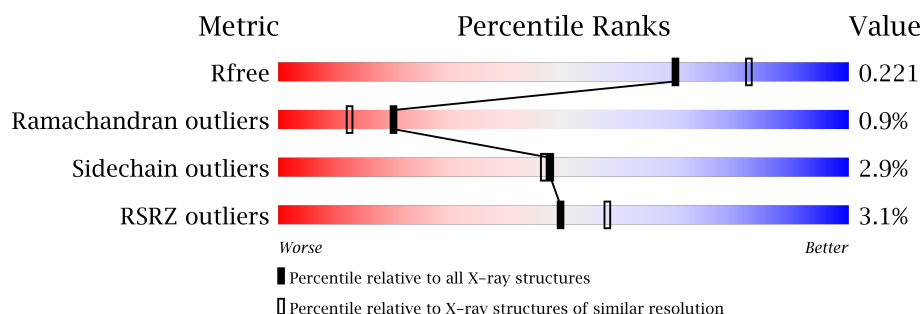
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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.



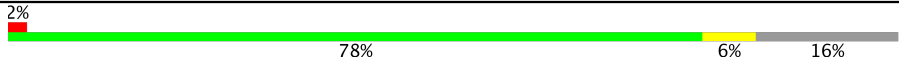

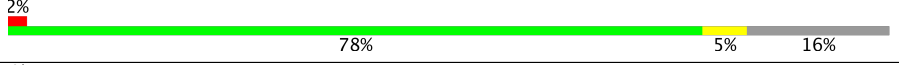

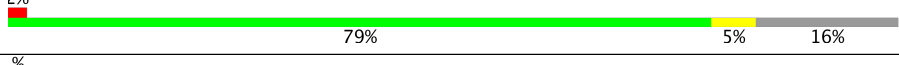
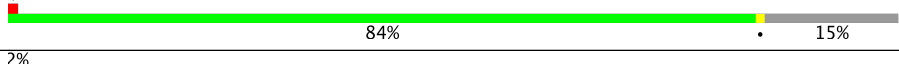
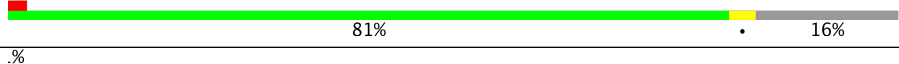

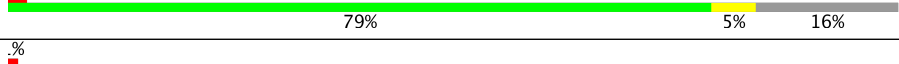


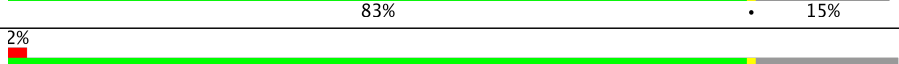
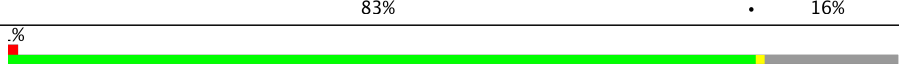
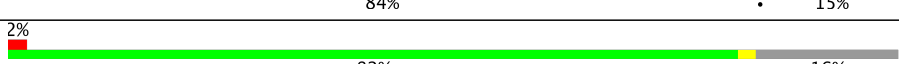

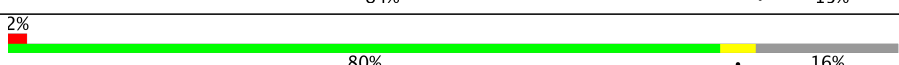
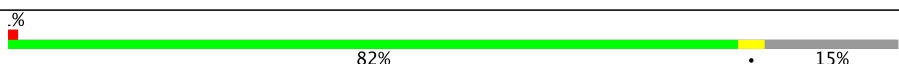
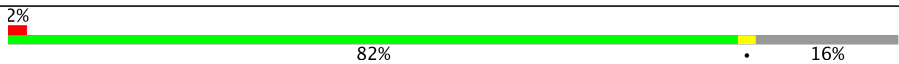
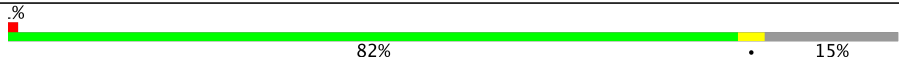


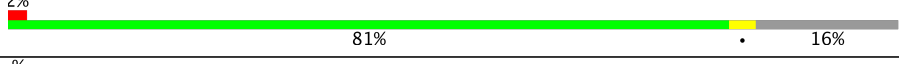
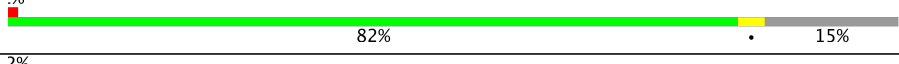


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1170 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1-A	216	<div> <div>0.1%</div> <div>83%</div> <div>15%</div> </div>
1	1-B	216	<div> <div>2%</div> <div>82%</div> <div>16%</div> </div>
1	10-A	216	<div> <div>0.1%</div> <div>81%</div> <div>15%</div> </div>
1	10-B	216	<div> <div>2%</div> <div>81%</div> <div>16%</div> </div>
1	11-A	216	<div> <div>0.1%</div> <div>84%</div> <div>15%</div> </div>
1	11-B	216	<div> <div>2%</div> <div>80%</div> <div>16%</div> </div>
1	12-A	216	<div> <div>0.1%</div> <div>83%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	12-B	216	
1	13-A	216	
1	13-B	216	
1	14-A	216	
1	14-B	216	
1	15-A	216	
1	15-B	216	
1	16-A	216	
1	16-B	216	
1	2-A	216	
1	2-B	216	
1	3-A	216	
1	3-B	216	
1	4-A	216	
1	4-B	216	
1	5-A	216	
1	5-B	216	
1	6-A	216	
1	6-B	216	
1	7-A	216	
1	7-B	216	
1	8-A	216	
1	8-B	216	
1	9-A	216	
1	9-B	216	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NO3	1-A	600	-	-	-	X
2	NO3	10-A	600	-	-	-	X
2	NO3	11-A	600	-	-	-	X
2	NO3	12-A	600	-	-	-	X
2	NO3	13-A	600	-	-	-	X
2	NO3	14-A	600	-	-	-	X
2	NO3	15-A	600	-	-	-	X
2	NO3	16-A	600	-	-	-	X
2	NO3	2-A	600	-	-	-	X
2	NO3	3-A	600	-	-	-	X
2	NO3	5-A	600	-	-	-	X
2	NO3	8-A	600	-	-	-	X
3	EDO	1-A	701	-	-	-	X
3	EDO	1-A	993	-	-	-	X
3	EDO	10-A	701	-	-	-	X
3	EDO	10-B	993	-	-	-	X
3	EDO	11-A	701	-	-	-	X
3	EDO	11-B	993	-	-	-	X
3	EDO	12-A	701	-	-	-	X
3	EDO	12-B	993	-	-	-	X
3	EDO	13-A	701	-	-	-	X
3	EDO	13-B	993	-	-	-	X
3	EDO	14-A	701	-	-	-	X
3	EDO	14-B	993	-	-	-	X
3	EDO	15-A	701	-	-	-	X
3	EDO	15-B	993	-	-	-	X
3	EDO	16-A	701	-	-	-	X
3	EDO	16-B	993	-	-	-	X
3	EDO	2-A	701	-	-	-	X
3	EDO	2-B	993	-	-	-	X
3	EDO	3-A	701	-	-	-	X
3	EDO	3-B	993	-	-	-	X
3	EDO	4-A	701	-	-	-	X
3	EDO	4-B	993	-	-	-	X
3	EDO	5-A	701	-	-	-	X
3	EDO	5-B	993	-	-	-	X
3	EDO	6-A	701	-	-	-	X
3	EDO	6-B	993	-	-	-	X
3	EDO	7-A	701	-	-	-	X
3	EDO	7-B	993	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	8-A	701	-	-	-	X
3	EDO	8-B	993	-	-	-	X
3	EDO	9-A	701	-	-	-	X
3	EDO	9-B	993	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50160 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 Lysine decarboxylase-like protein At5g11950.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	2-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	3-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	4-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	5-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	6-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	7-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	8-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	9-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	10-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	11-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	12-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	13-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	14-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	15-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			
1	16-A	184	Total	C	N	O	S	Se	0	0	0
			1411	896	243	262	2	8			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	2-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	3-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	4-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	5-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	6-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	7-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	8-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	9-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	10-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	11-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	12-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	13-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	14-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	15-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			
1	16-B	181	Total	C	N	O	S	Se	0	0	0
			1385	882	236	257	2	8			

