



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:17 PM UTC

PDB ID : 4ZM3 / pdb_00004zm3
Title : Crystal structure of PLP-Dependent 3-Aminobenzoate Synthase PctV wild-type
Authors : Hirayama, A.; Miyanaga, A.; Kudo, F.; Eguchi, T.
Deposited on : 2015-05-02
Resolution : 2.27 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

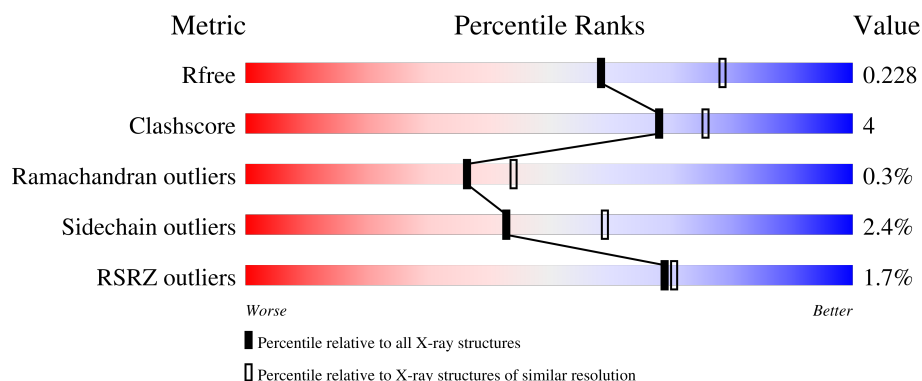
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	A	464	% 76% 7% • 16%
1	B	464	2% 74% 7% • 18%
1	C	464	2% 75% 7% • 17%
1	D	464	% 75% 7% • 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12181 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 Aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2960	1870	543	536	11			
1	B	381	Total	C	N	O	S	0	0	0
			2906	1836	534	526	10			
1	C	384	Total	C	N	O	S	0	0	0
			2925	1847	538	529	11			
1	D	387	Total	C	N	O	S	0	0	0
			2947	1859	540	536	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A8R0K5
A	-18	GLY	-	expression tag	UNP A8R0K5
A	-17	SER	-	expression tag	UNP A8R0K5
A	-16	SER	-	expression tag	UNP A8R0K5
A	-15	HIS	-	expression tag	UNP A8R0K5
A	-14	HIS	-	expression tag	UNP A8R0K5
A	-13	HIS	-	expression tag	UNP A8R0K5
A	-12	HIS	-	expression tag	UNP A8R0K5
A	-11	HIS	-	expression tag	UNP A8R0K5
A	-10	HIS	-	expression tag	UNP A8R0K5
A	-9	SER	-	expression tag	UNP A8R0K5
A	-8	SER	-	expression tag	UNP A8R0K5
A	-7	GLY	-	expression tag	UNP A8R0K5
A	-6	LEU	-	expression tag	UNP A8R0K5
A	-5	VAL	-	expression tag	UNP A8R0K5
A	-4	PRO	-	expression tag	UNP A8R0K5
A	-3	ARG	-	expression tag	UNP A8R0K5
A	-2	GLY	-	expression tag	UNP A8R0K5
A	-1	SER	-	expression tag	UNP A8R0K5
A	0	HIS	-	expression tag	UNP A8R0K5
B	-19	MET	-	expression tag	UNP A8R0K5

