



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 02:11 am BST

PDB ID : 6BFY
Title : Crystal structure of enolase from Escherichia coli with bound 2-phosphoglycerate substrate
Authors : Erlandsen, H.; Wright, D.; Krucinska, J.
Deposited on : 2017-10-27
Resolution : 1.81 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

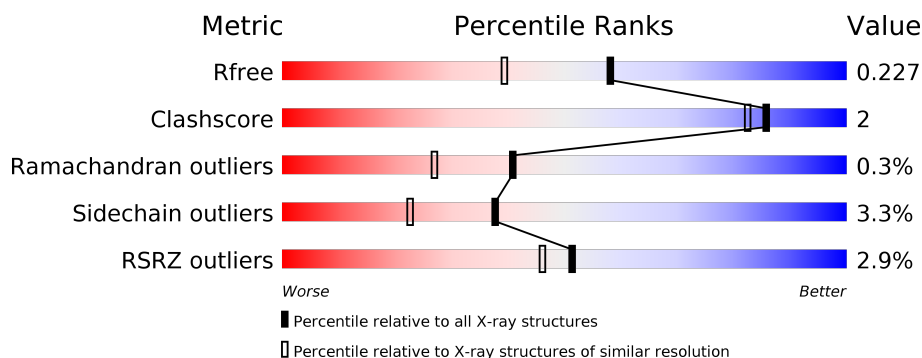
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	449	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	449	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	C	449	<div> <div></div> <div> <div></div> <div>89%</div> <div>7%</div> <div>..</div> </div> </div>
1	D	449	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>..</div> </div> </div>
1	E	449	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>
1	F	449	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>

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
4	SO4	D	805	-	-	-	X
5	GOL	D	806	-	X	-	-
5	GOL	F	505	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20818 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 Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3254	2036	559	644	15			
1	B	438	Total	C	N	O	S	0	0	0
			3249	2033	558	643	15			
1	C	439	Total	C	N	O	S	0	0	0
			3254	2036	559	644	15			
1	F	438	Total	C	N	O	S	0	0	0
			3245	2031	557	642	15			
1	D	438	Total	C	N	O	S	0	0	0
			3249	2033	558	643	15			
1	E	438	Total	C	N	O	S	0	1	0
			3258	2039	560	644	15			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	expression tag	UNP B7MLA0
A	-16	SER	-	expression tag	UNP B7MLA0
A	-15	HIS	-	expression tag	UNP B7MLA0
A	-14	MET	-	expression tag	UNP B7MLA0
A	-13	ALA	-	expression tag	UNP B7MLA0
A	-12	SER	-	expression tag	UNP B7MLA0
A	-11	MET	-	expression tag	UNP B7MLA0
A	-10	THR	-	expression tag	UNP B7MLA0
A	-9	GLY	-	expression tag	UNP B7MLA0
A	-8	GLY	-	expression tag	UNP B7MLA0
A	-7	GLN	-	expression tag	UNP B7MLA0
A	-6	GLN	-	expression tag	UNP B7MLA0
A	-5	MET	-	expression tag	UNP B7MLA0
A	-4	GLY	-	expression tag	UNP B7MLA0
A	-3	ARG	-	expression tag	UNP B7MLA0
A	-2	GLY	-	expression tag	UNP B7MLA0
A	-1	SER	-	expression tag	UNP B7MLA0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	expression tag	UNP B7MLA0
B	-16	SER	-	expression tag	UNP B7MLA0
B	-15	HIS	-	expression tag	UNP B7MLA0
B	-14	MET	-	expression tag	UNP B7MLA0
B	-13	ALA	-	expression tag	UNP B7MLA0
B	-12	SER	-	expression tag	UNP B7MLA0
B	-11	MET	-	expression tag	UNP B7MLA0
B	-10	THR	-	expression tag	UNP B7MLA0
B	-9	GLY	-	expression tag	UNP B7MLA0
B	-8	GLY	-	expression tag	UNP B7MLA0
B	-7	GLN	-	expression tag	UNP B7MLA0
B	-6	GLN	-	expression tag	UNP B7MLA0
B	-5	MET	-	expression tag	UNP B7MLA0
B	-4	GLY	-	expression tag	UNP B7MLA0
B	-3	ARG	-	expression tag	UNP B7MLA0
B	-2	GLY	-	expression tag	UNP B7MLA0
B	-1	SER	-	expression tag	UNP B7MLA0
C	-17	GLY	-	expression tag	UNP B7MLA0
C	-16	SER	-	expression tag	UNP B7MLA0
C	-15	HIS	-	expression tag	UNP B7MLA0
C	-14	MET	-	expression tag	UNP B7MLA0
C	-13	ALA	-	expression tag	UNP B7MLA0
C	-12	SER	-	expression tag	UNP B7MLA0
C	-11	MET	-	expression tag	UNP B7MLA0
C	-10	THR	-	expression tag	UNP B7MLA0
C	-9	GLY	-	expression tag	UNP B7MLA0
C	-8	GLY	-	expression tag	UNP B7MLA0
C	-7	GLN	-	expression tag	UNP B7MLA0
C	-6	GLN	-	expression tag	UNP B7MLA0
C	-5	MET	-	expression tag	UNP B7MLA0
C	-4	GLY	-	expression tag	UNP B7MLA0
C	-3	ARG	-	expression tag	UNP B7MLA0
C	-2	GLY	-	expression tag	UNP B7MLA0
C	-1	SER	-	expression tag	UNP B7MLA0
F	-17	GLY	-	expression tag	UNP B7MLA0
F	-16	SER	-	expression tag	UNP B7MLA0
F	-15	HIS	-	expression tag	UNP B7MLA0
F	-14	MET	-	expression tag	UNP B7MLA0
F	-13	ALA	-	expression tag	UNP B7MLA0
F	-12	SER	-	expression tag	UNP B7MLA0
F	-11	MET	-	expression tag	UNP B7MLA0
F	-10	THR	-	expression tag	UNP B7MLA0

