



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 03:24 am BST

PDB ID : 3UJ2  
Title : CRYSTAL STRUCTURE OF AN ENOLASE FROM ANAEROSTIPES CAC-  
CAE (EFI TARGET EFI-502054) WITH BOUND MG AND SULFATE  
Authors : Vetting, M.W.; Toro, R.; Bhosle, R.; Hillerich, B.; Washington, E.; Scott  
Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker,  
H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2011-11-07  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (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

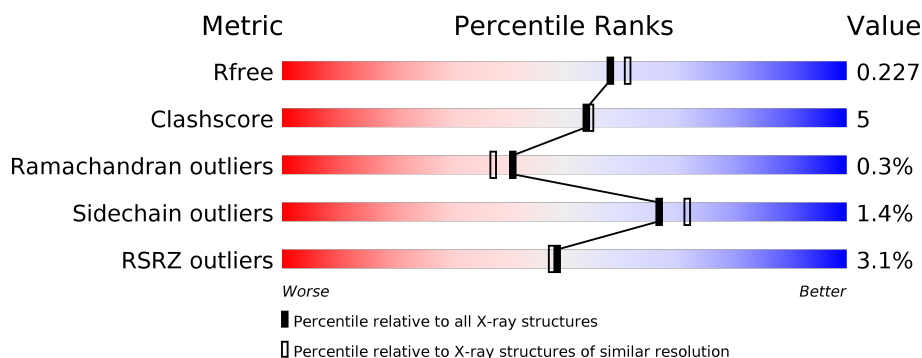
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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>84%</div> <div>10% 6%</div> </div>
1	B	449	<div>2%</div> <div>83%</div> <div>11% 6%</div>