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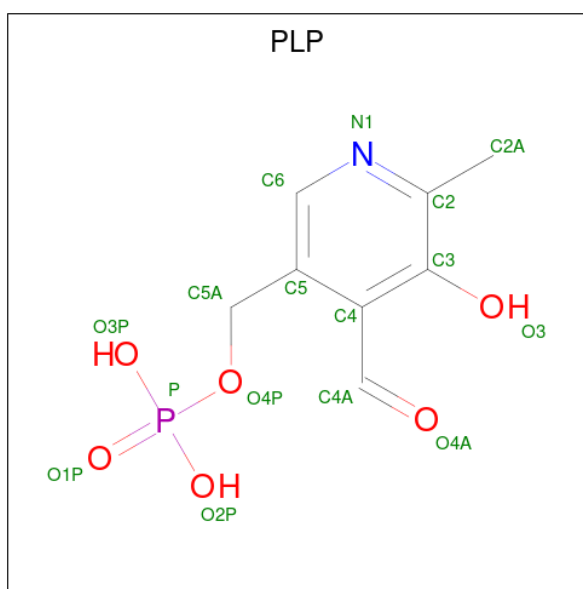
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A8R0K5
B	-17	SER	-	expression tag	UNP A8R0K5
B	-16	SER	-	expression tag	UNP A8R0K5
B	-15	HIS	-	expression tag	UNP A8R0K5
B	-14	HIS	-	expression tag	UNP A8R0K5
B	-13	HIS	-	expression tag	UNP A8R0K5
B	-12	HIS	-	expression tag	UNP A8R0K5
B	-11	HIS	-	expression tag	UNP A8R0K5
B	-10	HIS	-	expression tag	UNP A8R0K5
B	-9	SER	-	expression tag	UNP A8R0K5
B	-8	SER	-	expression tag	UNP A8R0K5
B	-7	GLY	-	expression tag	UNP A8R0K5
B	-6	LEU	-	expression tag	UNP A8R0K5
B	-5	VAL	-	expression tag	UNP A8R0K5
B	-4	PRO	-	expression tag	UNP A8R0K5
B	-3	ARG	-	expression tag	UNP A8R0K5
B	-2	GLY	-	expression tag	UNP A8R0K5
B	-1	SER	-	expression tag	UNP A8R0K5
B	0	HIS	-	expression tag	UNP A8R0K5
C	-19	MET	-	expression tag	UNP A8R0K5
C	-18	GLY	-	expression tag	UNP A8R0K5
C	-17	SER	-	expression tag	UNP A8R0K5
C	-16	SER	-	expression tag	UNP A8R0K5
C	-15	HIS	-	expression tag	UNP A8R0K5
C	-14	HIS	-	expression tag	UNP A8R0K5
C	-13	HIS	-	expression tag	UNP A8R0K5
C	-12	HIS	-	expression tag	UNP A8R0K5
C	-11	HIS	-	expression tag	UNP A8R0K5
C	-10	HIS	-	expression tag	UNP A8R0K5
C	-9	SER	-	expression tag	UNP A8R0K5
C	-8	SER	-	expression tag	UNP A8R0K5
C	-7	GLY	-	expression tag	UNP A8R0K5
C	-6	LEU	-	expression tag	UNP A8R0K5
C	-5	VAL	-	expression tag	UNP A8R0K5
C	-4	PRO	-	expression tag	UNP A8R0K5
C	-3	ARG	-	expression tag	UNP A8R0K5
C	-2	GLY	-	expression tag	UNP A8R0K5
C	-1	SER	-	expression tag	UNP A8R0K5
C	0	HIS	-	expression tag	UNP A8R0K5
D	-19	MET	-	expression tag	UNP A8R0K5
D	-18	GLY	-	expression tag	UNP A8R0K5
D	-17	SER	-	expression tag	UNP A8R0K5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A8R0K5
D	-15	HIS	-	expression tag	UNP A8R0K5
D	-14	HIS	-	expression tag	UNP A8R0K5
D	-13	HIS	-	expression tag	UNP A8R0K5
D	-12	HIS	-	expression tag	UNP A8R0K5
D	-11	HIS	-	expression tag	UNP A8R0K5
D	-10	HIS	-	expression tag	UNP A8R0K5
D	-9	SER	-	expression tag	UNP A8R0K5
D	-8	SER	-	expression tag	UNP A8R0K5
D	-7	GLY	-	expression tag	UNP A8R0K5
D	-6	LEU	-	expression tag	UNP A8R0K5
D	-5	VAL	-	expression tag	UNP A8R0K5
D	-4	PRO	-	expression tag	UNP A8R0K5
D	-3	ARG	-	expression tag	UNP A8R0K5
D	-2	GLY	-	expression tag	UNP A8R0K5
D	-1	SER	-	expression tag	UNP A8R0K5
D	0	HIS	-	expression tag	UNP A8R0K5

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



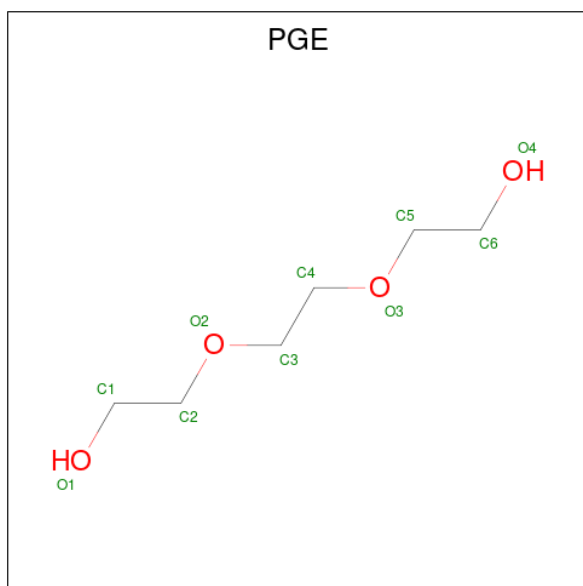
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