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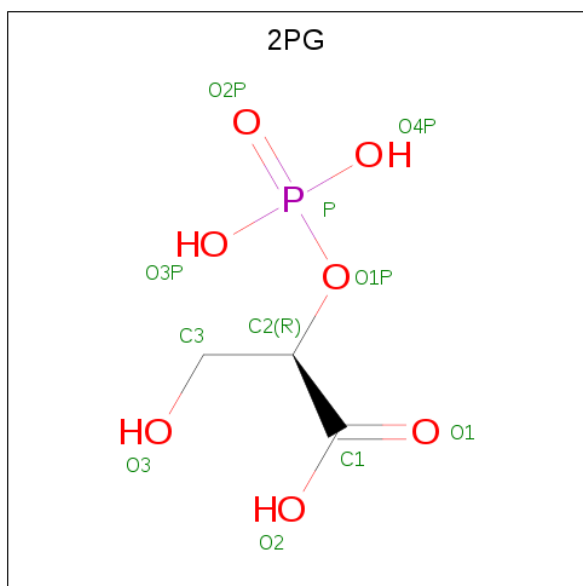
Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	GLY	-	expression tag	UNP B7MLA0
F	-8	GLY	-	expression tag	UNP B7MLA0
F	-7	GLN	-	expression tag	UNP B7MLA0
F	-6	GLN	-	expression tag	UNP B7MLA0
F	-5	MET	-	expression tag	UNP B7MLA0
F	-4	GLY	-	expression tag	UNP B7MLA0
F	-3	ARG	-	expression tag	UNP B7MLA0
F	-2	GLY	-	expression tag	UNP B7MLA0
F	-1	SER	-	expression tag	UNP B7MLA0
D	-17	GLY	-	expression tag	UNP B7MLA0
D	-16	SER	-	expression tag	UNP B7MLA0
D	-15	HIS	-	expression tag	UNP B7MLA0
D	-14	MET	-	expression tag	UNP B7MLA0
D	-13	ALA	-	expression tag	UNP B7MLA0
D	-12	SER	-	expression tag	UNP B7MLA0
D	-11	MET	-	expression tag	UNP B7MLA0
D	-10	THR	-	expression tag	UNP B7MLA0
D	-9	GLY	-	expression tag	UNP B7MLA0
D	-8	GLY	-	expression tag	UNP B7MLA0
D	-7	GLN	-	expression tag	UNP B7MLA0
D	-6	GLN	-	expression tag	UNP B7MLA0
D	-5	MET	-	expression tag	UNP B7MLA0
D	-4	GLY	-	expression tag	UNP B7MLA0
D	-3	ARG	-	expression tag	UNP B7MLA0
D	-2	GLY	-	expression tag	UNP B7MLA0
D	-1	SER	-	expression tag	UNP B7MLA0
E	-17	GLY	-	expression tag	UNP B7MLA0
E	-16	SER	-	expression tag	UNP B7MLA0
E	-15	HIS	-	expression tag	UNP B7MLA0
E	-14	MET	-	expression tag	UNP B7MLA0
E	-13	ALA	-	expression tag	UNP B7MLA0
E	-12	SER	-	expression tag	UNP B7MLA0
E	-11	MET	-	expression tag	UNP B7MLA0
E	-10	THR	-	expression tag	UNP B7MLA0
E	-9	GLY	-	expression tag	UNP B7MLA0
E	-8	GLY	-	expression tag	UNP B7MLA0
E	-7	GLN	-	expression tag	UNP B7MLA0
E	-6	GLN	-	expression tag	UNP B7MLA0
E	-5	MET	-	expression tag	UNP B7MLA0
E	-4	GLY	-	expression tag	UNP B7MLA0
E	-3	ARG	-	expression tag	UNP B7MLA0
E	-2	GLY	-	expression tag	UNP B7MLA0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP B7MLA0