There are 20 discrepancies between the modelled and reference sequences:

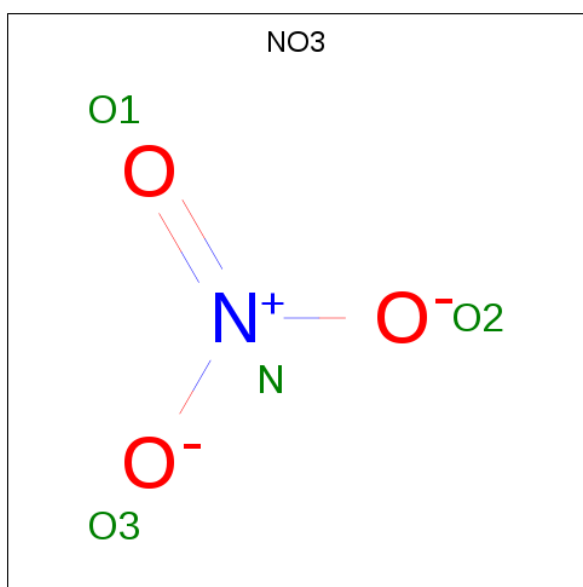
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q84MC2
A	54	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
A	77	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
A	95	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
A	102	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
A	119	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
A	125	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	181	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
A	184	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
A	192	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
B	1	SER	-	EXPRESSION TAG	UNP Q84MC2
B	54	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
B	77	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
B	95	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
B	102	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
B	119	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
B	125	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
B	181	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
B	184	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2
B	192	MSE	MET	MODIFIED RESIDUE	UNP Q84MC2

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	N	O	0	0
			4	1	3		
2	2-A	1	Total	N	O	0	0
			4	1	3		
2	3-A	1	Total	N	O	0	0
			4	1	3		
2	4-A	1	Total	N	O	0	0
			4	1	3		
2	5-A	1	Total	N	O	0	0
			4	1	3		

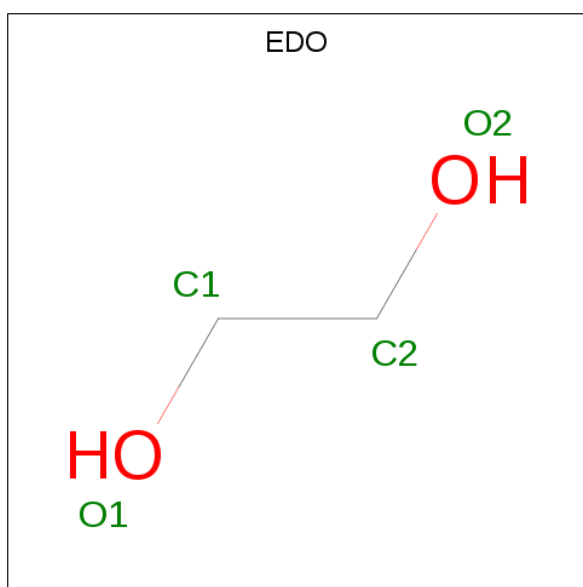
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	6-A	1	Total	N	O	0	0
			4	1	3		
2	7-A	1	Total	N	O	0	0
			4	1	3		
2	8-A	1	Total	N	O	0	0
			4	1	3		
2	9-A	1	Total	N	O	0	0
			4	1	3		
2	10-A	1	Total	N	O	0	0
			4	1	3		
2	11-A	1	Total	N	O	0	0
			4	1	3		
2	12-A	1	Total	N	O	0	0
			4	1	3		
2	13-A	1	Total	N	O	0	0
			4	1	3		
2	14-A	1	Total	N	O	0	0
			4	1	3		
2	15-A	1	Total	N	O	0	0
			4	1	3		
2	16-A	1	Total	N	O	0	0
			4	1	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	1	Total C O 4 2 2	0	0
3	2-A	1	Total C O 4 2 2	0	0
3	3-A	1	Total C O 4 2 2	0	0
3	4-A	1	Total C O 4 2 2	0	0
3	5-A	1	Total C O 4 2 2	0	0
3	6-A	1	Total C O 4 2 2	0	0
3	7-A	1	Total C O 4 2 2	0	0
3	8-A	1	Total C O 4 2 2	0	0
3	9-A	1	Total C O 4 2 2	0	0
3	10-A	1	Total C O 4 2 2	0	0
3	11-A	1	Total C O 4 2 2	0	0
3	12-A	1	Total C O 4 2 2	0	0
3	13-A	1	Total C O 4 2 2	0	0
3	14-A	1	Total C O 4 2 2	0	0
3	15-A	1	Total C O 4 2 2	0	0
3	16-A	1	Total C O 4 2 2	0	0
3	1-A	1	Total C O 4 2 2	0	0
3	2-A	1	Total C O 4 2 2	0	0
3	3-A	1	Total C O 4 2 2	0	0
3	4-A	1	Total C O 4 2 2	0	0
3	5-A	1	Total C O 4 2 2	0	0
3	6-A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	9-A	1	Total 4	C 2	O 2	0	0
3	10-A	1	Total 4	C 2	O 2	0	0
3	11-A	1	Total 4	C 2	O 2	0	0
3	12-A	1	Total 4	C 2	O 2	0	0
3	13-A	1	Total 4	C 2	O 2	0	0
3	14-A	1	Total 4	C 2	O 2	0	0
3	15-A	1	Total 4	C 2	O 2	0	0
3	16-A	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	9-B	1	Total 4	C 2	O 2	0	0
3	10-B	1	Total 4	C 2	O 2	0	0
3	11-B	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	12-B	1	Total 4	C 2	O 2	0	0
3	13-B	1	Total 4	C 2	O 2	0	0
3	14-B	1	Total 4	C 2	O 2	0	0
3	15-B	1	Total 4	C 2	O 2	0	0
3	16-B	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	9-B	1	Total 4	C 2	O 2	0	0
3	10-B	1	Total 4	C 2	O 2	0	0
3	11-B	1	Total 4	C 2	O 2	0	0
3	12-B	1	Total 4	C 2	O 2	0	0
3	13-B	1	Total 4	C 2	O 2	0	0
3	14-B	1	Total 4	C 2	O 2	0	0
3	15-B	1	Total 4	C 2	O 2	0	0
3	16-B	1	Total 4	C 2	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	155	Total O 155 155	0	0
4	2-A	155	Total O 155 155	0	0
4	3-A	157	Total O 157 157	0	0
4	4-A	155	Total O 155 155	0	0
4	5-A	162	Total O 162 162	0	0
4	6-A	153	Total O 153 153	0	0
4	7-A	159	Total O 159 159	0	0
4	8-A	158	Total O 158 158	0	0
4	9-A	162	Total O 162 162	0	0
4	10-A	151	Total O 151 151	0	0
4	11-A	151	Total O 151 151	0	0
4	12-A	152	Total O 152 152	0	0
4	13-A	155	Total O 155 155	0	0
4	14-A	154	Total O 154 154	0	0
4	15-A	155	Total O 155 155	0	0
4	16-A	158	Total O 158 158	0	0
4	1-B	164	Total O 164 164	0	0
4	2-B	164	Total O 164 164	0	0
4	3-B	162	Total O 162 162	0	0
4	4-B	164	Total O 164 164	0	0
4	5-B	157	Total O 157 157	0	0

*Continued on next page...*

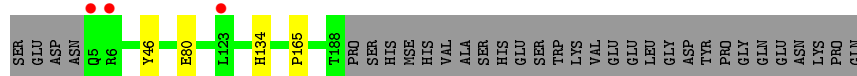
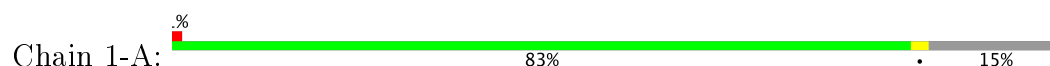
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	6-B	166	Total 166	O 166	0	0
4	7-B	160	Total 160	O 160	0	0
4	8-B	161	Total 161	O 161	0	0
4	9-B	157	Total 157	O 157	0	0
4	10-B	168	Total 168	O 168	0	0
4	11-B	168	Total 168	O 168	0	0
4	12-B	167	Total 167	O 167	0	0
4	13-B	164	Total 164	O 164	0	0
4	14-B	165	Total 165	O 165	0	0
4	15-B	164	Total 164	O 164	0	0
4	16-B	161	Total 161	O 161	0	0

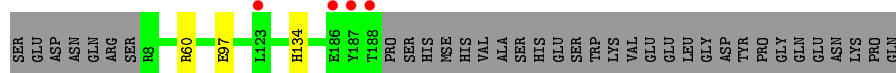
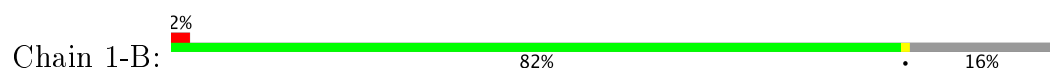
### 3 Residue-property plots [i](#)

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.