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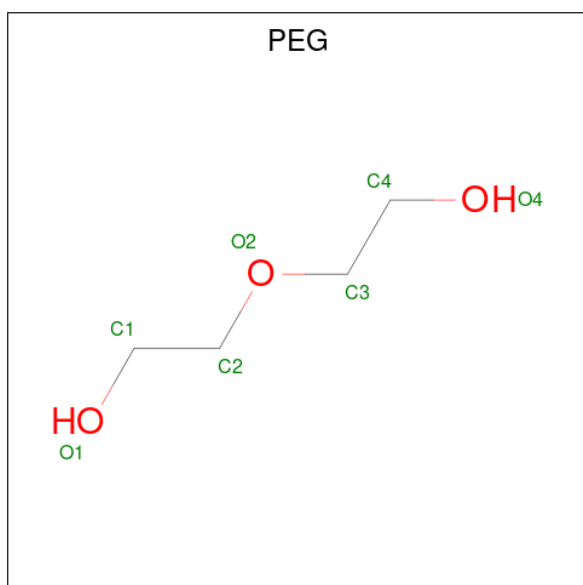
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0

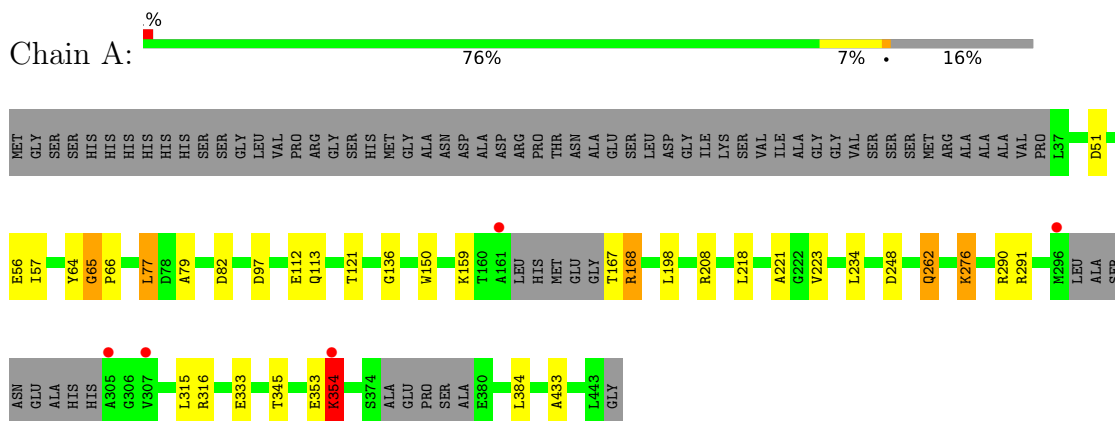
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	80	Total O 80 80	0	0
5	B	77	Total O 77 77	0	0
5	C	99	Total O 99 99	0	0
5	D	92	Total O 92 92	0	0

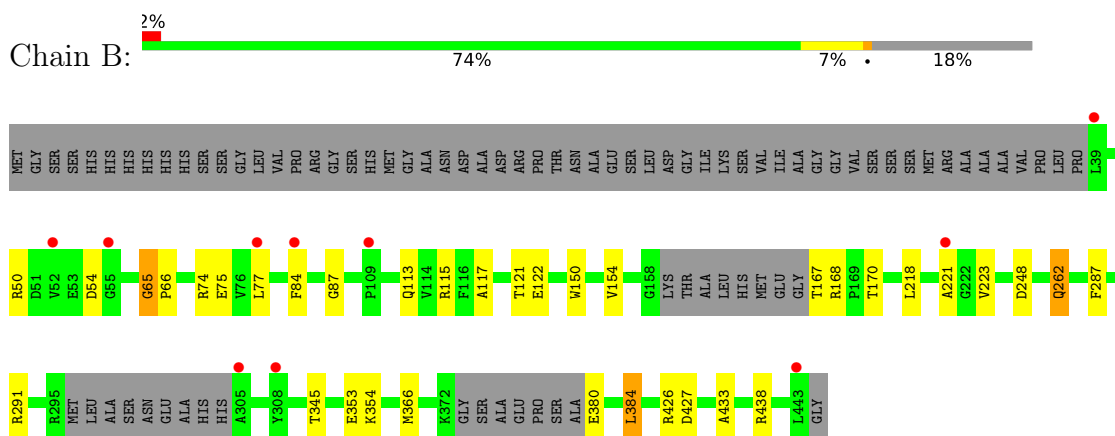
3 Residue-property plots [i](#)

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.