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Mol	Chain	Length	Quality of chain
1	G	449	<div><div>%</div><div><div></div><div>84%</div><div>10%</div><div>• 6%</div></div></div>
1	H	449	<div><div>7%</div><div><div></div><div>79%</div><div>14%</div><div>• 6%</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27374 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	1	0
			3209	2010	548	636	15			
1	B	423	Total	C	N	O	S	0	1	0
			3214	2016	548	636	14			
1	C	423	Total	C	N	O	S	0	1	0
			3212	2012	548	638	14			
1	D	423	Total	C	N	O	S	0	0	0
			3203	2007	547	635	14			
1	E	423	Total	C	N	O	S	0	0	0
			3203	2007	547	635	14			
1	F	423	Total	C	N	O	S	0	0	0
			3203	2007	547	635	14			
1	G	423	Total	C	N	O	S	0	0	0
			3203	2007	547	635	14			
1	H	423	Total	C	N	O	S	0	0	0
			3203	2007	547	635	14			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP B0MAG5
A	-20	HIS	-	EXPRESSION TAG	UNP B0MAG5
A	-19	HIS	-	EXPRESSION TAG	UNP B0MAG5
A	-18	HIS	-	EXPRESSION TAG	UNP B0MAG5
A	-17	HIS	-	EXPRESSION TAG	UNP B0MAG5
A	-16	HIS	-	EXPRESSION TAG	UNP B0MAG5
A	-15	HIS	-	EXPRESSION TAG	UNP B0MAG5
A	-14	SER	-	EXPRESSION TAG	UNP B0MAG5
A	-13	SER	-	EXPRESSION TAG	UNP B0MAG5
A	-12	GLY	-	EXPRESSION TAG	UNP B0MAG5
A	-11	VAL	-	EXPRESSION TAG	UNP B0MAG5
A	-10	ASP	-	EXPRESSION TAG	UNP B0MAG5
A	-9	LEU	-	EXPRESSION TAG	UNP B0MAG5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	EXPRESSION TAG	UNP B0MAG5
A	-7	THR	-	EXPRESSION TAG	UNP B0MAG5
A	-6	GLU	-	EXPRESSION TAG	UNP B0MAG5
A	-5	ASN	-	EXPRESSION TAG	UNP B0MAG5
A	-4	LEU	-	EXPRESSION TAG	UNP B0MAG5
A	-3	TYR	-	EXPRESSION TAG	UNP B0MAG5
A	-2	PHE	-	EXPRESSION TAG	UNP B0MAG5
A	-1	GLN	-	EXPRESSION TAG	UNP B0MAG5
A	0	SER	-	EXPRESSION TAG	UNP B0MAG5
B	-21	MET	-	EXPRESSION TAG	UNP B0MAG5
B	-20	HIS	-	EXPRESSION TAG	UNP B0MAG5
B	-19	HIS	-	EXPRESSION TAG	UNP B0MAG5
B	-18	HIS	-	EXPRESSION TAG	UNP B0MAG5
B	-17	HIS	-	EXPRESSION TAG	UNP B0MAG5
B	-16	HIS	-	EXPRESSION TAG	UNP B0MAG5
B	-15	HIS	-	EXPRESSION TAG	UNP B0MAG5
B	-14	SER	-	EXPRESSION TAG	UNP B0MAG5
B	-13	SER	-	EXPRESSION TAG	UNP B0MAG5
B	-12	GLY	-	EXPRESSION TAG	UNP B0MAG5
B	-11	VAL	-	EXPRESSION TAG	UNP B0MAG5
B	-10	ASP	-	EXPRESSION TAG	UNP B0MAG5
B	-9	LEU	-	EXPRESSION TAG	UNP B0MAG5
B	-8	GLY	-	EXPRESSION TAG	UNP B0MAG5
B	-7	THR	-	EXPRESSION TAG	UNP B0MAG5
B	-6	GLU	-	EXPRESSION TAG	UNP B0MAG5
B	-5	ASN	-	EXPRESSION TAG	UNP B0MAG5
B	-4	LEU	-	EXPRESSION TAG	UNP B0MAG5
B	-3	TYR	-	EXPRESSION TAG	UNP B0MAG5
B	-2	PHE	-	EXPRESSION TAG	UNP B0MAG5
B	-1	GLN	-	EXPRESSION TAG	UNP B0MAG5
B	0	SER	-	EXPRESSION TAG	UNP B0MAG5
C	-21	MET	-	EXPRESSION TAG	UNP B0MAG5
C	-20	HIS	-	EXPRESSION TAG	UNP B0MAG5
C	-19	HIS	-	EXPRESSION TAG	UNP B0MAG5
C	-18	HIS	-	EXPRESSION TAG	UNP B0MAG5
C	-17	HIS	-	EXPRESSION TAG	UNP B0MAG5
C	-16	HIS	-	EXPRESSION TAG	UNP B0MAG5
C	-15	HIS	-	EXPRESSION TAG	UNP B0MAG5
C	-14	SER	-	EXPRESSION TAG	UNP B0MAG5
C	-13	SER	-	EXPRESSION TAG	UNP B0MAG5
C	-12	GLY	-	EXPRESSION TAG	UNP B0MAG5
C	-11	VAL	-	EXPRESSION TAG	UNP B0MAG5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	ASP	-	EXPRESSION TAG	UNP B0MAG5
C	-9	LEU	-	EXPRESSION TAG	UNP B0MAG5
C	-8	GLY	-	EXPRESSION TAG	UNP B0MAG5
