



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:22 am GMT

PDB ID : 1XRH  
Title : Crystal Structure of Ureidoglycolate Dehydrogenase from Escherichia Coli  
Authors : Rajashankar, K.R.; Kniewel, R.; Lima, C.D.; Burley, S.K.; New York SGX  
Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2004-10-14  
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

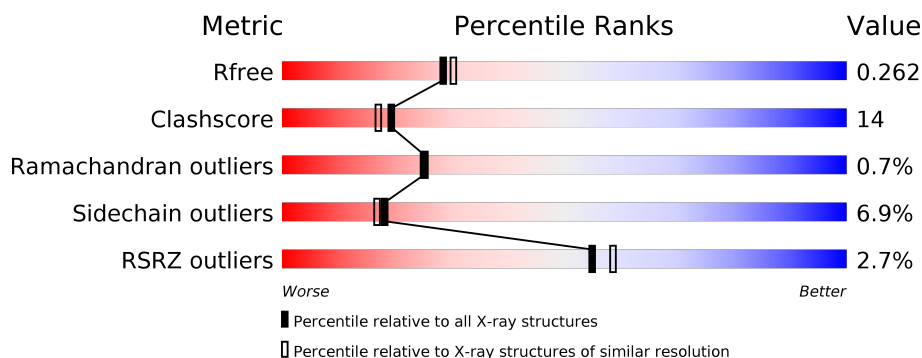
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	351	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>5%</div> </div> </div>
1	B	351	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div></div> </div> </div>
1	C	351	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div></div> </div> </div>
1	D	351	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div></div> </div> </div>
1	E	351	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div></div> </div> </div>
1	F	351	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	351	<div><div></div><div>3%</div><div></div><div>71%</div><div>22%</div><div></div><div></div></div>
1	H	351	<div><div></div><div>2%</div><div></div><div>75%</div><div>20%</div><div></div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21480 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 Ureidoglycolate Dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	Se	0	0	0
			2616	1647	457	497	3	12			
1	B	343	Total	C	N	O	S	Se	0	0	0
			2616	1647	457	497	3	12			
1	C	344	Total	C	N	O	S	Se	0	0	0
			2622	1650	458	499	3	12			
1	D	342	Total	C	N	O	S	Se	0	0	0
			2607	1642	456	494	3	12			
1	E	343	Total	C	N	O	S	Se	0	0	0
			2616	1647	457	497	3	12			
1	F	339	Total	C	N	O	S	Se	0	0	0
			2582	1626	453	488	3	12			
1	G	341	Total	C	N	O	S	Se	0	0	0
			2595	1633	455	492	3	12			
1	H	339	Total	C	N	O	S	Se	0	0	0
			2582	1626	453	488	3	12			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	CLONING ARTIFACT	UNP P77555
A	2	SER	-	CLONING ARTIFACT	UNP P77555
A	3	SER	MET	CLONING ARTIFACT	UNP P77555
A	94	MSE	MET	MODIFIED RESIDUE	UNP P77555
A	96	MSE	MET	MODIFIED RESIDUE	UNP P77555
A	116	MSE	MET	MODIFIED RESIDUE	UNP P77555
A	139	MSE	MET	MODIFIED RESIDUE	UNP P77555
A	145	MSE	MET	MODIFIED RESIDUE	UNP P77555
A	177	MSE	MET	MODIFIED RESIDUE	UNP P77555
A	195	MSE	MET	MODIFIED RESIDUE	UNP P77555
A	231	MSE	MET	MODIFIED RESIDUE	UNP P77555
A	232	MSE	MET	MODIFIED RESIDUE	UNP P77555
A	233	MSE	MET	MODIFIED RESIDUE	UNP P77555