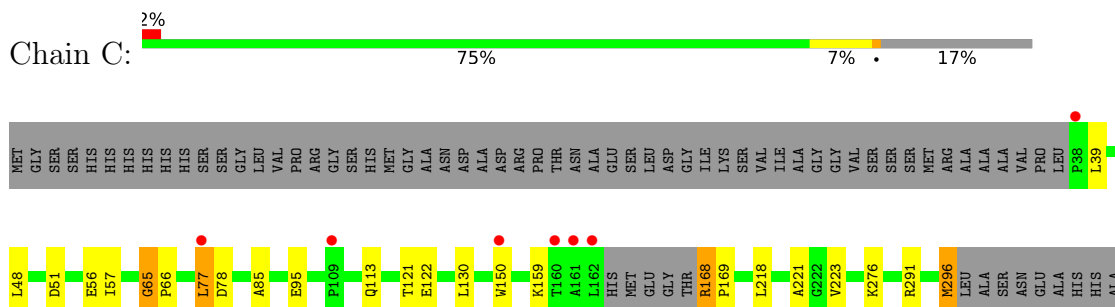
• Molecule 1: Aminotransferase

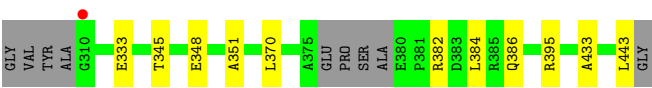


• Molecule 1: Aminotransferase

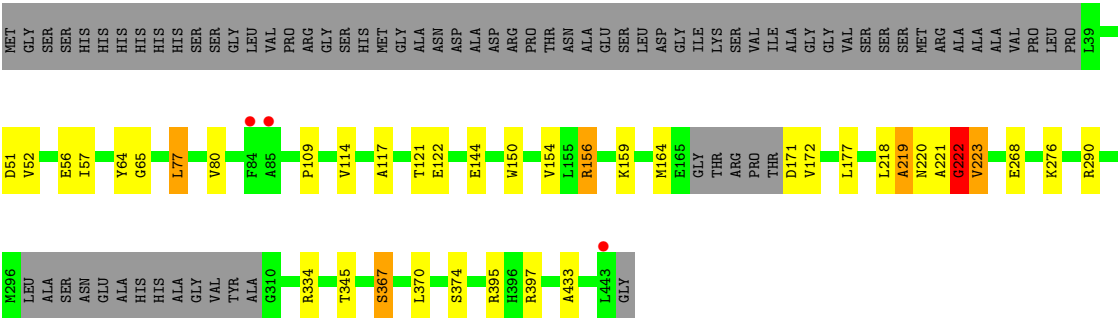
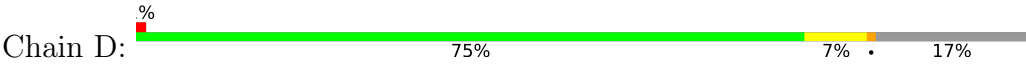


