



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:50 PM UTC

PDB ID : 2Q4D / pdb_00002q4d
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 : 2007-05-31
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

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>.

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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

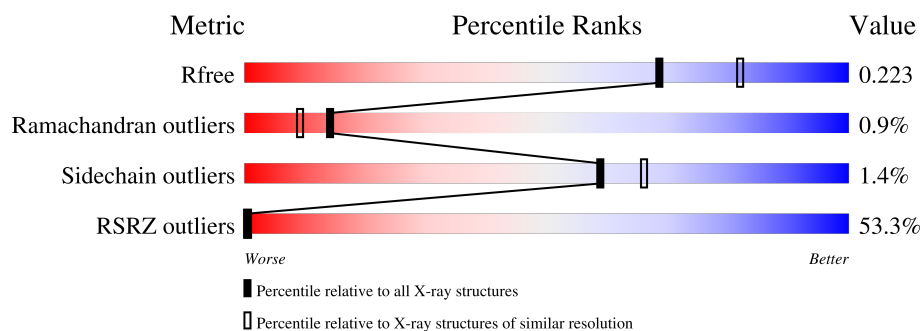
1 Overall quality at a glance

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}	180053	2057 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	216	44% 83% 15%
1	1-B	216	42% 83% 16%
1	10-A	216	83% 15%
1	10-B	216	83% 16%
1	11-A	216	83% 15%
1	11-B	216	81% 16%
1	12-A	216	83% 15%

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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	

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:

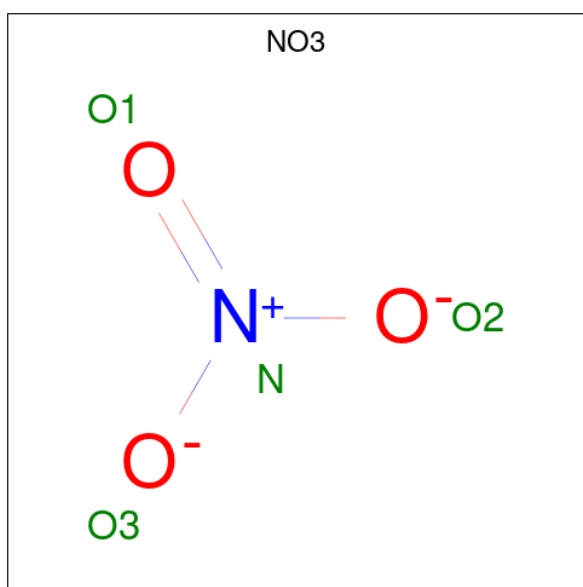
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q84MC2
A	54	MSE	MET	modified residue	UNP Q84MC2
A	77	MSE	MET	modified residue	UNP Q84MC2
A	95	MSE	MET	modified residue	UNP Q84MC2
A	102	MSE	MET	modified residue	UNP Q84MC2
A	119	MSE	MET	modified residue	UNP Q84MC2
A	125	MSE	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 (CCD ID: NO3) (formula: NO₃).



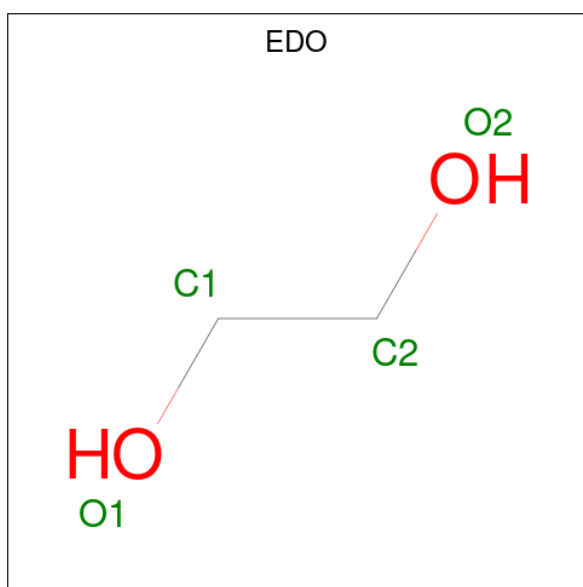
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	N	O	0	0
			4	1	3		
2	2-A	1	Total	N	O	0	0
			4	1	3		
2	3-A	1	Total	N	O	0	0
			4	1	3		
2	4-A	1	Total	N	O	0	0
			4	1	3		
2	5-A	1	Total	N	O	0	0
			4	1	3		

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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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