C	-7	THR	-	EXPRESSION TAG	UNP B0MAG5
C	-6	GLU	-	EXPRESSION TAG	UNP B0MAG5
C	-5	ASN	-	EXPRESSION TAG	UNP B0MAG5
C	-4	LEU	-	EXPRESSION TAG	UNP B0MAG5
C	-3	TYR	-	EXPRESSION TAG	UNP B0MAG5
C	-2	PHE	-	EXPRESSION TAG	UNP B0MAG5
C	-1	GLN	-	EXPRESSION TAG	UNP B0MAG5
C	0	SER	-	EXPRESSION TAG	UNP B0MAG5
D	-21	MET	-	EXPRESSION TAG	UNP B0MAG5
D	-20	HIS	-	EXPRESSION TAG	UNP B0MAG5
D	-19	HIS	-	EXPRESSION TAG	UNP B0MAG5
D	-18	HIS	-	EXPRESSION TAG	UNP B0MAG5
D	-17	HIS	-	EXPRESSION TAG	UNP B0MAG5
D	-16	HIS	-	EXPRESSION TAG	UNP B0MAG5
D	-15	HIS	-	EXPRESSION TAG	UNP B0MAG5
D	-14	SER	-	EXPRESSION TAG	UNP B0MAG5
D	-13	SER	-	EXPRESSION TAG	UNP B0MAG5
D	-12	GLY	-	EXPRESSION TAG	UNP B0MAG5
D	-11	VAL	-	EXPRESSION TAG	UNP B0MAG5
D	-10	ASP	-	EXPRESSION TAG	UNP B0MAG5
D	-9	LEU	-	EXPRESSION TAG	UNP B0MAG5
D	-8	GLY	-	EXPRESSION TAG	UNP B0MAG5
D	-7	THR	-	EXPRESSION TAG	UNP B0MAG5
D	-6	GLU	-	EXPRESSION TAG	UNP B0MAG5
D	-5	ASN	-	EXPRESSION TAG	UNP B0MAG5
D	-4	LEU	-	EXPRESSION TAG	UNP B0MAG5
D	-3	TYR	-	EXPRESSION TAG	UNP B0MAG5
D	-2	PHE	-	EXPRESSION TAG	UNP B0MAG5
D	-1	GLN	-	EXPRESSION TAG	UNP B0MAG5
D	0	SER	-	EXPRESSION TAG	UNP B0MAG5
E	-21	MET	-	EXPRESSION TAG	UNP B0MAG5
E	-20	HIS	-	EXPRESSION TAG	UNP B0MAG5
E	-19	HIS	-	EXPRESSION TAG	UNP B0MAG5
E	-18	HIS	-	EXPRESSION TAG	UNP B0MAG5
E	-17	HIS	-	EXPRESSION TAG	UNP B0MAG5
E	-16	HIS	-	EXPRESSION TAG	UNP B0MAG5
E	-15	HIS	-	EXPRESSION TAG	UNP B0MAG5
E	-14	SER	-	EXPRESSION TAG	UNP B0MAG5
E	-13	SER	-	EXPRESSION TAG	UNP B0MAG5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	GLY	-	EXPRESSION TAG	UNP B0MAG5
E	-11	VAL	-	EXPRESSION TAG	UNP B0MAG5
E	-10	ASP	-	EXPRESSION TAG	UNP B0MAG5
E	-9	LEU	-	EXPRESSION TAG	UNP B0MAG5
E	-8	GLY	-	EXPRESSION TAG	UNP B0MAG5
E	-7	THR	-	EXPRESSION TAG	UNP B0MAG5
E	-6	GLU	-	EXPRESSION TAG	UNP B0MAG5
E	-5	ASN	-	EXPRESSION TAG	UNP B0MAG5
E	-4	LEU	-	EXPRESSION TAG	UNP B0MAG5
E	-3	TYR	-	EXPRESSION TAG	UNP B0MAG5
E	-2	PHE	-	EXPRESSION TAG	UNP B0MAG5
E	-1	GLN	-	EXPRESSION TAG	UNP B0MAG5
E	0	SER	-	EXPRESSION TAG	UNP B0MAG5
F	-21	MET	-	EXPRESSION TAG	UNP B0MAG5
F	-20	HIS	-	EXPRESSION TAG	UNP B0MAG5
F	-19	HIS	-	EXPRESSION TAG	UNP B0MAG5
F	-18	HIS	-	EXPRESSION TAG	UNP B0MAG5
F	-17	HIS	-	EXPRESSION TAG	UNP B0MAG5
F	-16	HIS	-	EXPRESSION TAG	UNP B0MAG5
F	-15	HIS	-	EXPRESSION TAG	UNP B0MAG5
F	-14	SER	-	EXPRESSION TAG	UNP B0MAG5
F	-13	SER	-	EXPRESSION TAG	UNP B0MAG5
F	-12	GLY	-	EXPRESSION TAG	UNP B0MAG5
F	-11	VAL	-	EXPRESSION TAG	UNP B0MAG5
F	-10	ASP	-	EXPRESSION TAG	UNP B0MAG5
F	-9	LEU	-	EXPRESSION TAG	UNP B0MAG5
F	-8	GLY	-	EXPRESSION TAG	UNP B0MAG5
F	-7	THR	-	EXPRESSION TAG	UNP B0MAG5
F	-6	GLU	-	EXPRESSION TAG	UNP B0MAG5
F	-5	ASN	-	EXPRESSION TAG	UNP B0MAG5
F	-4	LEU	-	EXPRESSION TAG	UNP B0MAG5
F	-3	TYR	-	EXPRESSION TAG	UNP B0MAG5
F	-2	PHE	-	EXPRESSION TAG	UNP B0MAG5
F	-1	GLN	-	EXPRESSION TAG	UNP B0MAG5
F	0	SER	-	EXPRESSION TAG	UNP B0MAG5
G	-21	MET	-	EXPRESSION TAG	UNP B0MAG5
G	-20	HIS	-	EXPRESSION TAG	UNP B0MAG5
G	-19	HIS	-	EXPRESSION TAG	UNP B0MAG5
G	-18	HIS	-	EXPRESSION TAG	UNP B0MAG5
G	-17	HIS	-	EXPRESSION TAG	UNP B0MAG5
G	-16	HIS	-	EXPRESSION TAG	UNP B0MAG5
G	-15	HIS	-	EXPRESSION TAG	UNP B0MAG5