• Molecule 1: Aminotransferase





● Molecule 1: Aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.99Å 170.83Å 74.57Å 90.00° 98.33° 90.00°	Depositor
Resolution (Å)	42.85 – 2.27 42.85 – 2.27	Depositor EDS
% Data completeness (in resolution range)	94.8 (42.85-2.27) 94.8 (42.85-2.27)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.180 , 0.222 0.187 , 0.228	Depositor DCC
R_{free} test set	3225 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12181	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PLP, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.94	2/3016 (0.1%)	0.93	4/4089 (0.1%)
1	B	0.90	0/2961	0.94	6/4015 (0.1%)
1	C	0.95	0/2980	0.95	2/4038 (0.0%)
1	D	0.99	1/3003 (0.0%)	1.00	9/4070 (0.2%)
All	All	0.95	3/11960 (0.0%)	0.96	21/16212 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	219	ALA	CA-C	-5.36	1.44	1.52
1	A	77	LEU	N-CA	-5.34	1.39	1.46
1	A	77	LEU	CA-C	5.19	1.59	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	172	VAL	N-CA-C	7.58	119.75	108.46
1	D	220	ASN	N-CA-C	-6.73	104.17	112.38
1	D	290	ARG	CB-CG-CD	6.70	126.71	111.30
1	D	222	GLY	N-CA-C	6.40	128.34	113.18
1	D	80	VAL	N-CA-CB	6.30	118.64	110.57
1	C	39	LEU	N-CA-C	6.26	121.02	107.49
1	D	172	VAL	CB-CA-C	-6.24	100.90	110.50
1	A	77	LEU	CB-CA-C	6.20	122.58	110.67
1	A	262	GLN	CB-CA-C	-6.02	101.18	110.81
1	D	65	GLY	N-CA-C	5.98	124.53	112.34
1	A	354	LYS	CB-CG-CD	5.61	124.21	111.30
1	C	65	GLY	N-CA-C	5.43	123.41	112.34
1	B	65	GLY	N-CA-C	5.28	123.11	112.34
1	D	144	GLU	CB-CA-C	-5.25	101.70	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	367	SER	CB-CA-C	-5.18	100.78	109.48
1	B	154	VAL	CB-CA-C	-5.16	105.05	110.62
1	B	366	MET	N-CA-CB	-5.15	101.87	110.57
1	B	50	ARG	CA-C-N	5.11	130.26	120.97
1	B	50	ARG	C-N-CA	5.11	130.26	120.97
1	A	65	GLY	N-CA-C	5.07	122.69	112.34
1	B	262	GLN	CB-CA-C	-5.06	102.44	110.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2960	0	2982	26	1
1	B	2906	0	2922	21	1
1	C	2925	0	2950	26	0
1	D	2947	0	2961	26	0
2	A	16	0	7	1	0
2	B	16	0	8	1	0
2	C	16	0	8	0	0
2	D	16	0	7	0	0
3	C	10	0	14	2	0
4	D	21	0	30	0	0
5	A	80	0	0	0	0
5	B	77	0	0	1	0
5	C	99	0	0	0	0
5	D	92	0	0	1	0
All	All	12181	0	11889	86	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ARG:HD2	1:B:287:PHE:CE1	2.01	0.96
1:B:115:ARG:HD2	1:B:287:PHE:HE1	1.35	0.86
1:A:290:ARG:NH1	1:D:397:ARG:HD3	2.10	0.67
1:A:77:LEU:HB3	1:B:84:PHE:HB3	1.79	0.63
1:A:221:ALA:HB1	1:A:384:LEU:HD13	1.81	0.63
1:D:121:THR:HG21	1:D:150:TRP:CE2	2.33	0.63
1:A:113:GLN:HE21	1:A:291:ARG:HG2	1.65	0.62
1:C:85:ALA:HA	1:D:77:LEU:CD1	2.29	0.62
1:C:221:ALA:HB1	1:C:384:LEU:HD13	1.82	0.61
1:C:121:THR:HG21	1:C:150:TRP:CE2	2.35	0.61
1:A:290:ARG:HH11	1:D:397:ARG:HD3	1.65	0.61
1:A:353:GLU:C	1:A:354:LYS:HD3	2.26	0.61
1:C:85:ALA:HA	1:D:77:LEU:HD12	1.83	0.60
1:C:113:GLN:HE21	1:C:291:ARG:HG2	1.66	0.59
1:A:290:ARG:NH1	1:D:397:ARG:CD	2.66	0.59
1:B:353:GLU:O	1:B:354:LYS:CG	2.51	0.59
1:A:121:THR:HG21	1:A:150:TRP:CE2	2.38	0.58
1:B:121:THR:HG21	1:B:150:TRP:CE2	2.39	0.58
1:C:56:GLU:C	1:C:57:ILE:HG13	2.30	0.56
1:D:121:THR:HG21	1:D:150:TRP:CD2	2.41	0.56
1:B:353:GLU:O	1:B:354:LYS:HG3	2.06	0.55
1:D:334:ARG:NH2	5:D:602:HOH:O	2.33	0.55
1:C:348:GLU:HA	3:C:502:PGE:H42	1.89	0.55
1:C:130:LEU:CD1	1:C:296:MET:HB3	2.37	0.54
1:C:168:ARG:HG3	1:C:169:PRO:HD2	1.90	0.53
1:A:82:ASP:OD2	1:A:316:ARG:NH2	2.42	0.53