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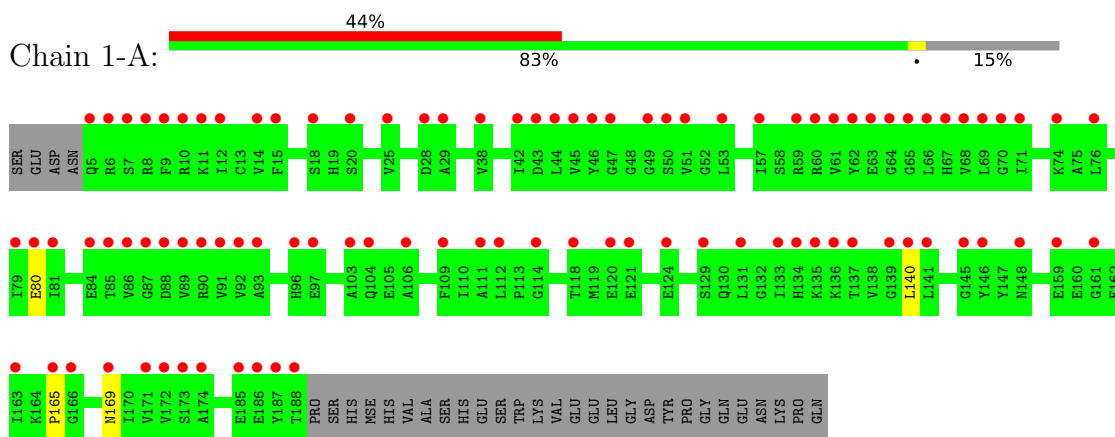
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	6-B	166	Total 166	O 166	0	0
4	7-B	160	Total 160	O 160	0	0
4	8-B	161	Total 161	O 161	0	0
4	9-B	157	Total 157	O 157	0	0
4	10-B	168	Total 168	O 168	0	0
4	11-B	168	Total 168	O 168	0	0
4	12-B	167	Total 167	O 167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

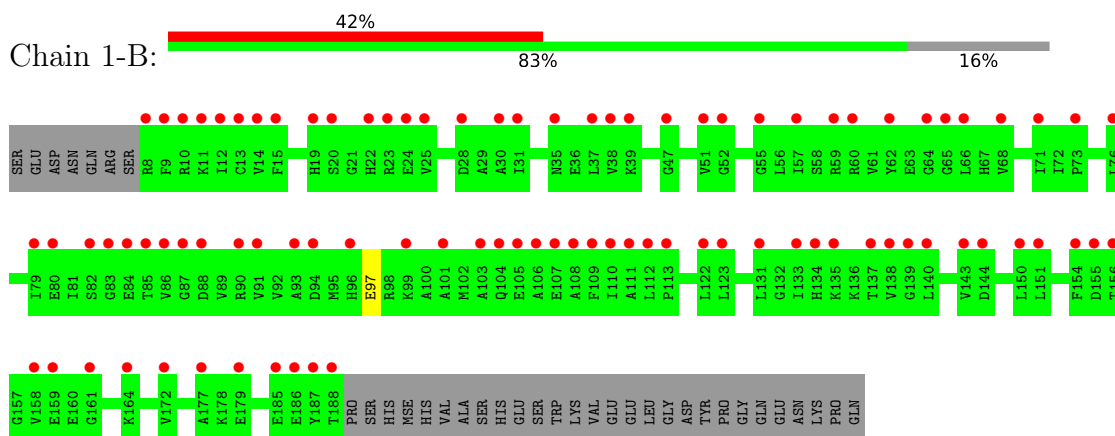
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

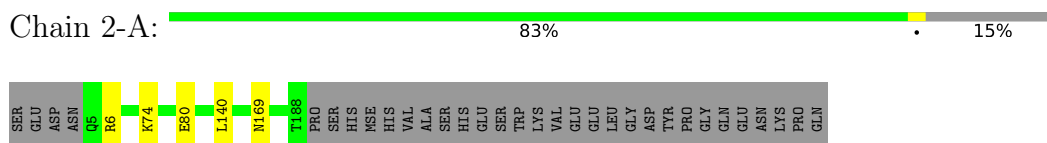
- Molecule 1: Lysine decarboxylase-like protein At5g11950



- Molecule 1: Lysine decarboxylase-like protein At5g11950

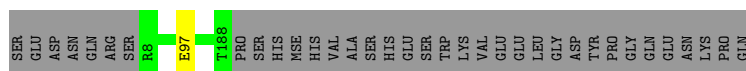


- Molecule 1: Lysine decarboxylase-like protein At5g11950



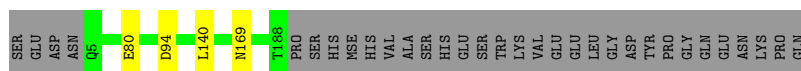
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 2-B:  83% 16%



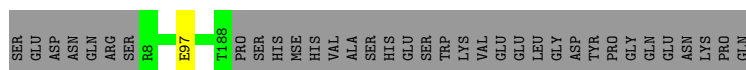
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 3-A:  83% 15%



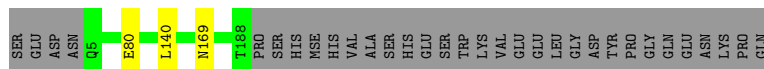
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 3-B:  83% 16%



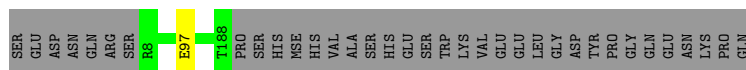
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 4-A:  84% 15%



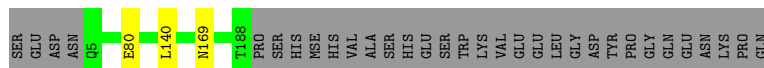
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 4-B:  83% 16%



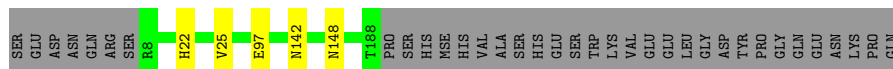
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 5-A:  84% 15%