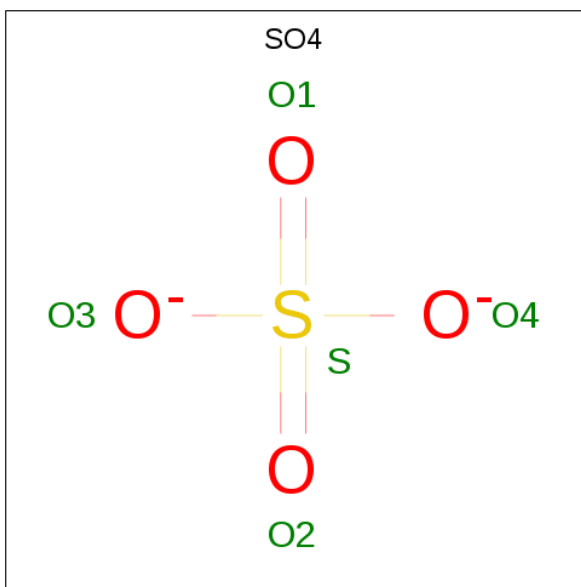
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	SER	-	EXPRESSION TAG	UNP B0MAG5
G	-13	SER	-	EXPRESSION TAG	UNP B0MAG5
G	-12	GLY	-	EXPRESSION TAG	UNP B0MAG5
G	-11	VAL	-	EXPRESSION TAG	UNP B0MAG5
G	-10	ASP	-	EXPRESSION TAG	UNP B0MAG5
G	-9	LEU	-	EXPRESSION TAG	UNP B0MAG5
G	-8	GLY	-	EXPRESSION TAG	UNP B0MAG5
G	-7	THR	-	EXPRESSION TAG	UNP B0MAG5
G	-6	GLU	-	EXPRESSION TAG	UNP B0MAG5
G	-5	ASN	-	EXPRESSION TAG	UNP B0MAG5
G	-4	LEU	-	EXPRESSION TAG	UNP B0MAG5
G	-3	TYR	-	EXPRESSION TAG	UNP B0MAG5
G	-2	PHE	-	EXPRESSION TAG	UNP B0MAG5
G	-1	GLN	-	EXPRESSION TAG	UNP B0MAG5
G	0	SER	-	EXPRESSION TAG	UNP B0MAG5
H	-21	MET	-	EXPRESSION TAG	UNP B0MAG5
H	-20	HIS	-	EXPRESSION TAG	UNP B0MAG5
H	-19	HIS	-	EXPRESSION TAG	UNP B0MAG5
H	-18	HIS	-	EXPRESSION TAG	UNP B0MAG5
H	-17	HIS	-	EXPRESSION TAG	UNP B0MAG5
H	-16	HIS	-	EXPRESSION TAG	UNP B0MAG5
H	-15	HIS	-	EXPRESSION TAG	UNP B0MAG5
H	-14	SER	-	EXPRESSION TAG	UNP B0MAG5
H	-13	SER	-	EXPRESSION TAG	UNP B0MAG5
H	-12	GLY	-	EXPRESSION TAG	UNP B0MAG5
H	-11	VAL	-	EXPRESSION TAG	UNP B0MAG5
H	-10	ASP	-	EXPRESSION TAG	UNP B0MAG5
H	-9	LEU	-	EXPRESSION TAG	UNP B0MAG5
H	-8	GLY	-	EXPRESSION TAG	UNP B0MAG5
H	-7	THR	-	EXPRESSION TAG	UNP B0MAG5
H	-6	GLU	-	EXPRESSION TAG	UNP B0MAG5
H	-5	ASN	-	EXPRESSION TAG	UNP B0MAG5
H	-4	LEU	-	EXPRESSION TAG	UNP B0MAG5
H	-3	TYR	-	EXPRESSION TAG	UNP B0MAG5
H	-2	PHE	-	EXPRESSION TAG	UNP B0MAG5
H	-1	GLN	-	EXPRESSION TAG	UNP B0MAG5
H	0	SER	-	EXPRESSION TAG	UNP B0MAG5