1:B:221:ALA:HB1	1:B:384:LEU:HG	1.92	0.52
1:D:64:TYR:O	1:D:276:LYS:HE3	2.10	0.52
1:A:79:ALA:HB1	1:A:316:ARG:NH1	2.26	0.51
1:B:221:ALA:HB1	1:B:384:LEU:CG	2.41	0.50
1:B:121:THR:HG21	1:B:150:TRP:CD2	2.47	0.50
1:C:121:THR:HG21	1:C:150:TRP:CD2	2.47	0.50
1:A:112:GLU:OE2	1:D:397:ARG:HD3	2.11	0.49
1:C:150:TRP:CZ2	1:D:122:GLU:HG3	2.46	0.49
1:D:218:LEU:O	1:D:223:VAL:HA	2.12	0.49
1:A:97:ASP:HA	1:A:315:LEU:HD23	1.94	0.49
1:A:113:GLN:HE21	1:A:291:ARG:CG	2.24	0.49
1:B:345:THR:CG2	1:B:433:ALA:HB2	2.43	0.48
1:C:351:ALA:HB3	3:C:502:PGE:H4	1.94	0.48
1:D:109:PRO:HB2	1:D:268:GLU:OE2	2.14	0.48
1:D:222:GLY:C	1:D:367:SER:HG	2.22	0.48
1:B:113:GLN:HE21	1:B:291:ARG:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ALA:C	1:D:221:ALA:N	2.66	0.48
1:B:354:LYS:HG3	1:B:354:LYS:O	2.12	0.47
1:C:48:LEU:HD13	1:C:56:GLU:OE2	2.13	0.47
1:C:95:GLU:HG2	1:D:52:VAL:HG12	1.95	0.47
1:C:345:THR:CG2	1:C:433:ALA:HB2	2.44	0.47
1:C:113:GLN:HE21	1:C:291:ARG:CG	2.27	0.47
1:A:51:ASP:C	1:A:51:ASP:OD1	2.57	0.47
1:D:345:THR:CG2	1:D:433:ALA:HB2	2.45	0.46
1:A:345:THR:CG2	1:A:433:ALA:HB2	2.45	0.46
1:A:113:GLN:NE2	1:A:291:ARG:HG2	2.30	0.46
1:C:51:ASP:OD1	1:C:51:ASP:C	2.57	0.45
1:A:218:LEU:O	1:A:223:VAL:HA	2.16	0.45
1:A:121:THR:HG21	1:A:150:TRP:CD2	2.51	0.45
1:B:218:LEU:O	1:B:223:VAL:HA	2.17	0.45
1:C:113:GLN:NE2	1:C:291:ARG:HG2	2.31	0.44
1:C:122:GLU:HG3	1:D:150:TRP:CZ2	2.52	0.44
1:C:218:LEU:O	1:C:223:VAL:HA	2.18	0.44
1:B:248:ASP:OD2	2:B:501:PLP:N1	2.51	0.43
1:A:136:GLY:HA3	1:D:177:LEU:HD22	1.99	0.43
1:D:56:GLU:C	1:D:57:ILE:HG13	2.42	0.43
1:A:65:GLY:N	1:A:66:PRO:CD	2.81	0.43
1:A:353:GLU:C	1:A:354:LYS:CD	2.91	0.43
1:D:154:VAL:O	1:D:156:ARG:HD3	2.19	0.43
1:A:248:ASP:OD2	2:A:501:PLP:N1	2.52	0.42
1:C:150:TRP:CZ2	1:D:122:GLU:HB2	2.54	0.42
1:B:113:GLN:HE21	1:B:291:ARG:CG	2.32	0.42
1:D:51:ASP:OD1	1:D:51:ASP:C	2.62	0.42
1:B:113:GLN:NE2	1:B:291:ARG:HG2	2.35	0.42
1:B:65:GLY:N	1:B:66:PRO:CD	2.83	0.42
1:C:65:GLY:N	1:C:66:PRO:CD	2.82	0.42
1:B:353:GLU:O	1:B:354:LYS:HG2	2.20	0.42
1:A:168:ARG:HE	1:A:168:ARG:HB3	1.59	0.41
1:C:370:LEU:HD23	1:C:395:ARG:HB3	2.01	0.41
1:C:382:ARG:HG2	1:C:386:GLN:OE1	2.20	0.41
1:D:117:ALA:HB1	1:D:122:GLU:CD	2.45	0.41
1:A:64:TYR:O	1:A:276:LYS:HE3	2.21	0.41
1:B:74:ARG:O	1:B:75:GLU:C	2.64	0.41
1:C:95:GLU:HG2	1:D:52:VAL:CG1	2.50	0.41
1:D:370:LEU:HD23	1:D:395:ARG:HB3	2.02	0.41
1:A:56:GLU:C	1:A:57:ILE:HG13	2.46	0.40
1:A:198:LEU:CD2	1:A:234:LEU:HD12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLY:HA2	5:B:638:HOH:O	2.21	0.40
1:B:117:ALA:HB1	1:B:122:GLU:CD	2.46	0.40
1:C:77:LEU:HD23	1:C:78:ASP:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:NH1	1:B:54:ASP:OD2[1_655]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/464 (82%)	370 (97%)	10 (3%)	1 (0%)	36	44
1	B	373/464 (80%)	364 (98%)	9 (2%)	0	100	100
1	C	376/464 (81%)	366 (97%)	9 (2%)	1 (0%)	36	44
1	D	381/464 (82%)	370 (97%)	9 (2%)	2 (0%)	24	29
All	All	1511/1856 (81%)	1470 (97%)	37 (2%)	4 (0%)	36	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	222	GLY
1	D	223	VAL
1	A	276	LYS
1	C	276	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/355 (84%)	294 (98%)	6 (2%)	48	65
1	B	294/355 (83%)	284 (97%)	10 (3%)	32	46
1	C	297/355 (84%)	291 (98%)	6 (2%)	48	65
1	D	299/355 (84%)	292 (98%)	7 (2%)	44	60
All	All	1190/1420 (84%)	1161 (98%)	29 (2%)	43	59