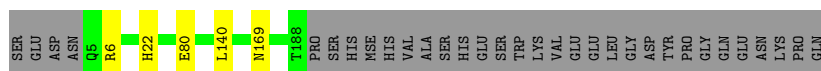
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 5-B:  81% 16%



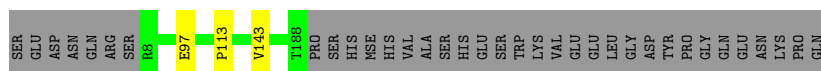
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 6-A:  83% 15%



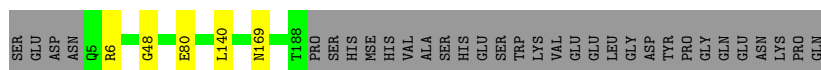
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 6-B:  82% 16%



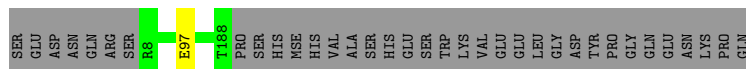
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 7-A:  83% 15%



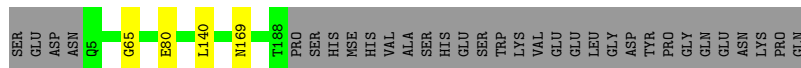
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 7-B:  83% 16%



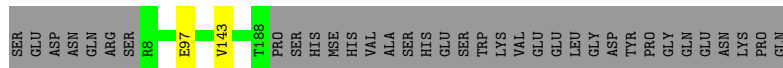
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 8-A:  83% 15%



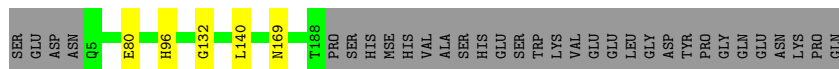
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 8-B:  83% 16%



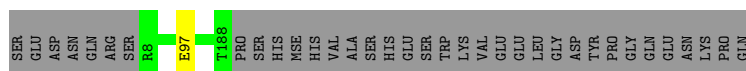
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 9-A:  83% 15%



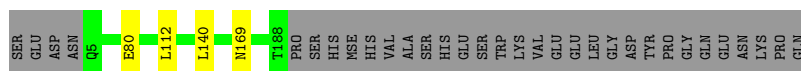
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 9-B:  83% 16%



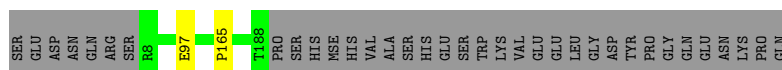
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 10-A:  83% 15%



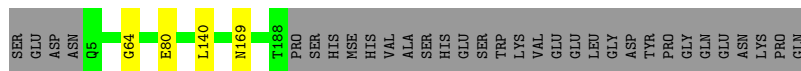
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 10-B:  83% 16%



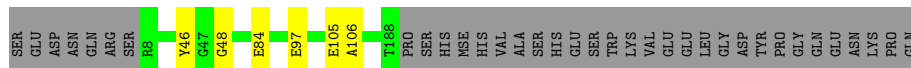
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 11-A:  83% 15%



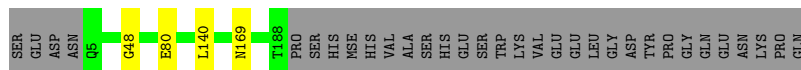
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 11-B:  81% 16%



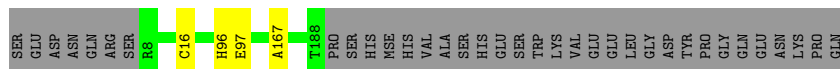
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 12-A:  83% 15%



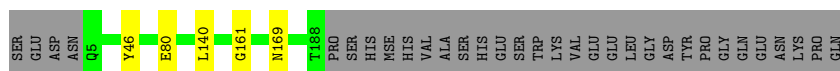
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 12-B:  82% 16%



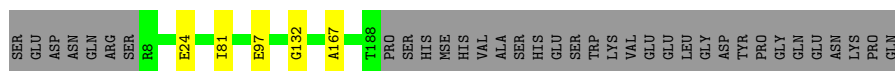
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 13-A:  83% 15%



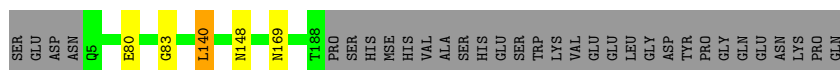
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 13-B:  81% 16%



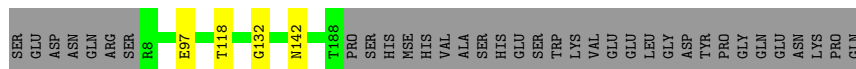
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 14-A:  83% 15%



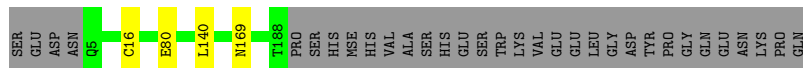
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 14-B:  82% 16%



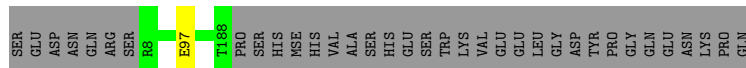
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 15-A:  83% 15%



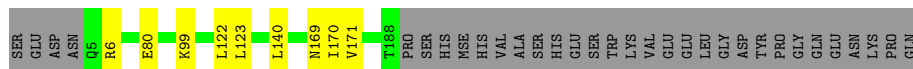
- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 15-B:  83% 16%



- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 16-A:  81% 15%



- Molecule 1: Lysine decarboxylase-like protein At5g11950

Chain 16-B:

82%

.