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	264	Total	O	0	0
			264	264		
4	B	252	Total	O	0	0
			252	252		
4	C	225	Total	O	0	0
			225	225		

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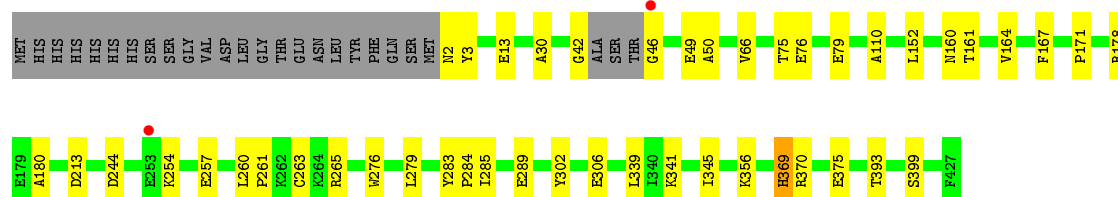
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	162	Total 162	O 162	0	0
4	E	183	Total 183	O 183	0	0
4	F	208	Total 208	O 208	0	0
4	G	176	Total 176	O 176	0	0
4	H	146	Total 146	O 146	0	0

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


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

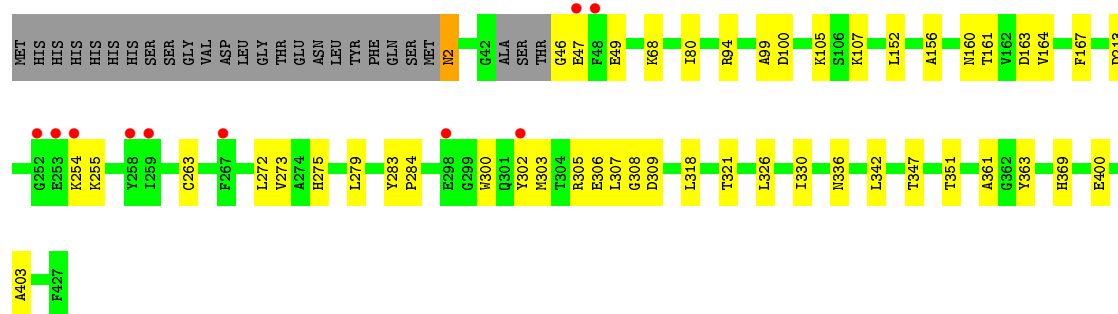
#### • Molecule 1: Enolase 1

Chain A: 




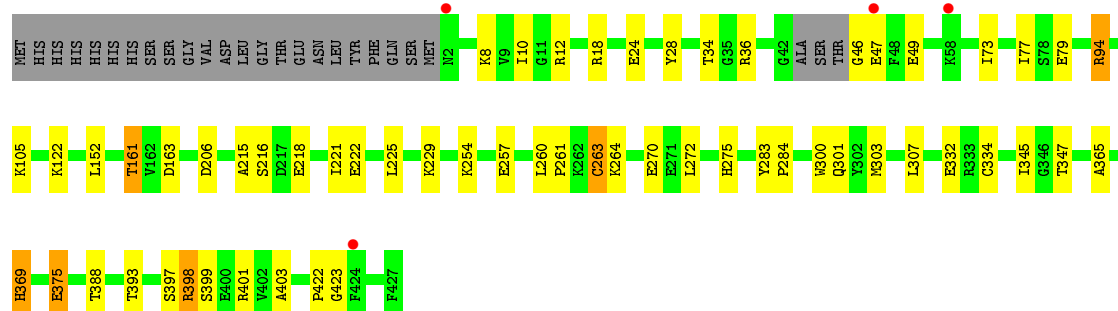
#### • Molecule 1: Enolase 1

Chain B: 




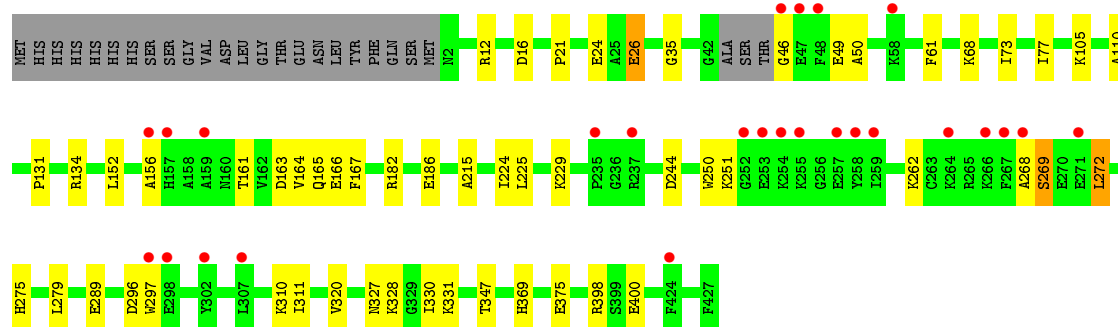
#### • Molecule 1: Enolase 1

Chain C: 