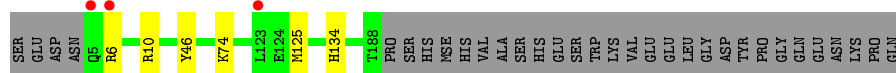
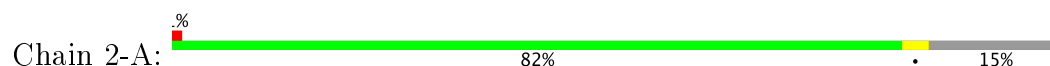
- Molecule 1: Lysine decarboxylase-like protein At5g11950



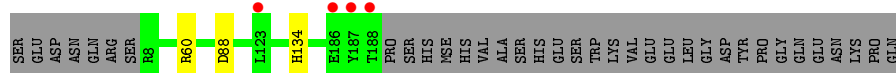
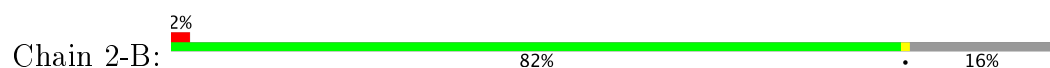
- Molecule 1: Lysine decarboxylase-like protein At5g11950



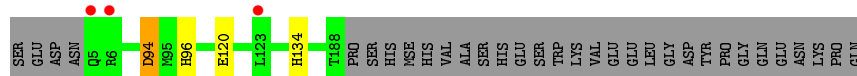
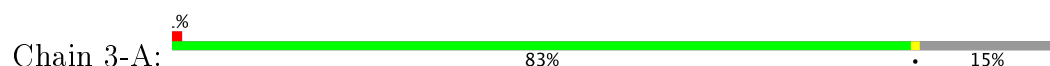
- Molecule 1: Lysine decarboxylase-like protein At5g11950



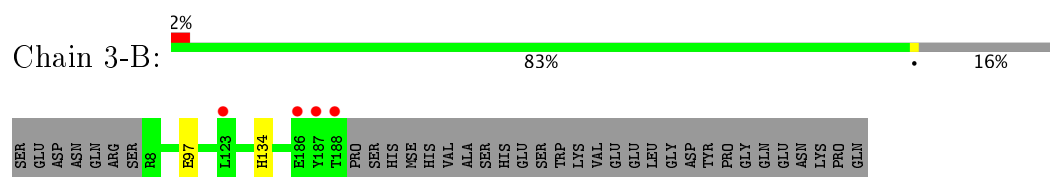
- Molecule 1: Lysine decarboxylase-like protein At5g11950



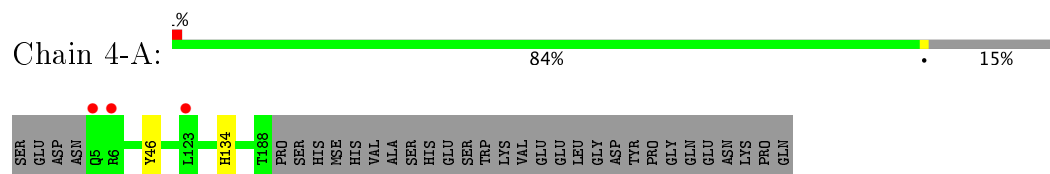
- Molecule 1: Lysine decarboxylase-like protein At5g11950



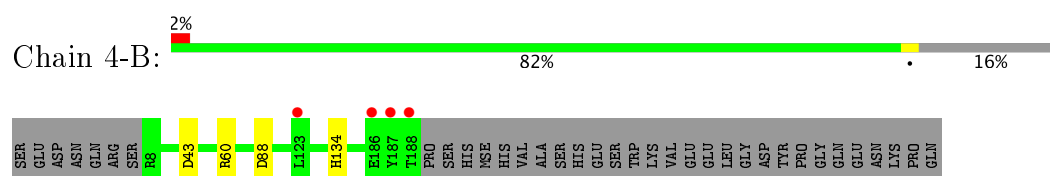
- Molecule 1: Lysine decarboxylase-like protein At5g11950



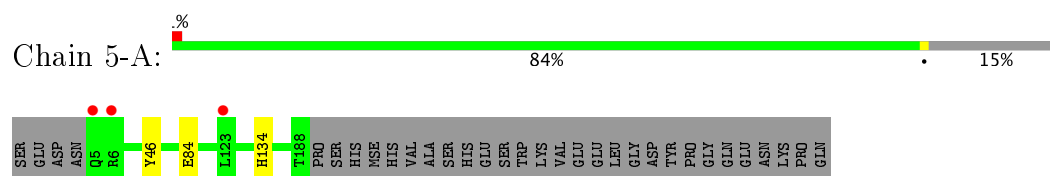
- Molecule 1: Lysine decarboxylase-like protein At5g11950



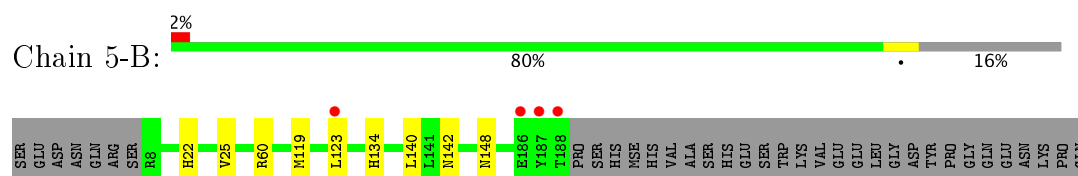
- Molecule 1: Lysine decarboxylase-like protein At5g11950



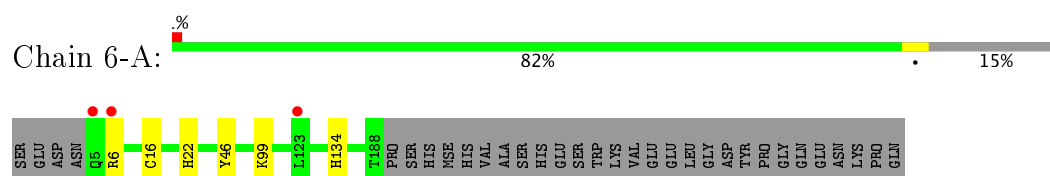
- Molecule 1: Lysine decarboxylase-like protein At5g11950



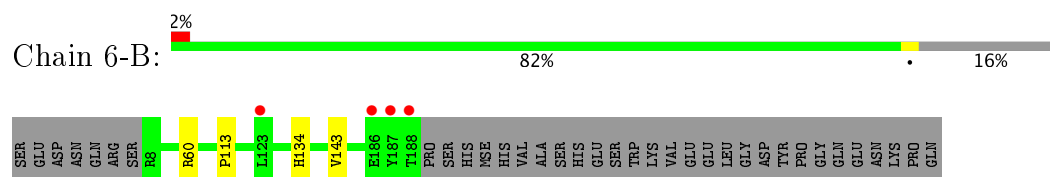
- Molecule 1: Lysine decarboxylase-like protein At5g11950