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LYS
1	A	167	THR
1	A	168	ARG
1	A	262	GLN
1	A	333	GLU
1	A	354	LYS
1	B	77	LEU
1	B	167	THR
1	B	168	ARG
1	B	170	THR
1	B	262	GLN
1	B	380	GLU
1	B	384	LEU
1	B	426	ARG
1	B	427	ASP
1	B	438	ARG
1	C	77	LEU
1	C	159	LYS
1	C	168	ARG
1	C	296	MET
1	C	333	GLU
1	C	443	LEU
1	D	77	LEU
1	D	114	VAL

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Mol	Chain	Res	Type
1	D	156	ARG
1	D	159	LYS
1	D	164	MET
1	D	171	ASP
1	D	374	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	83	GLN
1	A	113	GLN
1	A	118	ASN
1	A	292	HIS
1	A	340	GLN
1	B	113	GLN
1	B	311	ASN
1	B	340	GLN
1	C	113	GLN
1	C	340	GLN
1	D	113	GLN
1	D	292	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	PLP	C	501	-	16,16,16	2.99	4 (25%)	20,23,23	2.01	8 (40%)
4	PEG	D	502	-	6,6,6	0.59	0	5,5,5	0.86	0
4	PEG	D	504	-	6,6,6	0.77	0	5,5,5	0.61	0
3	PGE	C	502	-	9,9,9	0.64	0	8,8,8	0.79	0
4	PEG	D	503	-	6,6,6	0.61	0	5,5,5	0.43	0
2	PLP	D	501	-	16,16,16	2.32	3 (18%)	20,23,23	1.73	4 (20%)
2	PLP	B	501	-	16,16,16	3.10	6 (37%)	20,23,23	2.01	6 (30%)
2	PLP	A	501	-	16,16,16	3.13	4 (25%)	20,23,23	1.64	4 (20%)