- Molecule 2 is 2-PHOSPHOGLYCERIC ACID (three-letter code: 2PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			11	3	7	1		
2	B	1	Total	C	O	P	0	0
			11	3	7	1		
2	C	1	Total	C	O	P	0	0
			11	3	7	1		
2	F	1	Total	C	O	P	0	0
			11	3	7	1		
2	D	1	Total	C	O	P	0	0
			11	3	7	1		
2	E	1	Total	C	O	P	0	0
			11	3	7	1		

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

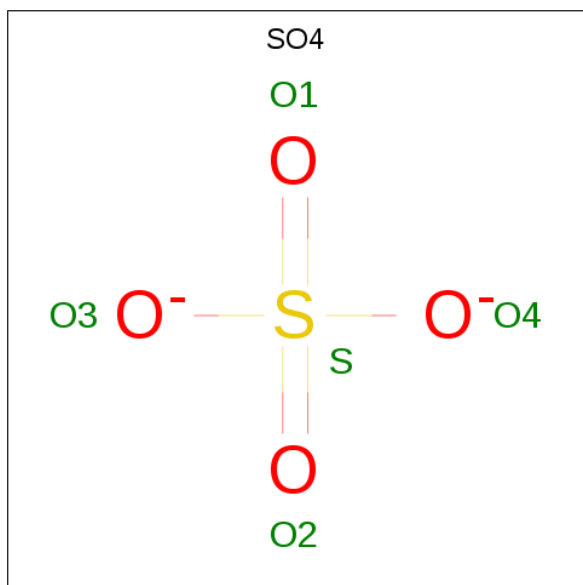
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		
3	F	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



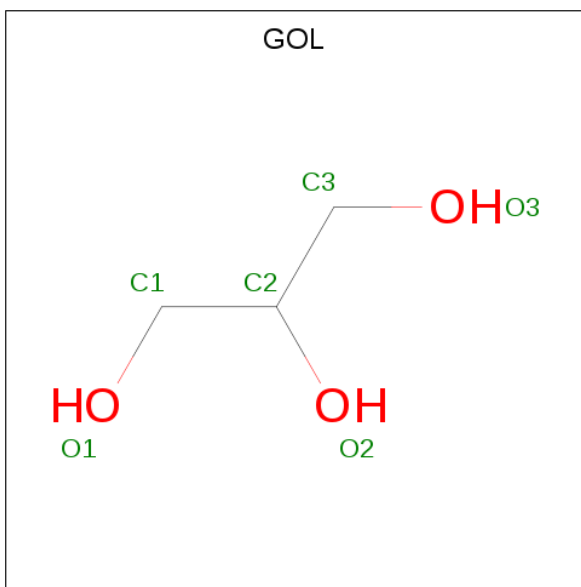
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