- Molecule 1: Lysine decarboxylase-like protein At5g11950

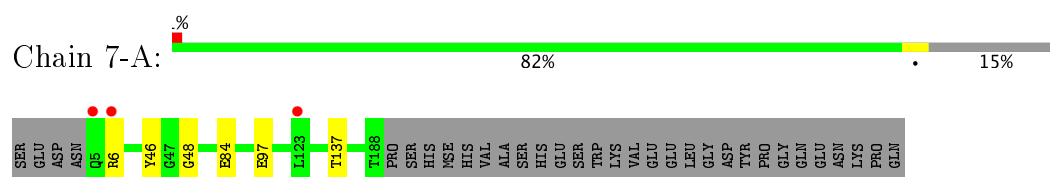


- Molecule 1: Lysine decarboxylase-like protein At5g11950

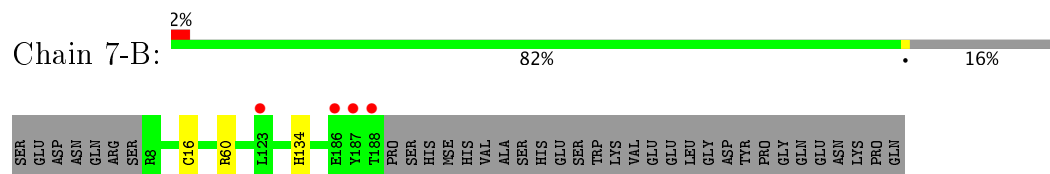


- Molecule 1: Lysine decarboxylase-like protein At5g11950

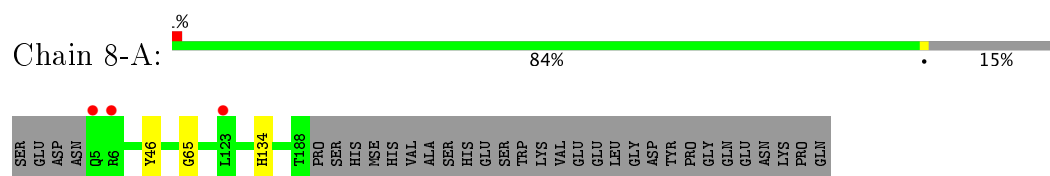




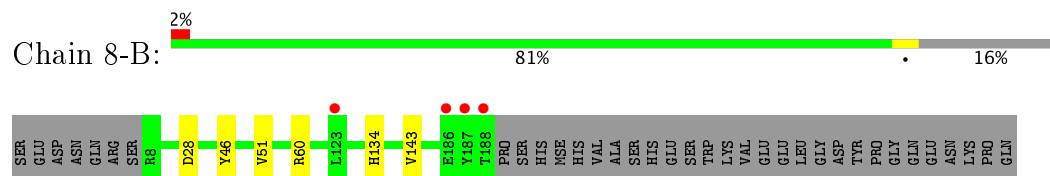
- Molecule 1: Lysine decarboxylase-like protein At5g11950



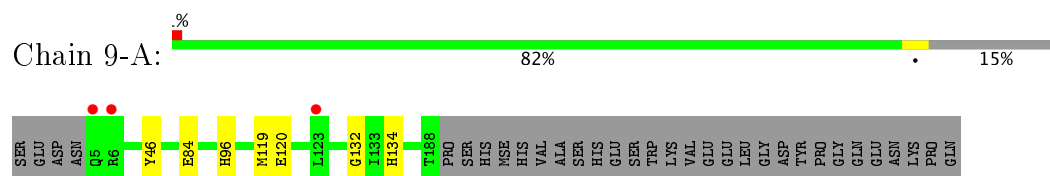
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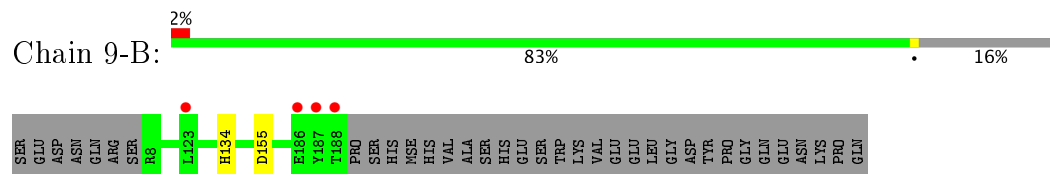
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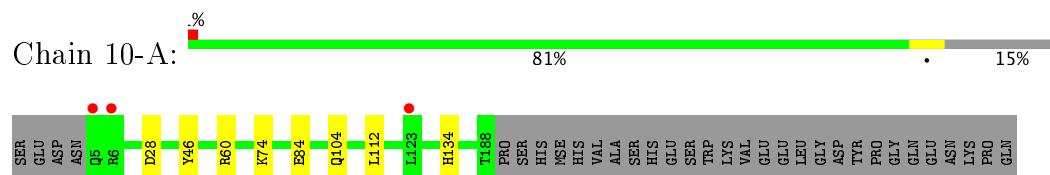
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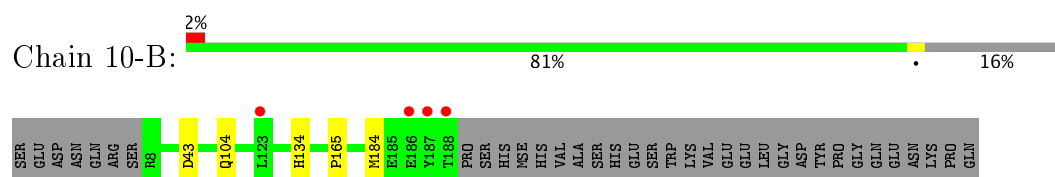
- Molecule 1: Lysine decarboxylase-like protein At5g11950



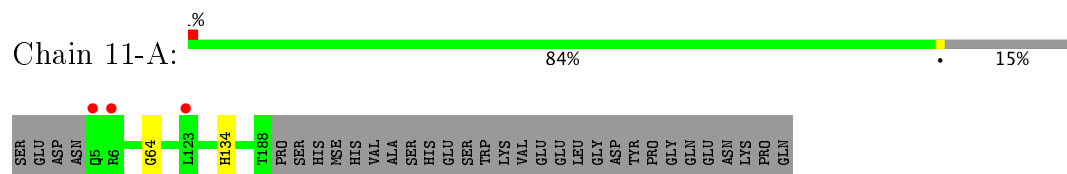
- Molecule 1: Lysine decarboxylase-like protein At5g11950



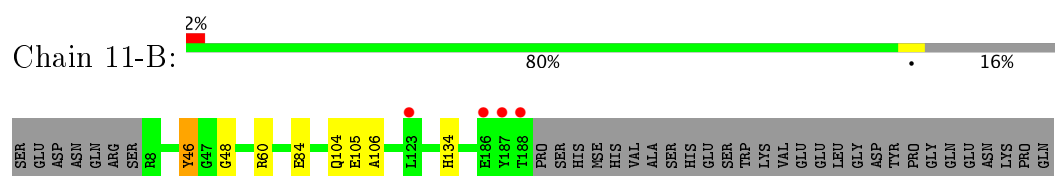
- Molecule 1: Lysine decarboxylase-like protein At5g11950



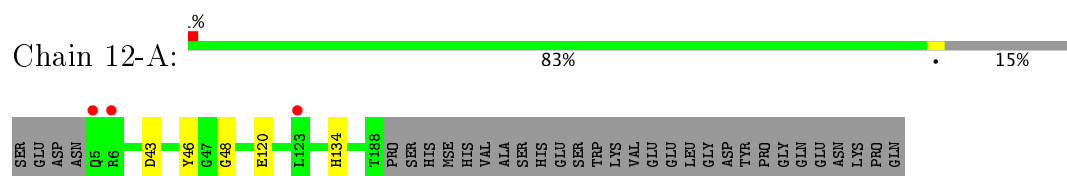
- Molecule 1: Lysine decarboxylase-like protein At5g11950



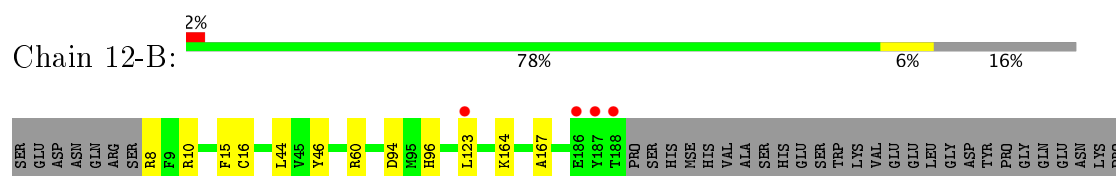
- Molecule 1: Lysine decarboxylase-like protein At5g11950



- Molecule 1: Lysine decarboxylase-like protein At5g11950

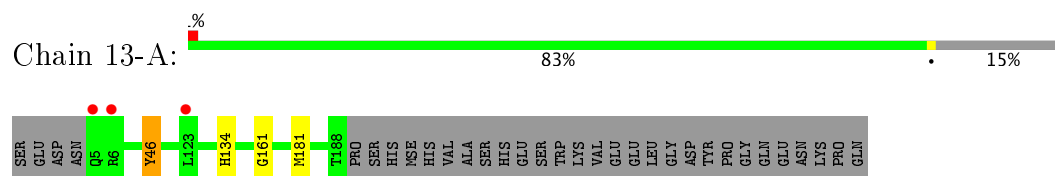


- Molecule 1: Lysine decarboxylase-like protein At5g11950

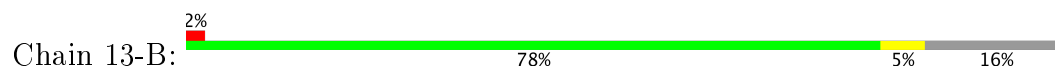


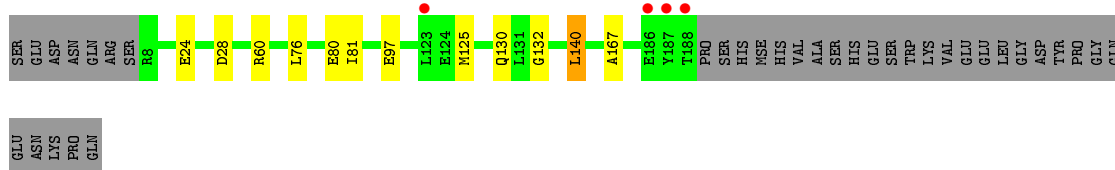
GLN

- Molecule 1: Lysine decarboxylase-like protein At5g11950

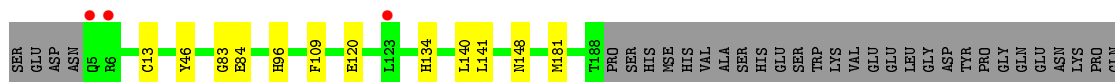
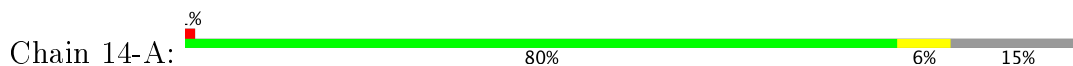