16%

SER	GLU	ASP	ASN	GLN	ARG	SER	R8	E97	Y116	L141	I170	T188	PRO	SER	HIS	MSE	HIS	VAL	ALA	SER	HIS	GLU	SER	TRP	LYS	VAL	GLU	GLU	LEU	GLY	ASP	TYR	PRO	GLY	GLN	GLU	ASN	LYS	PRO	GLN
-----	-----	-----	-----	-----	-----	-----	----	-----	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.59Å 80.43Å 50.71Å 90.00° 102.97° 90.00°	Depositor
Resolution (Å)	34.35 – 2.15 34.35 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.35-2.15) 99.1 (34.35-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.152 , 0.207 0.169 , 0.223	Depositor DCC
R_{free} test set	1300 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	50160	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.18	0/1426	0.35	0/1905
1	1-B	0.19	0/1400	0.36	0/1871
1	2-A	0.18	0/1426	0.35	0/1905
1	2-B	0.19	0/1400	0.36	0/1871
1	3-A	0.18	0/1426	0.35	0/1905
1	3-B	0.19	0/1400	0.36	0/1871
1	4-A	0.18	0/1426	0.35	0/1905
1	4-B	0.19	0/1400	0.36	0/1871
1	5-A	0.18	0/1426	0.35	0/1905
1	5-B	0.19	0/1400	0.36	0/1871
1	6-A	0.18	0/1426	0.35	0/1905
1	6-B	0.19	0/1400	0.36	0/1871
1	7-A	0.18	0/1426	0.35	0/1905
1	7-B	0.19	0/1400	0.36	0/1871
1	8-A	0.18	0/1426	0.35	0/1905
1	8-B	0.19	0/1400	0.36	0/1871
1	9-A	0.18	0/1426	0.35	0/1905
1	9-B	0.19	0/1400	0.36	0/1871
1	10-A	0.18	0/1426	0.35	0/1905
1	10-B	0.19	0/1400	0.36	0/1871
1	11-A	0.18	0/1426	0.35	0/1905
1	11-B	0.19	0/1400	0.36	0/1871
1	12-A	0.18	0/1426	0.35	0/1905
1	12-B	0.19	0/1400	0.36	0/1871
1	13-A	0.18	0/1426	0.35	0/1905
1	13-B	0.19	0/1400	0.36	0/1871
1	14-A	0.18	0/1426	0.35	0/1905
1	14-B	0.19	0/1400	0.36	0/1871
1	15-A	0.18	0/1426	0.35	0/1905
1	15-B	0.19	0/1400	0.36	0/1871
1	16-A	0.18	0/1426	0.35	0/1905
1	16-B	0.19	0/1400	0.36	0/1871

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.18	0/45216	0.36	0/60416

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	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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%)	24	20
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%)	11	7
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%)	24	20
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
1	5-B	179/216 (83%)	166 (93%)	9 (5%)	4 (2%)	5	1
1	6-A	182/216 (84%)	171 (94%)	9 (5%)	2 (1%)	11	7
1	6-B	179/216 (83%)	169 (94%)	8 (4%)	2 (1%)	11	7
1	7-A	182/216 (84%)	167 (92%)	13 (7%)	2 (1%)	11	7
1	7-B	179/216 (83%)	168 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-A	182/216 (84%)	170 (93%)	11 (6%)	1 (0%)	24	20
1	8-B	179/216 (83%)	162 (90%)	16 (9%)	1 (1%)	21	15
1	9-A	182/216 (84%)	171 (94%)	9 (5%)	2 (1%)	11	7
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%)	24	20
1	10-B	179/216 (83%)	161 (90%)	17 (10%)	1 (1%)	21	15
1	11-A	182/216 (84%)	169 (93%)	12 (7%)	1 (0%)	24	20
1	11-B	179/216 (83%)	160 (89%)	14 (8%)	5 (3%)	4	1
1	12-A	182/216 (84%)	173 (95%)	8 (4%)	1 (0%)	24	20
1	12-B	179/216 (83%)	157 (88%)	19 (11%)	3 (2%)	7	2
1	13-A	182/216 (84%)	163 (90%)	17 (9%)	2 (1%)	11	7
1	13-B	179/216 (83%)	158 (88%)	17 (10%)	4 (2%)	5	1
1	14-A	182/216 (84%)	165 (91%)	14 (8%)	3 (2%)	7	3
1	14-B	179/216 (83%)	157 (88%)	19 (11%)	3 (2%)	7	2
1	15-A	182/216 (84%)	177 (97%)	4 (2%)	1 (0%)	24	20
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%)	3	0
1	16-B	179/216 (83%)	155 (87%)	21 (12%)	3 (2%)	7	2
All	All	5776/6912 (84%)	5338 (92%)	386 (7%)	52 (1%)	14	9