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Chain	Residue	Modelled	Actual	Comment	Reference
A	253	MSE	MET	MODIFIED RESIDUE	UNP P77555
A	289	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	1	SER	-	CLONING ARTIFACT	UNP P77555
B	2	SER	-	CLONING ARTIFACT	UNP P77555
B	3	SER	MET	CLONING ARTIFACT	UNP P77555
B	94	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	96	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	116	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	139	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	145	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	177	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	195	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	231	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	232	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	233	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	253	MSE	MET	MODIFIED RESIDUE	UNP P77555
B	289	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	1	SER	-	CLONING ARTIFACT	UNP P77555
C	2	SER	-	CLONING ARTIFACT	UNP P77555
C	3	SER	MET	CLONING ARTIFACT	UNP P77555
C	94	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	96	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	116	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	139	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	145	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	177	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	195	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	231	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	232	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	233	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	253	MSE	MET	MODIFIED RESIDUE	UNP P77555
C	289	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	1	SER	-	CLONING ARTIFACT	UNP P77555
D	2	SER	-	CLONING ARTIFACT	UNP P77555
D	3	SER	MET	CLONING ARTIFACT	UNP P77555
D	94	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	96	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	116	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	139	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	145	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	177	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	195	MSE	MET	MODIFIED RESIDUE	UNP P77555

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Chain	Residue	Modelled	Actual	Comment	Reference
D	231	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	232	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	233	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	253	MSE	MET	MODIFIED RESIDUE	UNP P77555
D	289	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	1	SER	-	CLONING ARTIFACT	UNP P77555
E	2	SER	-	CLONING ARTIFACT	UNP P77555
E	3	SER	MET	CLONING ARTIFACT	UNP P77555
E	94	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	96	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	116	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	139	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	145	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	177	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	195	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	231	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	232	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	233	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	253	MSE	MET	MODIFIED RESIDUE	UNP P77555
E	289	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	1	SER	-	CLONING ARTIFACT	UNP P77555
F	2	SER	-	CLONING ARTIFACT	UNP P77555
F	3	SER	MET	CLONING ARTIFACT	UNP P77555
F	94	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	96	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	116	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	139	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	145	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	177	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	195	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	231	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	232	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	233	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	253	MSE	MET	MODIFIED RESIDUE	UNP P77555
F	289	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	1	SER	-	CLONING ARTIFACT	UNP P77555
G	2	SER	-	CLONING ARTIFACT	UNP P77555
G	3	SER	MET	CLONING ARTIFACT	UNP P77555
G	94	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	96	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	116	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	139	MSE	MET	MODIFIED RESIDUE	UNP P77555

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Chain	Residue	Modelled	Actual	Comment	Reference
G	145	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	177	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	195	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	231	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	232	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	233	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	253	MSE	MET	MODIFIED RESIDUE	UNP P77555
G	289	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	1	SER	-	CLONING ARTIFACT	UNP P77555
H	2	SER	-	CLONING ARTIFACT	UNP P77555
H	3	SER	MET	CLONING ARTIFACT	UNP P77555
H	94	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	96	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	116	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	139	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	145	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	177	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	195	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	231	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	232	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	233	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	253	MSE	MET	MODIFIED RESIDUE	UNP P77555
H	289	MSE	MET	MODIFIED RESIDUE	UNP P77555

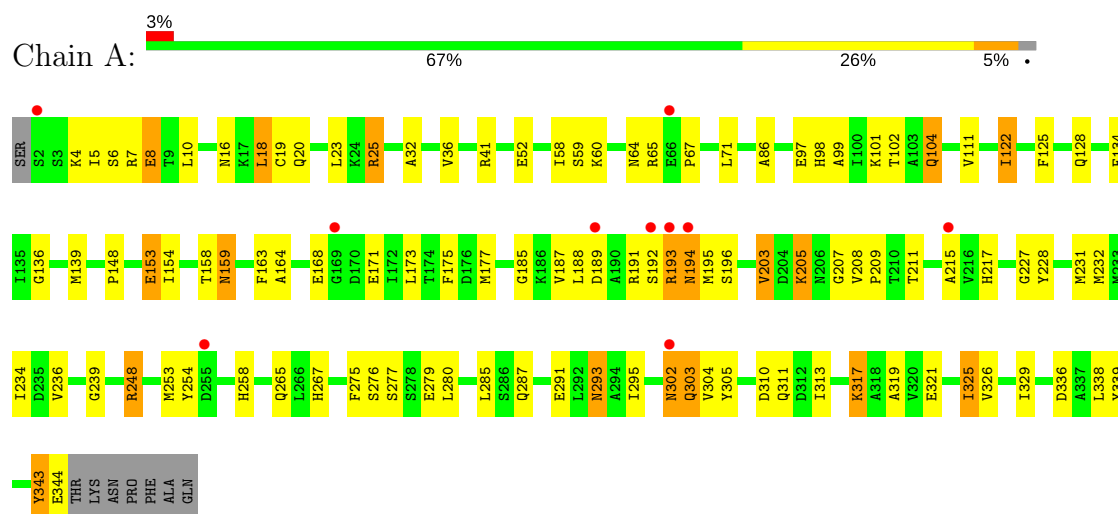
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	58	Total O 58 58	0	0
2	B	102	Total O 102 102	0	0
2	C	77	Total O 77 77	0	0
2	D	113	Total O 113 113	0	0
2	E	61	Total O 61 61	0	0
2	F	70	Total O 70 70	0	0
2	G	69	Total O 69 69	0	0
2	H	94	Total O 94 94	0	0