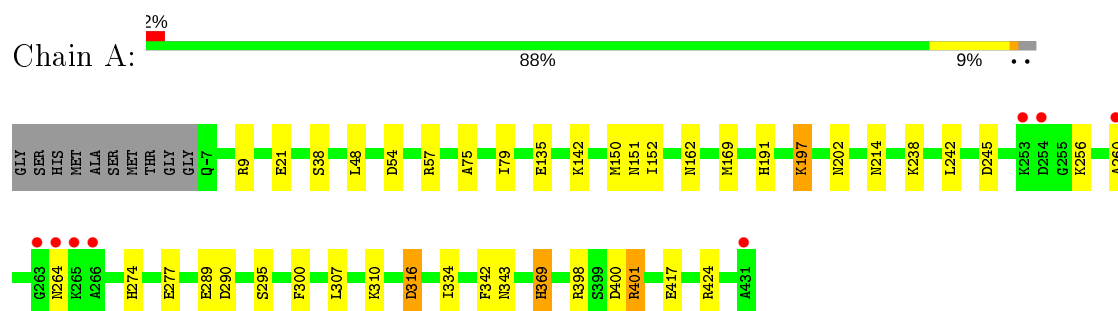
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	186	Total	O	0	0
			186	186		
6	B	209	Total	O	0	0
			209	209		
6	C	241	Total	O	0	0
			241	241		
6	F	123	Total	O	0	0
			123	123		
6	D	169	Total	O	0	0
			169	169		
6	E	175	Total	O	0	0
			175	175		

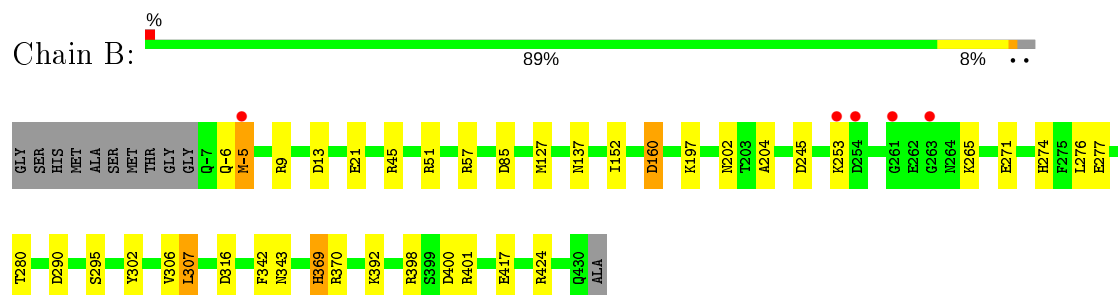
3 Residue-property plots [i](#)

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.