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%)	48	54
1	1-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	2-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	2-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	3-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	3-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	4-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	4-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	5-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	5-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	6-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	6-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	7-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	7-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	8-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	8-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	9-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	9-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	10-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	10-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	11-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	11-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	12-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	12-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	13-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	13-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	14-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	14-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	15-A	148/168 (88%)	145 (98%)	3 (2%)	48	54
1	15-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
1	16-A	148/168 (88%)	145 (98%)	3 (2%)	48	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	16-B	145/168 (86%)	144 (99%)	1 (1%)	76	82
All	All	4688/5376 (87%)	4624 (99%)	64 (1%)	59	66

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	15-A	140	LEU
1	15-B	97	GLU
1	7-A	80	GLU
1	6-B	97	GLU
1	16-A	80	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
1	9-A	19	HIS
1	16-B	19	HIS
1	10-B	149	ASN
1	16-A	169	ASN
1	15-A	19	HIS

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](#)

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	$\# Z > 2$
3	EDO	11-B	702	-	3,3,3	0.53	0	2,2,2	0.30	0
3	EDO	13-A	700	-	3,3,3	0.45	0	2,2,2	0.28	0
3	EDO	7-B	702	-	3,3,3	0.53	0	2,2,2	0.30	0
2	NO3	1-A	600	-	1,3,3	0.41	0	0,3,3	-	-
3	EDO	1-A	701	-	3,3,3	0.30	0	2,2,2	0.43	0
3	EDO	1-B	702	-	3,3,3	0.54	0	2,2,2	0.29	0
3	EDO	14-B	702	-	3,3,3	0.55	0	2,2,2	0.28	0
2	NO3	9-A	600	-	1,3,3	0.45	0	0,3,3	-	-
3	EDO	3-B	702	-	3,3,3	0.53	0	2,2,2	0.30	0
3	EDO	6-A	700	-	3,3,3	0.41	0	2,2,2	0.37	0
3	EDO	9-A	701	-	3,3,3	0.30	0	2,2,2	0.41	0
3	EDO	7-A	701	-	3,3,3	0.31	0	2,2,2	0.41	0
3	EDO	11-A	701	-	3,3,3	0.32	0	2,2,2	0.41	0
3	EDO	4-A	700	-	3,3,3	0.41	0	2,2,2	0.37	0
2	NO3	13-A	600	-	1,3,3	0.40	0	0,3,3	-	-
2	NO3	16-A	600	-	1,3,3	0.45	0	0,3,3	-	-
2	NO3	4-A	600	-	1,3,3	0.46	0	0,3,3	-	-
3	EDO	12-B	993	-	3,3,3	0.29	0	2,2,2	0.47	0
2	NO3	5-A	600	-	1,3,3	0.48	0	0,3,3	-	-
3	EDO	16-A	701	-	3,3,3	0.31	0	2,2,2	0.40	0
3	EDO	15-B	702	-	3,3,3	0.56	0	2,2,2	0.28	0
3	EDO	14-B	993	-	3,3,3	0.28	0	2,2,2	0.39	0
3	EDO	8-A	701	-	3,3,3	0.29	0	2,2,2	0.43	0
3	EDO	5-A	701	-	3,3,3	0.28	0	2,2,2	0.41	0
3	EDO	10-A	700	-	3,3,3	0.42	0	2,2,2	0.36	0
2	NO3	11-A	600	-	1,3,3	0.45	0	0,3,3	-	-
3	EDO	10-B	993	-	3,3,3	0.28	0	2,2,2	0.45	0
3	EDO	13-B	993	-	3,3,3	0.27	0	2,2,2	0.45	0
3	EDO	5-B	993	-	3,3,3	0.36	0	2,2,2	0.37	0
2	NO3	7-A	600	-	1,3,3	0.47	0	0,3,3	-	-
3	EDO	4-B	993	-	3,3,3	0.28	0	2,2,2	0.45	0
3	EDO	9-B	702	-	3,3,3	0.53	0	2,2,2	0.27	0
3	EDO	11-A	700	-	3,3,3	0.39	0	2,2,2	0.38	0
2	NO3	2-A	600	-	1,3,3	0.45	0	0,3,3	-	-
3	EDO	16-B	993	-	3,3,3	0.28	0	2,2,2	0.38	0
3	EDO	10-B	702	-	3,3,3	0.53	0	2,2,2	0.30	0
3	EDO	13-B	702	-	3,3,3	0.56	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	15-B	993	-	3,3,3	0.28	0	2,2,2	0.35	0