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	PLP	C	501	-	-	1/8/8/8	0/1/1/1
4	PEG	D	502	-	-	1/4/4/4	-
4	PEG	D	504	-	-	3/4/4/4	-
3	PGE	C	502	-	-	5/7/7/7	-
4	PEG	D	503	-	-	2/4/4/4	-
2	PLP	D	501	-	-	2/8/8/8	0/1/1/1
2	PLP	B	501	-	-	0/8/8/8	0/1/1/1
2	PLP	A	501	-	-	0/8/8/8	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PLP	C3-C2	9.97	1.51	1.41
2	A	501	PLP	C3-C2	9.84	1.51	1.41
2	C	501	PLP	C3-C2	9.42	1.50	1.41
2	D	501	PLP	C3-C2	6.26	1.47	1.41
2	D	501	PLP	C4-C5	5.53	1.49	1.42
2	A	501	PLP	C4-C5	5.44	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	PLP	C4-C3	4.63	1.48	1.41
2	B	501	PLP	C4-C3	4.19	1.48	1.41
2	C	501	PLP	C4-C5	4.12	1.47	1.42
2	A	501	PLP	C4-C3	3.84	1.47	1.41
2	B	501	PLP	C4-C5	3.77	1.47	1.42
2	C	501	PLP	C6-C5	2.95	1.43	1.37
2	D	501	PLP	C4-C3	2.95	1.46	1.41
2	A	501	PLP	C6-C5	2.67	1.43	1.37
2	B	501	PLP	C6-C5	2.19	1.42	1.37
2	B	501	PLP	C2-N1	2.17	1.37	1.33
2	B	501	PLP	C6-N1	2.04	1.38	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	PLP	C4-C3-C2	-4.05	117.86	120.14
2	B	501	PLP	O3-C3-C2	3.85	125.56	117.58
2	C	501	PLP	C3-C4-C4A	3.62	124.83	119.84
2	A	501	PLP	C3-C4-C5	-3.61	115.38	118.28
2	D	501	PLP	C3-C4-C5	-3.47	115.49	118.28
2	B	501	PLP	C2A-C2-C3	3.30	124.66	120.80
2	B	501	PLP	C4-C3-C2	-3.23	118.33	120.14
2	D	501	PLP	O3P-P-O4P	-3.21	98.29	106.67
2	D	501	PLP	O4A-C4A-C4	-3.18	117.26	124.80
2	B	501	PLP	O4P-C5A-C5	3.12	115.20	109.36
2	B	501	PLP	O4A-C4A-C4	-2.96	117.77	124.80
2	C	501	PLP	O3P-P-O2P	2.94	118.82	107.80
2	C	501	PLP	O2P-P-O4P	-2.60	99.89	106.67
2	C	501	PLP	O4A-C4A-C4	-2.60	118.64	124.80
2	A	501	PLP	O3P-P-O2P	2.53	117.27	107.80
2	C	501	PLP	C3-C4-C5	-2.52	116.25	118.28
2	A	501	PLP	O3P-P-O4P	-2.42	100.37	106.67
2	B	501	PLP	O4P-P-O1P	-2.37	100.04	106.44
2	A	501	PLP	C3-C4-C4A	2.27	122.96	119.84
2	D	501	PLP	C6-N1-C2	2.18	123.15	119.20
2	C	501	PLP	C6-N1-C2	2.14	123.09	119.20
2	C	501	PLP	O3P-P-O4P	-2.05	101.33	106.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	PLP	C5A-O4P-P-O2P
2	D	501	PLP	C5A-O4P-P-O1P
2	D	501	PLP	C5A-O4P-P-O3P
4	D	504	PEG	O2-C3-C4-O4
3	C	502	PGE	O2-C3-C4-O3
4	D	504	PEG	C1-C2-O2-C3
4	D	503	PEG	O1-C1-C2-O2
3	C	502	PGE	O1-C1-C2-O2
4	D	502	PEG	O2-C3-C4-O4
4	D	503	PEG	O2-C3-C4-O4
3	C	502	PGE	C6-C5-O3-C4
3	C	502	PGE	O3-C5-C6-O4
3	C	502	PGE	C3-C4-O3-C5
4	D	504	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	PGE	2	0
2	B	501	PLP	1	0
2	A	501	PLP	1	0

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	A	389/464 (83%)	-0.06	5 (1%) 75 76	19, 30, 55, 76	0
1	B	381/464 (82%)	0.08	10 (2%) 57 59	20, 34, 57, 87	0
1	C	384/464 (82%)	-0.14	8 (2%) 63 65	17, 29, 50, 70	0
1	D	387/464 (83%)	-0.07	3 (0%) 82 84	19, 29, 50, 66	0
All	All	1541/1856 (83%)	-0.05	26 (1%) 69 70	17, 31, 54, 87	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	ALA	4.1
1	B	39	LEU	3.8
1	B	109	PRO	3.4
1	A	161	ALA	3.2
1	C	310	GLY	3.0
1	C	38	PRO	2.8
1	B	55	GLY	2.5
1	C	77	LEU	2.5
1	C	150	TRP	2.4
1	A	296	MET	2.4
1	B	308	TYR	2.4
1	A	307	VAL	2.3
1	B	221	ALA	2.3
1	D	84	PHE	2.2
1	B	77	LEU	2.2
1	B	84	PHE	2.2
1	B	305	ALA	2.2
1	B	52	VAL	2.2
1	D	85	ALA	2.2
1	D	443	LEU	2.2
1	B	443	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	160	THR	2.1
1	A	354	LYS	2.1
1	C	162	LEU	2.1
1	C	161	ALA	2.0
1	C	109	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	PEG	D	503	7/7	0.82	0.14	44,48,57,57	0
4	PEG	D	504	7/7	0.89	0.11	42,45,47,47	0
3	PGE	C	502	10/10	0.90	0.10	38,43,46,49	0
2	PLP	D	501	16/16	0.93	0.09	29,36,45,55	0
4	PEG	D	502	7/7	0.93	0.12	34,38,40,41	0
2	PLP	B	501	16/16	0.94	0.08	25,31,40,48	0
2	PLP	C	501	16/16	0.96	0.07	20,26,30,32	0
2	PLP	A	501	16/16	0.96	0.08	19,28,38,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.