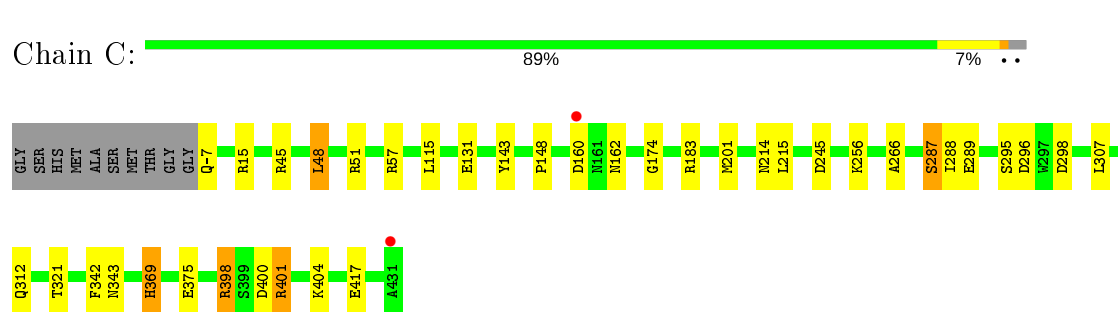
• Molecule 1: Enolase



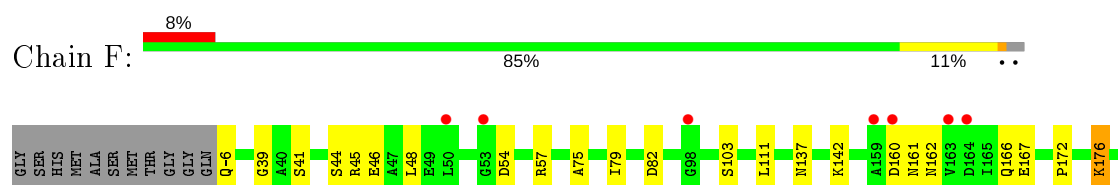
• Molecule 1: Enolase

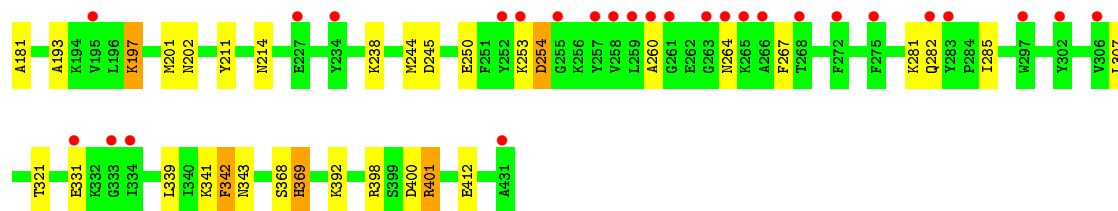


• Molecule 1: Enolase

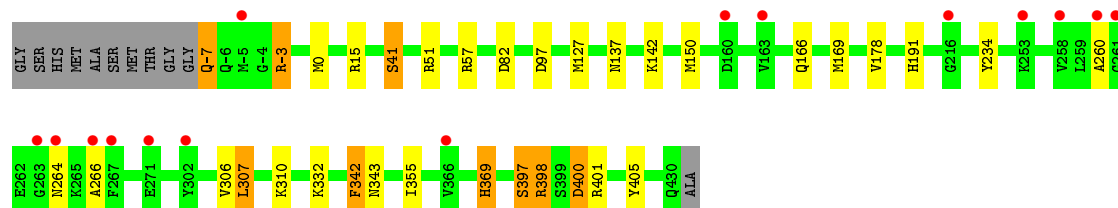
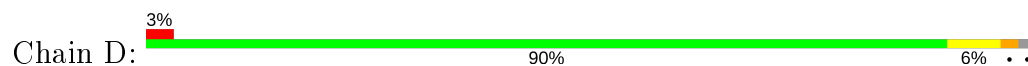


• Molecule 1: Enolase

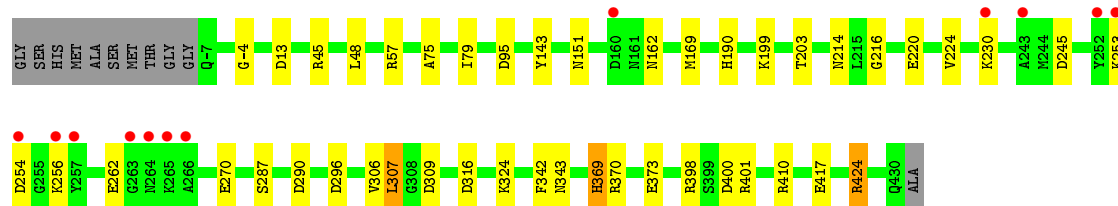
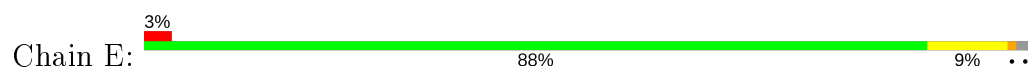




● Molecule 1: Enolase



● Molecule 1: Enolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.94Å 142.40Å 206.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.61 – 1.81 37.17 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (78.61-1.81) 100.0 (37.17-1.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.166 , 0.232 0.195 , 0.227	Depositor DCC
R_{free} test set	14043 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20818	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: GOL, MG, SO4, 2PG

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	1.28	7/3296 (0.2%)	1.11	10/4435 (0.2%)
1	B	1.33	7/3291 (0.2%)	1.14	18/4428 (0.4%)
1	C	1.34	11/3296 (0.3%)	1.14	15/4435 (0.3%)
1	D	1.29	4/3291 (0.1%)	1.11	9/4428 (0.2%)
1	E	1.21	4/3300 (0.1%)	1.09	11/4439 (0.2%)
1	F	1.23	6/3287 (0.2%)	1.09	6/4423 (0.1%)
All	All	1.28	39/19761 (0.2%)	1.11	69/26588 (0.3%)