3	EDO	12-A	701	-	3,3,3	0.33	0	2,2,2	0.40	0
2	NO3	10-A	600	-	1,3,3	0.45	0	0,3,3	-	-
3	EDO	9-A	700	-	3,3,3	0.41	0	2,2,2	0.37	0
2	NO3	8-A	600	-	1,3,3	0.48	0	0,3,3	-	-
3	EDO	10-A	701	-	3,3,3	0.37	0	2,2,2	0.38	0
3	EDO	3-A	701	-	3,3,3	0.29	0	2,2,2	0.42	0
3	EDO	8-B	702	-	3,3,3	0.53	0	2,2,2	0.30	0
3	EDO	3-B	993	-	3,3,3	0.28	0	2,2,2	0.44	0
3	EDO	2-B	993	-	3,3,3	0.29	0	2,2,2	0.41	0
3	EDO	15-A	700	-	3,3,3	0.44	0	2,2,2	0.31	0
3	EDO	7-A	700	-	3,3,3	0.41	0	2,2,2	0.37	0
2	NO3	14-A	600	-	1,3,3	0.44	0	0,3,3	-	-
3	EDO	2-A	701	-	3,3,3	0.31	0	2,2,2	0.42	0
3	EDO	2-A	700	-	3,3,3	0.41	0	2,2,2	0.36	0
3	EDO	12-B	702	-	3,3,3	0.53	0	2,2,2	0.32	0
3	EDO	11-B	993	-	3,3,3	0.28	0	2,2,2	0.50	0
3	EDO	4-A	701	-	3,3,3	0.38	0	2,2,2	0.35	0
3	EDO	6-B	702	-	3,3,3	0.54	0	2,2,2	0.29	0
2	NO3	3-A	600	-	1,3,3	0.44	0	0,3,3	-	-
3	EDO	1-B	700	-	3,3,3	0.41	0	2,2,2	0.38	0
2	NO3	12-A	600	-	1,3,3	0.46	0	0,3,3	-	-
3	EDO	9-B	993	-	3,3,3	0.30	0	2,2,2	0.42	0
3	EDO	1-A	993	-	3,3,3	0.30	0	2,2,2	0.43	0
3	EDO	2-B	702	-	3,3,3	0.54	0	2,2,2	0.31	0
3	EDO	14-A	701	-	3,3,3	0.30	0	2,2,2	0.42	0
3	EDO	7-B	993	-	3,3,3	0.28	0	2,2,2	0.45	0
3	EDO	3-A	700	-	3,3,3	0.42	0	2,2,2	0.35	0
3	EDO	4-B	702	-	3,3,3	0.54	0	2,2,2	0.31	0
3	EDO	6-A	701	-	3,3,3	0.31	0	2,2,2	0.41	0
2	NO3	6-A	600	-	1,3,3	0.45	0	0,3,3	-	-
3	EDO	16-A	700	-	3,3,3	0.39	0	2,2,2	0.37	0
3	EDO	14-A	700	-	3,3,3	0.41	0	2,2,2	0.38	0
2	NO3	15-A	600	-	1,3,3	0.47	0	0,3,3	-	-
3	EDO	16-B	702	-	3,3,3	0.55	0	2,2,2	0.27	0
3	EDO	12-A	700	-	3,3,3	0.44	0	2,2,2	0.30	0
3	EDO	15-A	701	-	3,3,3	0.31	0	2,2,2	0.42	0
3	EDO	5-A	700	-	3,3,3	0.42	0	2,2,2	0.35	0
3	EDO	6-B	993	-	3,3,3	0.28	0	2,2,2	0.45	0
3	EDO	8-B	993	-	3,3,3	0.28	0	2,2,2	0.46	0
3	EDO	8-A	700	-	3,3,3	0.40	0	2,2,2	0.38	0
3	EDO	5-B	702	-	3,3,3	0.52	0	2,2,2	0.31	0
3	EDO	13-A	701	-	3,3,3	0.30	0	2,2,2	0.44	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
3	EDO	7-B	993	-	-	0/1/1/1	-
3	EDO	12-A	701	-	-	1/1/1/1	-
3	EDO	13-A	701	-	-	1/1/1/1	-
3	EDO	11-B	702	-	-	0/1/1/1	-
3	EDO	3-A	700	-	-	0/1/1/1	-
3	EDO	9-A	700	-	-	0/1/1/1	-
3	EDO	4-B	702	-	-	0/1/1/1	-
3	EDO	12-B	993	-	-	0/1/1/1	-
3	EDO	6-A	701	-	-	0/1/1/1	-
3	EDO	10-A	701	-	-	1/1/1/1	-
3	EDO	3-A	701	-	-	1/1/1/1	-
3	EDO	8-B	702	-	-	0/1/1/1	-
3	EDO	16-A	701	-	-	1/1/1/1	-
3	EDO	3-B	993	-	-	0/1/1/1	-
3	EDO	2-B	993	-	-	0/1/1/1	-
3	EDO	15-B	702	-	-	0/1/1/1	-
3	EDO	16-A	700	-	-	0/1/1/1	-
3	EDO	14-A	700	-	-	0/1/1/1	-
3	EDO	15-A	700	-	-	1/1/1/1	-
3	EDO	16-B	702	-	-	0/1/1/1	-
3	EDO	8-A	701	-	-	1/1/1/1	-
3	EDO	13-A	700	-	-	1/1/1/1	-
3	EDO	7-A	700	-	-	0/1/1/1	-
3	EDO	7-B	702	-	-	0/1/1/1	-
3	EDO	5-A	701	-	-	1/1/1/1	-
3	EDO	10-A	700	-	-	0/1/1/1	-
3	EDO	12-A	700	-	-	1/1/1/1	-
3	EDO	14-B	993	-	-	1/1/1/1	-
3	EDO	2-A	701	-	-	1/1/1/1	-
3	EDO	2-A	700	-	-	0/1/1/1	-
3	EDO	10-B	993	-	-	0/1/1/1	-
3	EDO	12-B	702	-	-	1/1/1/1	-
3	EDO	15-A	701	-	-	1/1/1/1	-
3	EDO	13-B	993	-	-	0/1/1/1	-
3	EDO	11-B	993	-	-	0/1/1/1	-
3	EDO	5-B	993	-	-	1/1/1/1	-
3	EDO	4-A	701	-	-	1/1/1/1	-
3	EDO	1-A	701	-	-	1/1/1/1	-
3	EDO	5-A	700	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	1-B	702	-	-	0/1/1/1	-
3	EDO	14-B	702	-	-	0/1/1/1	-
3	EDO	4-B	993	-	-	0/1/1/1	-
3	EDO	6-B	702	-	-	0/1/1/1	-
3	EDO	3-B	702	-	-	0/1/1/1	-
3	EDO	9-B	702	-	-	0/1/1/1	-
3	EDO	6-A	700	-	-	0/1/1/1	-
3	EDO	6-B	993	-	-	0/1/1/1	-
3	EDO	8-B	993	-	-	0/1/1/1	-
3	EDO	11-A	700	-	-	0/1/1/1	-
3	EDO	9-A	701	-	-	1/1/1/1	-
3	EDO	1-B	700	-	-	1/1/1/1	-
3	EDO	9-B	993	-	-	0/1/1/1	-
3	EDO	16-B	993	-	-	1/1/1/1	-
3	EDO	8-A	700	-	-	1/1/1/1	-
3	EDO	7-A	701	-	-	1/1/1/1	-
3	EDO	11-A	701	-	-	0/1/1/1	-
3	EDO	10-B	702	-	-	0/1/1/1	-
3	EDO	1-A	993	-	-	0/1/1/1	-
3	EDO	13-B	702	-	-	0/1/1/1	-
3	EDO	5-B	702	-	-	1/1/1/1	-
3	EDO	15-B	993	-	-	1/1/1/1	-
3	EDO	4-A	700	-	-	0/1/1/1	-
3	EDO	2-B	702	-	-	0/1/1/1	-
3	EDO	14-A	701	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	5-A	701	EDO	O1-C1-C2-O2
3	8-A	701	EDO	O1-C1-C2-O2
3	9-A	701	EDO	O1-C1-C2-O2
3	13-A	701	EDO	O1-C1-C2-O2
3	1-A	701	EDO	O1-C1-C2-O2