- Molecule 1: Lysine decarboxylase-like protein At5g11950

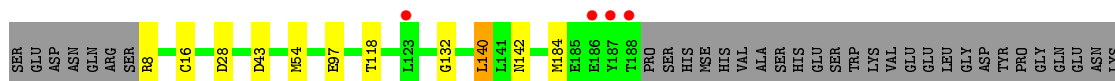
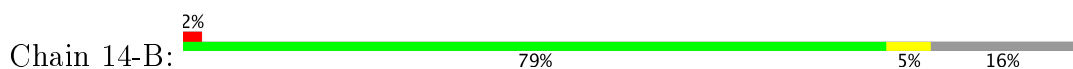




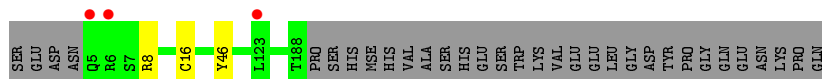
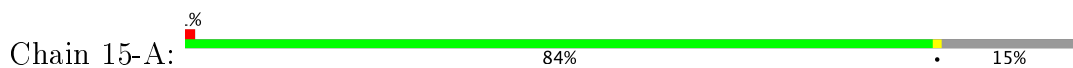
- Molecule 1: Lysine decarboxylase-like protein At5g11950



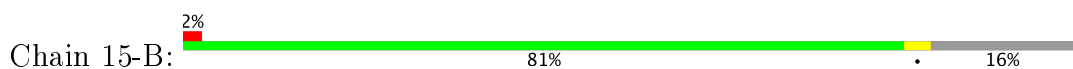
- Molecule 1: Lysine decarboxylase-like protein At5g11950



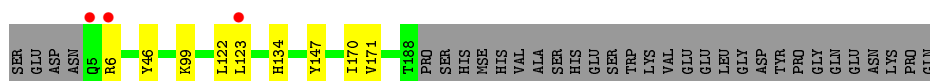
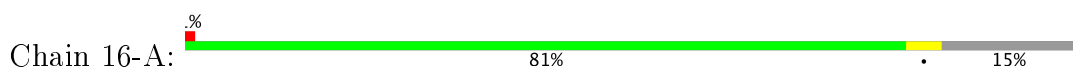
- Molecule 1: Lysine decarboxylase-like protein At5g11950



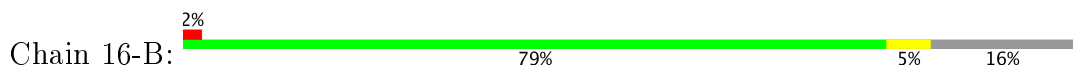
- Molecule 1: Lysine decarboxylase-like protein At5g11950

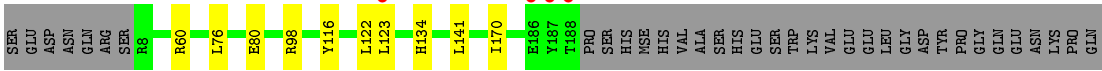


- Molecule 1: Lysine decarboxylase-like protein At5g11950



- Molecule 1: Lysine decarboxylase-like protein At5g11950





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.59Å 80.43Å 50.71Å 90.00° 102.97° 90.00°	Depositor
Resolution (Å)	34.35 – 2.15 35.45 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.35-2.15) 99.1 (35.45-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.152 , 0.207 0.170 , 0.221	Depositor DCC
$R_{free}$ test set	1300 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 72.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	50160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: EDO, NO3

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	1-A	0.34	0/1426	0.53	0/1905
1	1-B	0.34	0/1400	0.54	0/1871
1	2-A	0.33	0/1426	0.55	0/1905
1	2-B	0.34	0/1400	0.54	0/1871
1	3-A	0.34	0/1426	0.54	0/1905
1	3-B	0.34	0/1400	0.54	0/1871
1	4-A	0.33	0/1426	0.54	0/1905
1	4-B	0.34	0/1400	0.54	0/1871
1	5-A	0.35	0/1426	0.54	0/1905
1	5-B	0.34	0/1400	0.54	0/1871
1	6-A	0.34	0/1426	0.54	0/1905
1	6-B	0.34	0/1400	0.55	0/1871
1	7-A	0.34	0/1426	0.54	0/1905
1	7-B	0.35	0/1400	0.54	0/1871
1	8-A	0.34	0/1426	0.54	0/1905
1	8-B	0.35	0/1400	0.55	0/1871
1	9-A	0.35	0/1426	0.56	0/1905
1	9-B	0.34	0/1400	0.55	0/1871
1	10-A	0.35	0/1426	0.53	0/1905
1	10-B	0.34	0/1400	0.55	0/1871
1	11-A	0.34	0/1426	0.54	0/1905
1	11-B	0.34	0/1400	0.54	0/1871
1	12-A	0.33	0/1426	0.54	0/1905
1	12-B	0.34	0/1400	0.55	0/1871
1	13-A	0.38	0/1426	0.62	0/1905
1	13-B	0.38	0/1400	0.62	2/1871 (0.1%)
1	14-A	0.39	0/1426	0.59	0/1905
1	14-B	0.38	0/1400	0.63	1/1871 (0.1%)
1	15-A	0.38	0/1426	0.61	0/1905
1	15-B	0.37	0/1400	0.62	1/1871 (0.1%)
1	16-A	0.38	0/1426	0.61	0/1905
1	16-B	0.38	0/1400	0.60	0/1871

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.35	0/45216	0.56	4/60416 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	13-B	140	LEU	CA-CB-CG	6.08	129.29	115.30
1	15-B	140	LEU	CA-CB-CG	5.83	128.71	115.30
1	14-B	140	LEU	CA-CB-CG	5.44	127.81	115.30
1	13-B	60	ARG	NE-CZ-NH1	-5.01	117.80	120.30