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	GLU	CD-OE2	-8.66	1.16	1.25
1	C	287	SER	CA-CB	8.10	1.65	1.52
1	E	287	SER	CA-CB	7.32	1.64	1.52
1	A	21	GLU	CD-OE1	7.02	1.33	1.25
1	C	375	GLU	CG-CD	6.78	1.62	1.51

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	F	57	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	A	424	ARG	NE-CZ-NH1	-9.31	115.64	120.30
1	B	424	ARG	NE-CZ-NH1	-8.89	115.86	120.30
1	D	-7	GLN	CB-CA-C	8.88	128.16	110.40

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	3254	0	3278	14	0
1	B	3249	0	3273	12	0
1	C	3254	0	3278	13	0
1	D	3249	0	3273	12	0
1	E	3258	0	3285	13	0
1	F	3245	0	3270	26	0
2	A	11	0	4	0	0
2	B	11	0	4	0	0
2	C	11	0	4	0	0
2	D	11	0	4	0	0
2	E	11	0	4	0	0
2	F	11	0	4	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	1	0
4	C	25	0	0	0	0
4	D	10	0	0	0	0
4	E	20	0	0	1	0
4	F	5	0	0	0	0
5	D	6	0	8	0	0
5	E	6	0	8	0	0
5	F	6	0	6	0	0
6	A	186	0	0	1	0
6	B	209	0	0	1	0
6	C	241	0	0	1	0
6	D	169	0	0	3	0
6	E	175	0	0	1	0
6	F	123	0	0	1	0
All	All	20818	0	19703	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 88 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:C:201:MET:CE	1:C:215:LEU:HD23	1.78	1.13
1:F:167:GLU:OE1	1:F:392:LYS:HE2	1.60	1.01
1:C:201:MET:HE1	1:C:215:LEU:HD23	1.38	0.99
1:C:201:MET:HE2	1:C:215:LEU:HD23	1.52	0.91
1:A:197:LYS:HA	1:A:197:LYS:HE2	1.59	0.85

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	A	437/449 (97%)	425 (97%)	11 (2%)	1 (0%)	47	33
1	B	436/449 (97%)	418 (96%)	17 (4%)	1 (0%)	47	33
1	C	437/449 (97%)	426 (98%)	10 (2%)	1 (0%)	47	33
1	D	436/449 (97%)	419 (96%)	15 (3%)	2 (0%)	29	15
1	E	437/449 (97%)	422 (97%)	13 (3%)	2 (0%)	29	15
1	F	436/449 (97%)	424 (97%)	10 (2%)	2 (0%)	29	15
All	All	2619/2694 (97%)	2534 (97%)	76 (3%)	9 (0%)	41	27

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	254	ASP
1	D	266	ALA
1	E	-4	GLY
1	B	398	ARG
1	C	398	ARG

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	331/337 (98%)	319 (96%)	12 (4%)	35	19
1	B	331/337 (98%)	321 (97%)	10 (3%)	41	26
1	C	331/337 (98%)	325 (98%)	6 (2%)	59	48
1	D	331/337 (98%)	321 (97%)	10 (3%)	41	26
1	E	332/337 (98%)	319 (96%)	13 (4%)	32	17
1	F	330/337 (98%)	315 (96%)	15 (4%)	27	12
All	All	1986/2022 (98%)	1920 (97%)	66 (3%)	38	23

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	142	LYS
1	F	282	GLN
1	E	342	PHE
1	F	176	LYS
1	F	238	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	171	GLN
1	F	166	GLN
1	E	214	ASN
1	C	303	GLN
1	F	171	GLN