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	176/216 (81%)	2.44	95 (53%) 0 0	1, 1, 2, 4	176 (100%)
1	1-B	173/216 (80%)	2.46	91 (52%) 0 0	1, 2, 2, 4	173 (100%)
1	2-A	0/216	-	-	-	-
1	2-B	0/216	-	-	-	-
1	3-A	0/216	-	-	-	-
1	3-B	0/216	-	-	-	-
1	4-A	0/216	-	-	-	-
1	4-B	0/216	-	-	-	-
1	5-A	0/216	-	-	-	-
1	5-B	0/216	-	-	-	-
1	6-A	0/216	-	-	-	-
1	6-B	0/216	-	-	-	-
1	7-A	0/216	-	-	-	-
1	7-B	0/216	-	-	-	-
1	8-A	0/216	-	-	-	-
1	8-B	0/216	-	-	-	-
1	9-A	0/216	-	-	-	-
1	9-B	0/216	-	-	-	-
1	10-A	0/216	-	-	-	-
1	10-B	0/216	-	-	-	-
1	11-A	0/216	-	-	-	-
1	11-B	0/216	-	-	-	-
1	12-A	0/216	-	-	-	-
1	12-B	0/216	-	-	-	-
1	13-A	0/216	-	-	-	-
1	13-B	0/216	-	-	-	-
1	14-A	0/216	-	-	-	-
1	14-B	0/216	-	-	-	-
1	15-A	0/216	-	-	-	-
1	15-B	0/216	-	-	-	-
1	16-A	0/216	-	-	-	-
1	16-B	0/216	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	349/6912 (5%)	2.45	186 (53%) 0 0	1, 1, 2, 4	349 (100%)

The worst 5 of 186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	111	ALA	12.0
1	1-A	70	GLY	10.2
1	1-B	188	THR	8.8
1	1-A	89	VAL	6.9
1	1-B	187	TYR	6.9