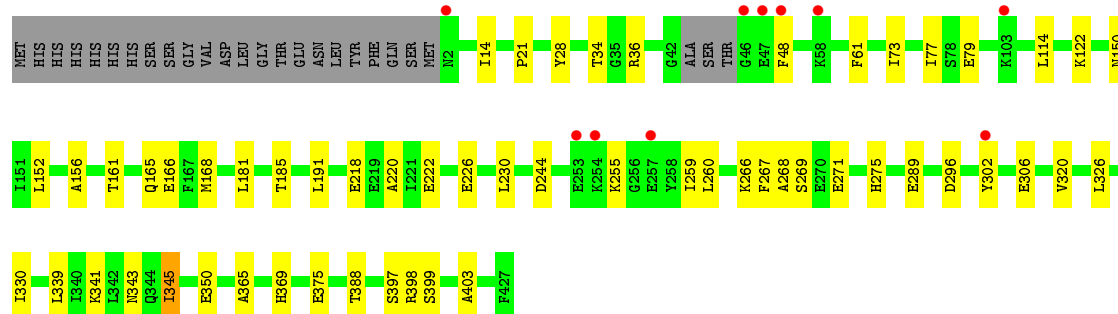
- Molecule 1: Enolase 1

Chain D: 




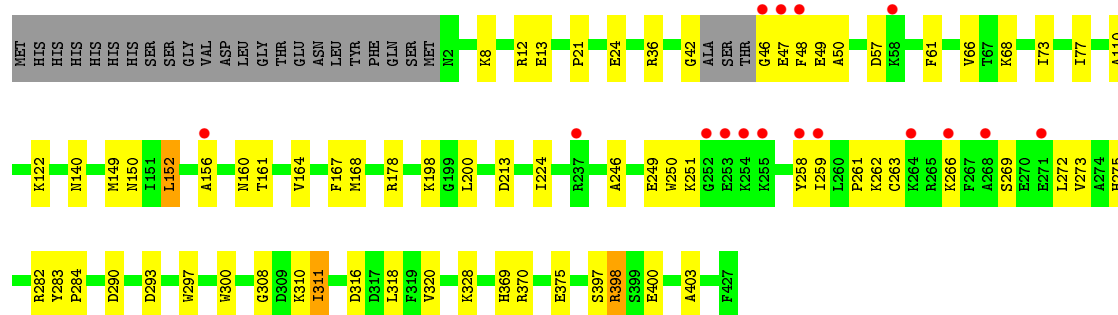
- Molecule 1: Enolase 1

Chain E: 




- Molecule 1: Enolase 1

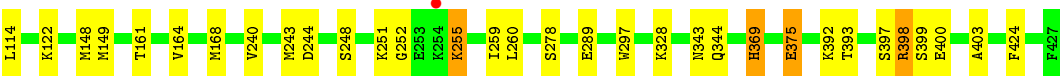
Chain F: 



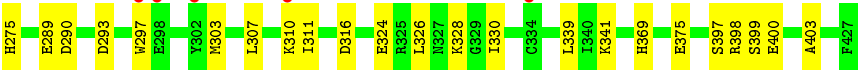
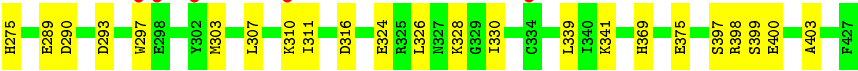
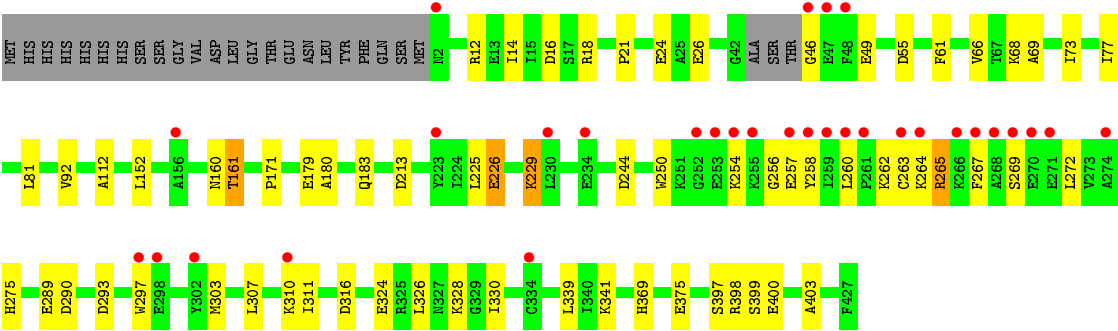
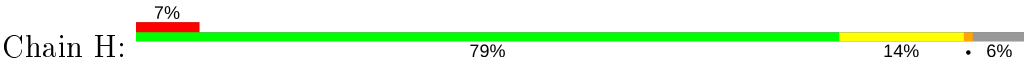
- Molecule 1: Enolase 1