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 ⓘ

Of 43 ligands modelled in this entry, 12 are monoatomic - leaving 31 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	E	506	-	4,4,4	0.51	0	6,6,6	0.57	0
4	SO4	D	801	-	4,4,4	0.52	0	6,6,6	1.07	0
4	SO4	C	506	-	4,4,4	0.23	0	6,6,6	1.49	1 (16%)
4	SO4	A	507	-	4,4,4	0.63	0	6,6,6	1.11	1 (16%)
5	GOL	F	505	-	5,5,5	1.52	1 (20%)	5,5,5	2.75	4 (80%)
5	GOL	D	806	-	5,5,5	0.89	0	5,5,5	2.64	4 (80%)
2	2PG	F	501	3	7,10,10	2.50	3 (42%)	8,14,14	1.53	2 (25%)
4	SO4	C	508	-	4,4,4	0.62	0	6,6,6	0.73	0
4	SO4	A	505	-	4,4,4	0.48	0	6,6,6	0.61	0
2	2PG	A	501	3	7,10,10	2.81	3 (42%)	8,14,14	2.28	3 (37%)
4	SO4	D	805	-	4,4,4	0.81	0	6,6,6	0.79	0
4	SO4	F	504	-	4,4,4	0.43	0	6,6,6	1.22	1 (16%)
4	SO4	C	507	-	4,4,4	0.57	0	6,6,6	0.67	0
4	SO4	A	504	-	4,4,4	1.14	1 (25%)	6,6,6	0.58	0
4	SO4	B	504	-	4,4,4	0.63	0	6,6,6	0.51	0
4	SO4	B	508	-	4,4,4	0.81	0	6,6,6	1.64	2 (33%)
5	GOL	E	508	-	5,5,5	0.35	0	5,5,5	1.84	1 (20%)
4	SO4	B	507	-	4,4,4	0.61	0	6,6,6	0.63	0
4	SO4	E	507	-	4,4,4	0.64	0	6,6,6	0.91	0
4	SO4	B	506	-	4,4,4	0.46	0	6,6,6	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	505	-	4,4,4	0.39	0	6,6,6	0.86	0
4	SO4	B	505	-	4,4,4	0.59	0	6,6,6	0.56	0
4	SO4	A	506	-	4,4,4	0.76	0	6,6,6	0.71	0
2	2PG	C	501	3	7,10,10	2.05	4 (57%)	8,14,14	1.68	2 (25%)
2	2PG	B	501	3	7,10,10	2.20	2 (28%)	8,14,14	1.59	2 (25%)
4	SO4	C	504	-	4,4,4	0.74	0	6,6,6	1.46	2 (33%)
4	SO4	A	508	-	4,4,4	0.54	0	6,6,6	0.59	0
4	SO4	E	505	-	4,4,4	0.57	0	6,6,6	1.27	1 (16%)
2	2PG	E	502	3	7,10,10	1.93	1 (14%)	8,14,14	1.78	2 (25%)
4	SO4	E	501	-	4,4,4	0.64	0	6,6,6	1.19	0
2	2PG	D	802	3	7,10,10	1.60	2 (28%)	8,14,14	1.22	1 (12%)

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
5	GOL	E	508	-	-	4/4/4/4	-
5	GOL	F	505	-	-	2/4/4/4	-
2	2PG	C	501	3	-	0/7/11/11	-
2	2PG	B	501	3	-	0/7/11/11	-
2	2PG	F	501	3	-	0/7/11/11	-
5	GOL	D	806	-	-	2/4/4/4	-
2	2PG	E	502	3	-	1/7/11/11	-
2	2PG	A	501	3	-	0/7/11/11	-
2	2PG	D	802	3	-	0/7/11/11	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	2PG	P-O1P	5.03	1.68	1.59
2	A	501	2PG	O1P-C2	-5.02	1.39	1.45
2	F	501	2PG	O1P-C2	-4.77	1.39	1.45
2	E	502	2PG	O1P-C2	-4.58	1.39	1.45
2	B	501	2PG	O1P-C2	-4.27	1.40	1.45

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	2PG	P-O1P-C2	-4.72	112.20	123.04
5	D	806	GOL	O3-C3-C2	-4.06	90.73	110.20
2	C	501	2PG	P-O1P-C2	-3.68	114.58	123.04
5	F	505	GOL	O2-C2-C1	-3.60	93.25	109.12
2	E	502	2PG	P-O1P-C2	-3.51	114.99	123.04