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	1-A	1411	0	1430	0	0
1	1-B	1385	0	1404	0	0
1	2-A	1411	0	1430	0	0
1	2-B	1385	0	1404	0	0
1	3-A	1411	0	1430	0	0
1	3-B	1385	0	1404	0	0
1	4-A	1411	0	1430	0	0
1	4-B	1385	0	1404	0	0
1	5-A	1411	0	1430	0	0
1	5-B	1385	0	1404	0	0
1	6-A	1411	0	1430	0	0
1	6-B	1385	0	1404	0	0
1	7-A	1411	0	1430	0	0
1	7-B	1385	0	1404	0	0
1	8-A	1411	0	1430	0	0
1	8-B	1385	0	1404	0	0
1	9-A	1411	0	1430	0	0
1	9-B	1385	0	1404	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10-A	1411	0	1430	0	0
1	10-B	1385	0	1404	0	0
1	11-A	1411	0	1430	0	0
1	11-B	1385	0	1404	0	0
1	12-A	1411	0	1430	0	0
1	12-B	1385	0	1404	0	0
1	13-A	1411	0	1430	0	0
1	13-B	1385	0	1404	0	0
1	14-A	1411	0	1430	0	0
1	14-B	1385	0	1404	0	0
1	15-A	1411	0	1430	0	0
1	15-B	1385	0	1404	0	0
1	16-A	1411	0	1430	0	0
1	16-B	1385	0	1404	0	0
2	1-A	4	0	0	0	0
2	2-A	4	0	0	0	0
2	3-A	4	0	0	0	0
2	4-A	4	0	0	0	0
2	5-A	4	0	0	0	0
2	6-A	4	0	0	0	0
2	7-A	4	0	0	0	0
2	8-A	4	0	0	0	0
2	9-A	4	0	0	0	0
2	10-A	4	0	0	0	0
2	11-A	4	0	0	0	0
2	12-A	4	0	0	0	0
2	13-A	4	0	0	0	0
2	14-A	4	0	0	0	0
2	15-A	4	0	0	0	0
2	16-A	4	0	0	0	0
3	1-A	8	0	12	0	0
3	1-B	8	0	12	0	0
3	2-A	8	0	12	0	0
3	2-B	8	0	12	0	0
3	3-A	8	0	12	0	0
3	3-B	8	0	12	0	0
3	4-A	8	0	12	0	0
3	4-B	8	0	12	0	0
3	5-A	8	0	12	0	0
3	5-B	8	0	12	0	0
3	6-A	8	0	12	0	0
3	6-B	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7-A	8	0	12	0	0
3	7-B	8	0	12	0	0
3	8-A	8	0	12	0	0
3	8-B	8	0	12	0	0
3	9-A	8	0	12	0	0
3	9-B	8	0	12	0	0
3	10-A	8	0	12	0	0
3	10-B	8	0	12	0	0
3	11-A	8	0	12	0	0
3	11-B	8	0	12	0	0
3	12-A	8	0	12	0	0
3	12-B	8	0	12	0	0
3	13-A	8	0	12	0	0
3	13-B	8	0	12	0	0
3	14-A	8	0	12	0	0
3	14-B	8	0	12	0	0
3	15-A	8	0	12	0	0
3	15-B	8	0	12	0	0
3	16-A	8	0	12	0	0
3	16-B	8	0	12	0	0
4	1-A	155	0	0	0	0
4	1-B	164	0	0	0	0
4	2-A	155	0	0	0	0
4	2-B	164	0	0	0	0
4	3-A	157	0	0	0	0
4	3-B	162	0	0	0	0
4	4-A	155	0	0	0	0
4	4-B	164	0	0	0	0
4	5-A	162	0	0	0	0
4	5-B	157	0	0	0	0
4	6-A	153	0	0	0	0
4	6-B	166	0	0	0	0
4	7-A	159	0	0	0	0
4	7-B	160	0	0	0	0
4	8-A	158	0	0	0	0
4	8-B	161	0	0	0	0
4	9-A	162	0	0	0	0
4	9-B	157	0	0	0	0
4	10-A	151	0	0	0	0
4	10-B	168	0	0	0	0
4	11-A	151	0	0	0	0
4	11-B	168	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	12-A	152	0	0	0	0
4	12-B	167	0	0	0	0
4	13-A	155	0	0	0	0
4	13-B	164	0	0	0	0
4	14-A	154	0	0	0	0
4	14-B	165	0	0	0	0
4	15-A	155	0	0	0	0
4	15-B	164	0	0	0	0
4	16-A	158	0	0	0	0
4	16-B	161	0	0	0	0
All	All	50160	0	45728	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	182/216 (84%)	169 (93%)	12 (7%)	1 (0%)	32	25
1	1-B	179/216 (83%)	162 (90%)	17 (10%)	0	100	100
1	2-A	182/216 (84%)	168 (92%)	12 (7%)	2 (1%)	17	9
1	2-B	179/216 (83%)	175 (98%)	4 (2%)	0	100	100
1	3-A	182/216 (84%)	170 (93%)	11 (6%)	1 (0%)	32	25
1	3-B	179/216 (83%)	170 (95%)	9 (5%)	0	100	100
1	4-A	182/216 (84%)	174 (96%)	8 (4%)	0	100	100
1	4-B	179/216 (83%)	170 (95%)	9 (5%)	0	100	100
1	5-A	182/216 (84%)	166 (91%)	16 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-B	179/216 (83%)	166 (93%)	9 (5%)	4 (2%)	8	2
1	6-A	182/216 (84%)	171 (94%)	9 (5%)	2 (1%)	17	9
1	6-B	179/216 (83%)	169 (94%)	8 (4%)	2 (1%)	17	9
1	7-A	182/216 (84%)	167 (92%)	13 (7%)	2 (1%)	17	9
1	7-B	179/216 (83%)	168 (94%)	11 (6%)	0	100	100
1	8-A	182/216 (84%)	170 (93%)	11 (6%)	1 (0%)	32	25
1	8-B	179/216 (83%)	162 (90%)	16 (9%)	1 (1%)	28	20
1	9-A	182/216 (84%)	171 (94%)	9 (5%)	2 (1%)	17	9
1	9-B	179/216 (83%)	169 (94%)	10 (6%)	0	100	100
1	10-A	182/216 (84%)	167 (92%)	14 (8%)	1 (0%)	32	25
1	10-B	179/216 (83%)	161 (90%)	17 (10%)	1 (1%)	28	20
1	11-A	182/216 (84%)	169 (93%)	12 (7%)	1 (0%)	32	25
1	11-B	179/216 (83%)	160 (89%)	14 (8%)	5 (3%)	6	1
1	12-A	182/216 (84%)	173 (95%)	8 (4%)	1 (0%)	32	25
1	12-B	179/216 (83%)	157 (88%)	19 (11%)	3 (2%)	11	4
1	13-A	182/216 (84%)	163 (90%)	17 (9%)	2 (1%)	17	9
1	13-B	179/216 (83%)	158 (88%)	17 (10%)	4 (2%)	8	2
1	14-A	182/216 (84%)	165 (91%)	14 (8%)	3 (2%)	11	4
1	14-B	179/216 (83%)	157 (88%)	19 (11%)	3 (2%)	11	4
1	15-A	182/216 (84%)	177 (97%)	4 (2%)	1 (0%)	32	25
1	15-B	179/216 (83%)	174 (97%)	5 (3%)	0	100	100
1	16-A	182/216 (84%)	165 (91%)	11 (6%)	6 (3%)	4	1
1	16-B	179/216 (83%)	155 (87%)	21 (12%)	3 (2%)	11	4
All	All	5776/6912 (84%)	5338 (92%)	386 (7%)	52 (1%)	20	12

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	5-B	142	ASN
1	6-B	143	VAL
1	8-B	143	VAL
1	11-B	46	TYR
1	14-A	148	ASN

### 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	1-A	148/168 (88%)	145 (98%)	3 (2%)	60	64
1	1-B	145/168 (86%)	142 (98%)	3 (2%)	59	62
1	2-A	148/168 (88%)	144 (97%)	4 (3%)	50	51
1	2-B	145/168 (86%)	142 (98%)	3 (2%)	59	62
1	3-A	148/168 (88%)	144 (97%)	4 (3%)	50	51
1	3-B	145/168 (86%)	143 (99%)	2 (1%)	71	77
1	4-A	148/168 (88%)	146 (99%)	2 (1%)	71	77
1	4-B	145/168 (86%)	141 (97%)	4 (3%)	49	49
1	5-A	148/168 (88%)	145 (98%)	3 (2%)	60	64
1	5-B	145/168 (86%)	140 (97%)	5 (3%)	42	40
1	6-A	148/168 (88%)	144 (97%)	4 (3%)	50	51
1	6-B	145/168 (86%)	143 (99%)	2 (1%)	71	77
1	7-A	148/168 (88%)	144 (97%)	4 (3%)	50	51
1	7-B	145/168 (86%)	142 (98%)	3 (2%)	59	62
1	8-A	148/168 (88%)	146 (99%)	2 (1%)	71	77
1	8-B	145/168 (86%)	140 (97%)	5 (3%)	42	40
1	9-A	148/168 (88%)	143 (97%)	5 (3%)	42	40
1	9-B	145/168 (86%)	143 (99%)	2 (1%)	71	77
1	10-A	148/168 (88%)	141 (95%)	7 (5%)	30	26
1	10-B	145/168 (86%)	141 (97%)	4 (3%)	49	49
1	11-A	148/168 (88%)	147 (99%)	1 (1%)	87	91
1	11-B	145/168 (86%)	141 (97%)	4 (3%)	49	49
1	12-A	148/168 (88%)	144 (97%)	4 (3%)	50	51
1	12-B	145/168 (86%)	136 (94%)	9 (6%)	21	15
1	13-A	148/168 (88%)	145 (98%)	3 (2%)	60	64
1	13-B	145/168 (86%)	138 (95%)	7 (5%)	30	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	14-A	148/168 (88%)	139 (94%)	9 (6%)	22	16
1	14-B	145/168 (86%)	137 (94%)	8 (6%)	25	19
1	15-A	148/168 (88%)	146 (99%)	2 (1%)	71	77
1	15-B	145/168 (86%)	138 (95%)	7 (5%)	30	25
1	16-A	148/168 (88%)	145 (98%)	3 (2%)	60	64
1	16-B	145/168 (86%)	138 (95%)	7 (5%)	30	25
All	All	4688/5376 (87%)	4553 (97%)	135 (3%)	48	46