Chain G: 





● Molecule 1: Enolase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	282.35Å 282.21Å 119.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.03 – 2.00 46.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	63.6 (46.03-2.00) 63.1 (46.03-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, $R_{free}$	0.172 , 0.231 0.171 , 0.227	Depositor DCC
$R_{free}$ test set	1398 reflections (0.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.042 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	27374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8004e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4

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	0.41	0/3257	0.56	0/4394
1	B	0.41	0/3263	0.55	0/4402
1	C	0.39	0/3260	0.55	0/4398
1	D	0.37	0/3251	0.52	0/4386
1	E	0.36	0/3251	0.52	0/4386
1	F	0.38	0/3251	0.54	0/4386
1	G	0.35	0/3251	0.52	0/4386
1	H	0.34	0/3251	0.51	0/4386
All	All	0.38	0/26035	0.53	0/35124

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 [i](#)

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	3209	0	3178	29	0
1	B	3214	0	3182	29	0
1	C	3212	0	3179	39	0
1	D	3203	0	3174	33	0
1	E	3203	0	3174	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3203	0	3174	45	0
1	G	3203	0	3174	33	0
1	H	3203	0	3174	46	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	15	0	0	0	0
2	H	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	264	0	0	2	0
4	B	252	0	0	2	0
4	C	225	0	0	5	0
4	D	162	0	0	2	0
4	E	183	0	0	2	0
4	F	208	0	0	4	0
4	G	176	0	0	2	0
4	H	146	0	0	2	0
All	All	27374	0	25409	272	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 5.

The worst 5 of 272 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:H:46:GLY:HA3	1:H:49:GLU:OE2	1.83	0.78
1:A:263:CYS:SG	1:A:265:ARG:HB2	2.26	0.76
1:H:326:LEU:O	1:H:330:ILE:HG13	1.90	0.70
1:F:160:ASN:HB3	1:F:213:ASP:HA	1.73	0.70
1:A:283:TYR:HB2	1:A:285:ILE:HD12	1.73	0.69

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	420/449 (94%)	406 (97%)	14 (3%)	0	100	100
1	B	420/449 (94%)	404 (96%)	14 (3%)	2 (0%)	29	23
1	C	420/449 (94%)	404 (96%)	15 (4%)	1 (0%)	47	44
1	D	419/449 (93%)	400 (96%)	17 (4%)	2 (0%)	29	23
1	E	419/449 (93%)	405 (97%)	13 (3%)	1 (0%)	47	44
1	F	419/449 (93%)	398 (95%)	18 (4%)	3 (1%)	22	16
1	G	419/449 (93%)	405 (97%)	13 (3%)	1 (0%)	47	44
1	H	419/449 (93%)	401 (96%)	18 (4%)	0	100	100
All	All	3355/3592 (93%)	3223 (96%)	122 (4%)	10 (0%)	41	37

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	ALA
1	D	156	ALA
1	E	156	ALA
1	F	156	ALA
1	F	308	GLY

### 5.3.2 Protein sidechains [i](#)

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	332/354 (94%)	328 (99%)	4 (1%)	71	76
1	B	332/354 (94%)	328 (99%)	4 (1%)	71	76
1	C	332/354 (94%)	325 (98%)	7 (2%)	53	57
1	D	331/354 (94%)	327 (99%)	4 (1%)	71	76
1	E	331/354 (94%)	329 (99%)	2 (1%)	86	90
1	F	331/354 (94%)	327 (99%)	4 (1%)	71	76
1	G	331/354 (94%)	327 (99%)	4 (1%)	71	76
1	H	331/354 (94%)	323 (98%)	8 (2%)	49	51
All	All	2651/2832 (94%)	2614 (99%)	37 (1%)	67	72

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	269	SER
1	E	369	HIS
1	H	229	LYS
1	D	272	LEU
1	D	369	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	327	ASN
1	C	2	ASN
1	F	2	ASN
1	H	2	ASN