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NO3	1-A	600	4/4	0.40	0.25	65,66,66,66	4
2	NO3	2-A	600	4/4	-	-	66,66,66,66	4
2	NO3	3-A	600	4/4	-	-	66,66,66,66	4
2	NO3	4-A	600	4/4	-	-	65,65,65,66	4
2	NO3	5-A	600	4/4	-	-	66,66,66,66	4
2	NO3	6-A	600	4/4	-	-	65,65,65,66	4
2	NO3	7-A	600	4/4	-	-	62,62,62,63	4
2	NO3	8-A	600	4/4	-	-	65,65,65,66	4
2	NO3	9-A	600	4/4	-	-	61,61,62,62	4
2	NO3	10-A	600	4/4	-	-	65,65,66,66	4
2	NO3	11-A	600	4/4	-	-	66,66,66,66	4
2	NO3	12-A	600	4/4	-	-	66,66,66,66	4
2	NO3	13-A	600	4/4	-	-	65,65,65,66	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NO3	14-A	600	4/4	-	-	66,66,66,66	4
2	NO3	15-A	600	4/4	-	-	66,66,66,67	4
2	NO3	16-A	600	4/4	-	-	66,66,66,67	4
3	EDO	1-B	702	4/4	0.60	0.30	44,47,48,48	4
3	EDO	2-A	701	4/4	-	-	40,42,42,46	4
3	EDO	3-A	701	4/4	-	-	46,46,47,49	4
3	EDO	4-A	701	4/4	-	-	37,38,38,38	4
3	EDO	5-A	701	4/4	-	-	42,44,45,48	4
3	EDO	6-A	701	4/4	-	-	43,43,44,46	4
3	EDO	7-A	701	4/4	-	-	46,46,47,49	4
3	EDO	8-A	701	4/4	-	-	45,45,46,48	4
3	EDO	9-A	701	4/4	-	-	45,45,45,48	4
3	EDO	10-A	701	4/4	-	-	43,43,44,44	4
3	EDO	11-A	701	4/4	-	-	47,47,48,50	4
3	EDO	12-A	701	4/4	-	-	47,47,48,49	4
3	EDO	13-A	701	4/4	-	-	44,44,45,48	4
3	EDO	14-A	701	4/4	-	-	48,49,49,51	4
3	EDO	15-A	701	4/4	-	-	48,49,49,51	4
3	EDO	16-A	701	4/4	-	-	47,48,48,51	4
3	EDO	2-A	700	4/4	-	-	54,54,55,55	4
3	EDO	3-A	700	4/4	-	-	53,54,54,54	4
3	EDO	4-A	700	4/4	-	-	53,54,54,55	4
3	EDO	5-A	700	4/4	-	-	53,54,54,54	4
3	EDO	6-A	700	4/4	-	-	53,54,54,55	4
3	EDO	7-A	700	4/4	-	-	54,55,55,55	4
3	EDO	8-A	700	4/4	-	-	54,55,55,55	4
3	EDO	9-A	700	4/4	-	-	54,54,54,55	4
3	EDO	10-A	700	4/4	-	-	53,54,54,55	4
3	EDO	11-A	700	4/4	-	-	53,54,54,54	4
3	EDO	12-A	700	4/4	-	-	52,54,54,54	4
3	EDO	13-A	700	4/4	-	-	53,54,55,55	4
3	EDO	14-A	700	4/4	-	-	54,54,55,55	4
3	EDO	15-A	700	4/4	-	-	53,54,55,55	4
3	EDO	16-A	700	4/4	-	-	54,54,54,55	4
3	EDO	1-A	701	4/4	0.72	0.22	44,44,44,48	4
3	EDO	1-A	993	4/4	0.80	0.23	43,43,43,50	4
3	EDO	1-B	700	4/4	0.86	0.22	54,55,55,55	4
3	EDO	2-B	702	4/4	-	-	44,47,48,48	4
3	EDO	3-B	702	4/4	-	-	44,47,48,48	4
3	EDO	4-B	702	4/4	-	-	44,47,48,48	4
3	EDO	5-B	702	4/4	-	-	46,47,48,49	4
3	EDO	6-B	702	4/4	-	-	44,47,48,48	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	7-B	702	4/4	-	-	44,48,48,48	4
3	EDO	8-B	702	4/4	-	-	44,47,48,48	4
3	EDO	9-B	702	4/4	-	-	44,47,48,48	4
3	EDO	10-B	702	4/4	-	-	44,47,48,48	4
3	EDO	11-B	702	4/4	-	-	43,47,48,48	4
3	EDO	12-B	702	4/4	-	-	45,48,48,48	4
3	EDO	13-B	702	4/4	-	-	44,48,48,49	4
3	EDO	14-B	702	4/4	-	-	44,47,49,49	4
3	EDO	15-B	702	4/4	-	-	44,47,49,49	4
3	EDO	16-B	702	4/4	-	-	44,48,48,48	4
3	EDO	2-B	993	4/4	-	-	42,43,44,50	4
3	EDO	3-B	993	4/4	-	-	43,44,44,50	4
3	EDO	4-B	993	4/4	-	-	43,44,44,50	4
3	EDO	5-B	993	4/4	-	-	38,40,41,46	4
3	EDO	6-B	993	4/4	-	-	44,45,45,50	4
3	EDO	7-B	993	4/4	-	-	43,44,44,50	4
3	EDO	8-B	993	4/4	-	-	43,44,44,50	4
3	EDO	9-B	993	4/4	-	-	43,44,44,50	4
3	EDO	10-B	993	4/4	-	-	42,43,44,50	4
3	EDO	11-B	993	4/4	-	-	42,43,44,50	4
3	EDO	12-B	993	4/4	-	-	42,43,44,50	4
3	EDO	13-B	993	4/4	-	-	43,44,45,52	4
3	EDO	14-B	993	4/4	-	-	43,43,45,51	4
3	EDO	15-B	993	4/4	-	-	43,44,45,51	4
3	EDO	16-B	993	4/4	-	-	42,43,45,52	4

6.5 Other polymers [i](#)

There are no such residues in this entry.