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	10-A	46	TYR
1	11-B	134	HIS
1	15-B	184	MSE
1	10-A	60	ARG
1	10-B	104	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	7-B	134	HIS
1	9-A	169	ASN
1	15-B	104	GLN
1	8-A	19	HIS
1	8-B	19	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

80 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	NO3	1-A	600	-	1,3,3	0.41	0	0,3,3	0.00	-
3	EDO	1-A	701	-	3,3,3	0.33	0	2,2,2	0.41	0
3	EDO	1-A	993	-	3,3,3	0.32	0	2,2,2	0.42	0
3	EDO	1-B	700	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	1-B	702	-	3,3,3	0.57	0	2,2,2	0.27	0
2	NO3	10-A	600	-	1,3,3	0.45	0	0,3,3	0.00	-
3	EDO	10-A	700	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	10-A	701	-	3,3,3	0.40	0	2,2,2	0.36	0
3	EDO	10-B	702	-	3,3,3	0.56	0	2,2,2	0.27	0
3	EDO	10-B	993	-	3,3,3	0.31	0	2,2,2	0.43	0
2	NO3	11-A	600	-	1,3,3	0.46	0	0,3,3	0.00	-
3	EDO	11-A	700	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	11-A	701	-	3,3,3	0.35	0	2,2,2	0.39	0
3	EDO	11-B	702	-	3,3,3	0.57	0	2,2,2	0.27	0
3	EDO	11-B	993	-	3,3,3	0.30	0	2,2,2	0.49	0
2	NO3	12-A	600	-	1,3,3	0.47	0	0,3,3	0.00	-
3	EDO	12-A	700	-	3,3,3	0.48	0	2,2,2	0.28	0
3	EDO	12-A	701	-	3,3,3	0.36	0	2,2,2	0.38	0
3	EDO	12-B	702	-	3,3,3	0.56	0	2,2,2	0.29	0
3	EDO	12-B	993	-	3,3,3	0.31	0	2,2,2	0.46	0
2	NO3	13-A	600	-	1,3,3	0.40	0	0,3,3	0.00	-
3	EDO	13-A	700	-	3,3,3	0.49	0	2,2,2	0.26	0
3	EDO	13-A	701	-	3,3,3	0.32	0	2,2,2	0.43	0
3	EDO	13-B	702	-	3,3,3	0.59	0	2,2,2	0.21	0
3	EDO	13-B	993	-	3,3,3	0.29	0	2,2,2	0.43	0
2	NO3	14-A	600	-	1,3,3	0.45	0	0,3,3	0.00	-
3	EDO	14-A	700	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	14-A	701	-	3,3,3	0.33	0	2,2,2	0.40	0
3	EDO	14-B	702	-	3,3,3	0.59	0	2,2,2	0.26	0
3	EDO	14-B	993	-	3,3,3	0.30	0	2,2,2	0.37	0
2	NO3	15-A	600	-	1,3,3	0.48	0	0,3,3	0.00	-
3	EDO	15-A	700	-	3,3,3	0.48	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	15-A	701	-	3,3,3	0.33	0	2,2,2	0.40	0
3	EDO	15-B	702	-	3,3,3	0.59	0	2,2,2	0.26	0
3	EDO	15-B	993	-	3,3,3	0.29	0	2,2,2	0.33	0
2	NO3	16-A	600	-	1,3,3	0.45	0	0,3,3	0.00	-
3	EDO	16-A	700	-	3,3,3	0.42	0	2,2,2	0.35	0
3	EDO	16-A	701	-	3,3,3	0.34	0	2,2,2	0.38	0
3	EDO	16-B	702	-	3,3,3	0.58	0	2,2,2	0.25	0
3	EDO	16-B	993	-	3,3,3	0.29	0	2,2,2	0.37	0
2	NO3	2-A	600	-	1,3,3	0.45	0	0,3,3	0.00	-
3	EDO	2-A	700	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	2-A	701	-	3,3,3	0.34	0	2,2,2	0.41	0
3	EDO	2-B	702	-	3,3,3	0.57	0	2,2,2	0.29	0
3	EDO	2-B	993	-	3,3,3	0.30	0	2,2,2	0.39	0
2	NO3	3-A	600	-	1,3,3	0.44	0	0,3,3	0.00	-
3	EDO	3-A	700	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	3-A	701	-	3,3,3	0.31	0	2,2,2	0.40	0
3	EDO	3-B	702	-	3,3,3	0.56	0	2,2,2	0.28	0
3	EDO	3-B	993	-	3,3,3	0.30	0	2,2,2	0.42	0
2	NO3	4-A	600	-	1,3,3	0.47	0	0,3,3	0.00	-
3	EDO	4-A	700	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	4-A	701	-	3,3,3	0.40	0	2,2,2	0.33	0
3	EDO	4-B	702	-	3,3,3	0.57	0	2,2,2	0.28	0
3	EDO	4-B	993	-	3,3,3	0.30	0	2,2,2	0.44	0
2	NO3	5-A	600	-	1,3,3	0.50	0	0,3,3	0.00	-
3	EDO	5-A	700	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	5-A	701	-	3,3,3	0.31	0	2,2,2	0.40	0
3	EDO	5-B	702	-	3,3,3	0.55	0	2,2,2	0.29	0
3	EDO	5-B	993	-	3,3,3	0.39	0	2,2,2	0.36	0
2	NO3	6-A	600	-	1,3,3	0.46	0	0,3,3	0.00	-
3	EDO	6-A	700	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	6-A	701	-	3,3,3	0.34	0	2,2,2	0.39	0
3	EDO	6-B	702	-	3,3,3	0.57	0	2,2,2	0.27	0
3	EDO	6-B	993	-	3,3,3	0.29	0	2,2,2	0.44	0
2	NO3	7-A	600	-	1,3,3	0.48	0	0,3,3	0.00	-
3	EDO	7-A	700	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	7-A	701	-	3,3,3	0.34	0	2,2,2	0.39	0
3	EDO	7-B	702	-	3,3,3	0.56	0	2,2,2	0.27	0
3	EDO	7-B	993	-	3,3,3	0.30	0	2,2,2	0.44	0
2	NO3	8-A	600	-	1,3,3	0.49	0	0,3,3	0.00	-
3	EDO	8-A	700	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	8-A	701	-	3,3,3	0.31	0	2,2,2	0.42	0
3	EDO	8-B	702	-	3,3,3	0.57	0	2,2,2	0.28	0
3	EDO	8-B	993	-	3,3,3	0.30	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NO3	9-A	600	-	1,3,3	0.45	0	0,3,3	0.00	-
3	EDO	9-A	700	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	9-A	701	-	3,3,3	0.33	0	2,2,2	0.39	0
3	EDO	9-B	702	-	3,3,3	0.56	0	2,2,2	0.24	0
3	EDO	9-B	993	-	3,3,3	0.32	0	2,2,2	0.40	0

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	NO3	1-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	1-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	993	-	-	0/1/1/1	0/0/0/0
3	EDO	1-B	700	-	-	0/1/1/1	0/0/0/0
3	EDO	1-B	702	-	-	0/1/1/1	0/0/0/0
2	NO3	10-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	10-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	10-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	10-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	11-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	11-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	11-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	11-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	12-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	12-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	12-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	12-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	13-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	13-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	13-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	13-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	14-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	14-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	14-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	14-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	15-A	600	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	15-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	15-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	15-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	16-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	16-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	16-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	16-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	2-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	2-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	2-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	2-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	3-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	3-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	3-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	3-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	4-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	4-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	4-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	4-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	5-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	5-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	5-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	5-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	6-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	6-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	6-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	6-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	7-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	7-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	7-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	7-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	8-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	8-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	701	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	8-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	8-B	993	-	-	0/1/1/1	0/0/0/0
2	NO3	9-A	600	-	-	0/0/0/0	0/0/0/0
3	EDO	9-A	700	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	701	-	-	0/1/1/1	0/0/0/0
3	EDO	9-B	702	-	-	0/1/1/1	0/0/0/0
3	EDO	9-B	993	-	-	0/1/1/1	0/0/0/0