### 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 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	$\# Z  > 2$
2	SO4	B	430	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	C	429	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	D	428	-	4,4,4	0.18	0	6,6,6	0.17	0
2	SO4	H	428	-	4,4,4	0.15	0	6,6,6	0.35	0
2	SO4	B	428	-	4,4,4	0.19	0	6,6,6	0.36	0
2	SO4	A	428	-	4,4,4	0.11	0	6,6,6	0.33	0
2	SO4	A	430	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	C	428	-	4,4,4	0.07	0	6,6,6	0.33	0
2	SO4	G	430	-	4,4,4	0.12	0	6,6,6	0.36	0
2	SO4	E	428	-	4,4,4	0.12	0	6,6,6	0.22	0
2	SO4	G	428	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	C	430	-	4,4,4	0.10	0	6,6,6	0.15	0
2	SO4	G	429	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	B	429	-	4,4,4	0.19	0	6,6,6	0.30	0
2	SO4	A	429	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SO4	D	429	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	F	429	-	4,4,4	0.15	0	6,6,6	0.21	0
2	SO4	E	429	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	H	429	-	4,4,4	0.12	0	6,6,6	0.11	0
2	SO4	F	428	-	4,4,4	0.19	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	423/449 (94%)	-0.38	2 (0%) 91 90	7, 19, 48, 79	0
1	B	423/449 (94%)	-0.19	10 (2%) 59 57	7, 21, 63, 99	0
1	C	423/449 (94%)	-0.29	4 (0%) 84 83	9, 25, 54, 81	0
1	D	423/449 (94%)	0.14	26 (6%) 21 20	14, 32, 75, 108	0
1	E	423/449 (94%)	-0.08	10 (2%) 59 57	14, 30, 63, 90	0
1	F	423/449 (94%)	-0.11	16 (3%) 40 39	10, 27, 69, 110	0
1	G	423/449 (94%)	-0.18	5 (1%) 79 78	16, 31, 57, 86	0
1	H	423/449 (94%)	0.16	31 (7%) 15 14	15, 36, 78, 118	0
All	All	3384/3592 (94%)	-0.12	104 (3%) 49 48	7, 28, 65, 118	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	GLY	6.0
1	D	259	ILE	5.1
1	H	271	GLU	5.0
1	D	252	GLY	5.0
1	H	254	LYS	4.9

### 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	D	430	1/1	0.80	0.11	44,44,44,44	0
2	SO4	C	430	5/5	0.83	0.19	72,88,90,94	0
2	SO4	A	430	5/5	0.87	0.15	87,91,103,108	0
2	SO4	B	430	5/5	0.89	0.14	81,82,94,100	0
3	MG	H	430	1/1	0.90	0.10	58,58,58,58	0
2	SO4	G	429	5/5	0.91	0.13	81,89,98,101	0
3	MG	F	430	1/1	0.95	0.06	41,41,41,41	0
3	MG	B	431	1/1	0.95	0.08	34,34,34,34	0
3	MG	G	431	1/1	0.95	0.11	32,32,32,32	0
3	MG	E	430	1/1	0.96	0.05	37,37,37,37	0
3	MG	C	431	1/1	0.96	0.07	36,36,36,36	0
2	SO4	G	428	5/5	0.97	0.10	53,57,60,68	0
2	SO4	D	428	5/5	0.98	0.08	39,51,56,63	0
2	SO4	H	428	5/5	0.98	0.11	25,41,47,64	0
2	SO4	D	429	5/5	0.98	0.11	38,43,49,62	0
2	SO4	G	430	5/5	0.98	0.11	32,33,43,49	0
3	MG	A	431	1/1	0.98	0.06	27,27,27,27	0
2	SO4	E	429	5/5	0.99	0.09	39,54,62,63	0
2	SO4	B	429	5/5	0.99	0.11	31,39,39,44	0
2	SO4	F	428	5/5	0.99	0.10	37,38,45,56	0
2	SO4	H	429	5/5	0.99	0.06	48,49,55,59	0
2	SO4	F	429	5/5	0.99	0.08	36,37,39,41	0
2	SO4	C	429	5/5	0.99	0.07	39,40,50,51	0
2	SO4	A	428	5/5	0.99	0.09	31,33,35,36	0
2	SO4	A	429	5/5	0.99	0.06	40,44,49,55	0
2	SO4	B	428	5/5	0.99	0.08	36,36,37,44	0
2	SO4	C	428	5/5	0.99	0.11	25,33,44,54	0
2	SO4	E	428	5/5	0.99	0.12	34,41,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.