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	806	GOL	C1-C2-C3-O3
5	E	508	GOL	O1-C1-C2-C3
5	E	508	GOL	C1-C2-C3-O3
5	F	505	GOL	C1-C2-C3-O3
5	E	508	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	2PG	1	0
4	B	507	SO4	1	0
4	E	507	SO4	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	439/449 (97%)	-0.08	8 (1%) 68 64	13, 23, 42, 63	0
1	B	438/449 (97%)	-0.19	5 (1%) 80 78	14, 21, 39, 66	0
1	C	439/449 (97%)	-0.29	2 (0%) 91 89	12, 20, 38, 54	0
1	D	438/449 (97%)	-0.04	15 (3%) 45 39	13, 22, 47, 67	0
1	E	438/449 (97%)	-0.09	12 (2%) 54 49	13, 25, 46, 68	0
1	F	438/449 (97%)	0.39	34 (7%) 13 10	15, 29, 56, 82	0
All	All	2630/2694 (97%)	-0.05	76 (2%) 51 46	12, 23, 46, 82	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	431	ALA	8.1
1	F	258	VAL	6.8
1	D	263	GLY	5.9
1	F	260	ALA	4.9
1	F	266	ALA	4.8

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. 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	SO4	D	805	5/5	0.35	0.41	68,78,115,131	0
5	GOL	F	505	6/6	0.79	0.21	29,33,39,73	0
4	SO4	A	507	5/5	0.82	0.19	54,57,95,102	0
4	SO4	B	504	5/5	0.85	0.19	51,61,92,110	0
5	GOL	E	508	6/6	0.86	0.12	32,39,49,49	0
4	SO4	C	507	5/5	0.89	0.16	53,53,70,87	0
4	SO4	E	507	5/5	0.89	0.17	52,52,56,85	0
5	GOL	D	806	6/6	0.90	0.15	27,34,39,66	0
3	MG	F	503	1/1	0.90	0.27	48,48,48,48	0
4	SO4	A	508	5/5	0.92	0.18	33,65,70,97	0
4	SO4	F	504	5/5	0.93	0.19	48,59,65,70	0
4	SO4	B	507	5/5	0.95	0.11	26,60,61,70	0
4	SO4	A	506	5/5	0.95	0.09	40,44,45,58	0
4	SO4	C	506	5/5	0.96	0.09	40,41,60,67	0
3	MG	D	804	1/1	0.96	0.07	36,36,36,36	0
2	2PG	F	501	11/11	0.96	0.15	25,29,36,37	0
4	SO4	C	508	5/5	0.96	0.21	27,58,65,71	0
4	SO4	C	504	5/5	0.96	0.08	38,41,44,49	0
4	SO4	E	501	5/5	0.96	0.12	36,39,47,64	0
4	SO4	E	505	5/5	0.96	0.11	43,44,47,66	0
4	SO4	D	801	5/5	0.97	0.10	35,37,44,68	0
4	SO4	B	506	5/5	0.97	0.09	36,39,41,48	0
4	SO4	B	505	5/5	0.97	0.10	40,42,48,57	0
4	SO4	A	504	5/5	0.97	0.11	38,40,42,44	0
4	SO4	A	505	5/5	0.97	0.16	43,44,51,55	0
3	MG	F	502	1/1	0.97	0.05	31,31,31,31	0
2	2PG	A	501	11/11	0.97	0.09	16,19,22,23	0
3	MG	C	502	1/1	0.97	0.05	19,19,19,19	0
2	2PG	D	802	11/11	0.97	0.14	18,23,28,29	0
2	2PG	C	501	11/11	0.98	0.10	14,16,21,21	0
2	2PG	B	501	11/11	0.98	0.09	16,17,19,19	0
3	MG	D	803	1/1	0.98	0.08	28,28,28,28	0
3	MG	E	503	1/1	0.98	0.04	25,25,25,25	0
4	SO4	E	506	5/5	0.98	0.17	39,44,52,60	0
4	SO4	B	508	5/5	0.98	0.15	34,39,43,49	0
3	MG	B	503	1/1	0.98	0.07	28,28,28,28	0
3	MG	A	503	1/1	0.98	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	502	1/1	0.98	0.04	27,27,27,27	0
2	2PG	E	502	11/11	0.98	0.08	18,20,26,29	0
3	MG	E	504	1/1	0.98	0.09	34,34,34,34	0
3	MG	A	502	1/1	0.98	0.04	29,29,29,29	0
3	MG	C	503	1/1	0.99	0.08	27,27,27,27	0
4	SO4	C	505	5/5	0.99	0.05	32,34,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.