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

### 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	1-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	1-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	2-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	2-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	3-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	3-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	4-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	4-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	5-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	5-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	6-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	6-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	7-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	7-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	8-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	8-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	9-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	9-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	10-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	10-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	11-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	11-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)
1	12-A	176/216 (81%)	-0.10	3 (1%) 70 76	12, 23, 39, 71	176 (100%)
1	12-B	173/216 (80%)	-0.07	4 (2%) 61 68	12, 23, 36, 62	173 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	13-A	176/216 (81%)	-0.10	3 (1%)	70	76	12, 23, 39, 71	176 (100%)
1	13-B	173/216 (80%)	-0.07	4 (2%)	61	68	12, 23, 36, 62	173 (100%)
1	14-A	176/216 (81%)	-0.10	3 (1%)	70	76	12, 23, 39, 71	176 (100%)
1	14-B	173/216 (80%)	-0.07	4 (2%)	61	68	12, 23, 36, 62	173 (100%)
1	15-A	176/216 (81%)	-0.10	3 (1%)	70	76	12, 23, 39, 71	176 (100%)
1	15-B	173/216 (80%)	-0.07	4 (2%)	61	68	12, 23, 36, 62	173 (100%)
1	16-A	176/216 (81%)	-0.10	3 (1%)	70	76	12, 23, 39, 71	176 (100%)
1	16-B	173/216 (80%)	-0.07	4 (2%)	61	68	12, 23, 36, 62	173 (100%)
All	All	5584/6912 (80%)	-0.09	112 (2%)	49	72	12, 24, 38, 71	5584 (100%)

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	188	THR	3.5
1	2-B	188	THR	3.5
1	3-B	188	THR	3.5
1	4-B	188	THR	3.5
1	5-B	188	THR	3.5

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	11-A	701	4/4	0.92	0.30	10.53	47,47,48,50	4
3	EDO	3-A	701	4/4	0.92	0.30	10.53	46,46,47,49	4
3	EDO	2-A	701	4/4	0.92	0.30	10.53	40,42,42,46	4
3	EDO	10-A	701	4/4	0.92	0.30	10.53	43,43,44,44	4
3	EDO	13-A	701	4/4	0.92	0.30	10.53	44,44,45,48	4
3	EDO	16-A	701	4/4	0.92	0.30	10.53	47,48,48,51	4
3	EDO	12-A	701	4/4	0.92	0.30	10.53	47,47,48,49	4
3	EDO	1-A	701	4/4	0.92	0.30	10.53	44,44,44,48	4
3	EDO	15-A	701	4/4	0.92	0.30	10.53	48,49,49,51	4
3	EDO	4-A	701	4/4	0.92	0.30	10.53	37,38,38,38	4
3	EDO	9-A	701	4/4	0.92	0.30	10.53	45,45,45,48	4
3	EDO	6-A	701	4/4	0.92	0.30	10.53	43,43,44,46	4
3	EDO	14-A	701	4/4	0.92	0.30	10.53	48,49,49,51	4
3	EDO	7-A	701	4/4	0.92	0.30	10.53	46,46,47,49	4
3	EDO	5-A	701	4/4	0.92	0.30	10.53	42,44,45,48	4
3	EDO	8-A	701	4/4	0.92	0.30	4.63	45,45,46,48	4
2	NO3	1-A	600	4/4	0.94	0.31	4.16	65,66,66,66	4
2	NO3	14-A	600	4/4	0.94	0.31	3.99	66,66,66,66	4
2	NO3	2-A	600	4/4	0.94	0.31	3.99	66,66,66,66	4
2	NO3	10-A	600	4/4	0.94	0.31	3.99	65,65,66,66	4
2	NO3	3-A	600	4/4	0.94	0.31	3.99	66,66,66,66	4
2	NO3	15-A	600	4/4	0.94	0.31	3.99	66,66,66,67	4
2	NO3	11-A	600	4/4	0.94	0.31	3.99	66,66,66,66	4
2	NO3	12-A	600	4/4	0.94	0.31	3.99	66,66,66,66	4
2	NO3	16-A	600	4/4	0.94	0.31	3.99	66,66,66,67	4
2	NO3	5-A	600	4/4	0.94	0.31	3.89	66,66,66,66	4
2	NO3	13-A	600	4/4	0.94	0.31	3.85	65,65,65,66	4
2	NO3	8-A	600	4/4	0.94	0.31	3.84	65,65,65,66	4
3	EDO	8-B	993	4/4	0.94	0.21	3.46	43,44,44,50	4
3	EDO	12-B	993	4/4	0.94	0.21	3.46	42,43,44,50	4
3	EDO	6-B	993	4/4	0.94	0.21	3.36	44,45,45,50	4
3	EDO	16-B	993	4/4	0.94	0.21	3.36	42,43,45,52	4
3	EDO	4-B	993	4/4	0.94	0.21	3.36	43,44,44,50	4
3	EDO	9-B	993	4/4	0.94	0.21	3.36	43,44,44,50	4
3	EDO	2-B	993	4/4	0.94	0.21	3.36	42,43,44,50	4
3	EDO	11-B	993	4/4	0.94	0.21	3.36	42,43,44,50	4
3	EDO	7-B	993	4/4	0.94	0.21	3.36	43,44,44,50	4
3	EDO	3-B	993	4/4	0.94	0.21	3.36	43,44,44,50	4
3	EDO	10-B	993	4/4	0.94	0.21	3.34	42,43,44,50	4
3	EDO	15-B	993	4/4	0.94	0.21	3.17	43,44,45,51	4
3	EDO	14-B	993	4/4	0.94	0.21	3.17	43,43,45,51	4
3	EDO	13-B	993	4/4	0.94	0.21	3.17	43,44,45,52	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	1-A	993	4/4	0.93	0.20	2.83	43,43,43,50	4
3	EDO	5-B	993	4/4	0.94	0.21	2.71	38,40,41,46	4
3	EDO	16-A	700	4/4	0.94	0.15	1.59	54,54,54,55	4
3	EDO	12-A	700	4/4	0.94	0.15	1.59	52,54,54,54	4
3	EDO	15-A	700	4/4	0.94	0.15	1.59	53,54,55,55	4
3	EDO	12-B	702	4/4	0.84	0.15	0.31	45,48,48,48	4
3	EDO	15-B	702	4/4	0.84	0.15	0.31	44,47,49,49	4
3	EDO	11-B	702	4/4	0.84	0.15	0.25	43,47,48,48	4
3	EDO	2-B	702	4/4	0.84	0.15	0.25	44,47,48,48	4
3	EDO	14-B	702	4/4	0.84	0.15	0.25	44,47,49,49	4
3	EDO	4-B	702	4/4	0.84	0.15	0.25	44,47,48,48	4
3	EDO	5-B	702	4/4	0.84	0.15	0.04	46,47,48,49	4
3	EDO	8-B	702	4/4	0.84	0.15	0.04	44,47,48,48	4
3	EDO	13-B	702	4/4	0.84	0.15	0.04	44,48,48,49	4
3	EDO	1-B	702	4/4	0.84	0.15	-0.02	44,47,48,48	4
3	EDO	9-B	702	4/4	0.84	0.15	-0.02	44,47,48,48	4
3	EDO	7-B	702	4/4	0.84	0.15	-0.02	44,48,48,48	4
3	EDO	10-B	702	4/4	0.84	0.15	-0.02	44,47,48,48	4
3	EDO	6-B	702	4/4	0.84	0.15	-0.02	44,47,48,48	4
3	EDO	3-B	702	4/4	0.84	0.15	-0.24	44,47,48,48	4
3	EDO	16-B	702	4/4	0.84	0.15	-0.24	44,48,48,48	4
3	EDO	14-A	700	4/4	0.94	0.15	-	54,54,55,55	4
3	EDO	3-A	700	4/4	0.94	0.15	-	53,54,54,54	4
3	EDO	4-A	700	4/4	0.94	0.15	-	53,54,54,55	4
2	NO3	9-A	600	4/4	0.94	0.31	-	61,61,62,62	4
3	EDO	9-A	700	4/4	0.94	0.15	-	54,54,54,55	4
3	EDO	7-A	700	4/4	0.94	0.15	-	54,55,55,55	4
2	NO3	7-A	600	4/4	0.94	0.31	-	62,62,62,63	4
3	EDO	5-A	700	4/4	0.94	0.15	-	53,54,54,54	4
2	NO3	4-A	600	4/4	0.94	0.31	-	65,65,65,66	4
3	EDO	13-A	700	4/4	0.94	0.15	-	53,54,55,55	4
3	EDO	11-A	700	4/4	0.94	0.15	-	53,54,54,54	4
3	EDO	1-B	700	4/4	0.91	0.13	-	54,55,55,55	4
2	NO3	6-A	600	4/4	0.94	0.31	-	65,65,65,66	4
3	EDO	6-A	700	4/4	0.94	0.15	-	53,54,54,55	4
3	EDO	10-A	700	4/4	0.94	0.15	-	53,54,54,55	4
3	EDO	8-A	700	4/4	0.94	0.15	-	54,55,55,55	4
3	EDO	2-A	700	4/4	0.94	0.15	-	54,54,55,55	4

## 6.5 Other polymers ⓘ

There are no such residues in this entry.