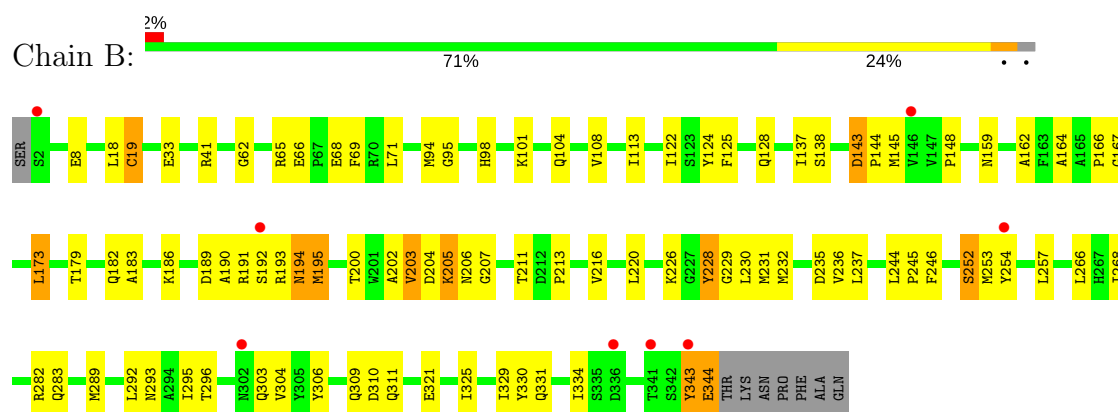
### 3 Residue-property plots

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.

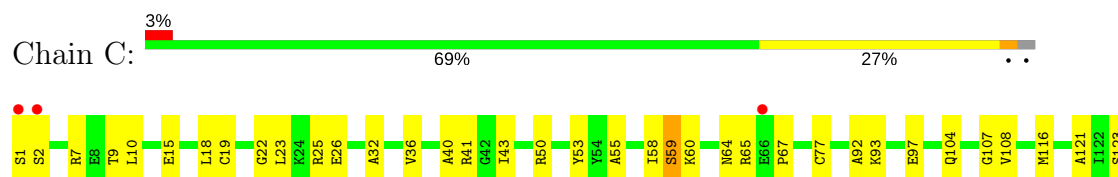
#### • Molecule 1: Ureidoglycolate Dehydrogenase



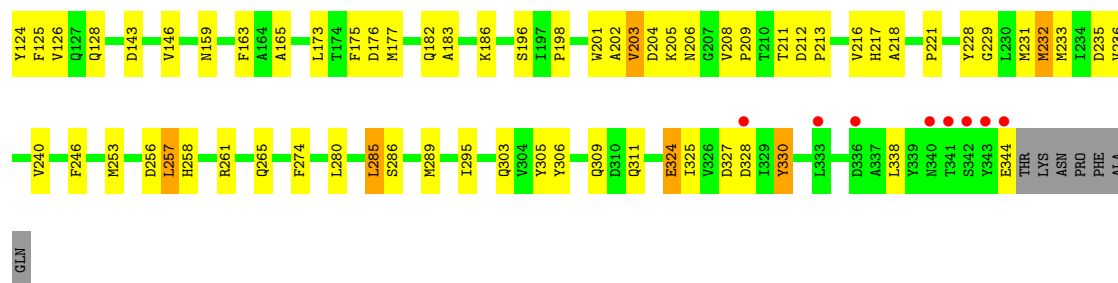
#### • Molecule 1: Ureidoglycolate Dehydrogenase



#### • Molecule 1: Ureidoglycolate Dehydrogenase







• Molecule 1: Ureidoglycolate Dehydrogenase

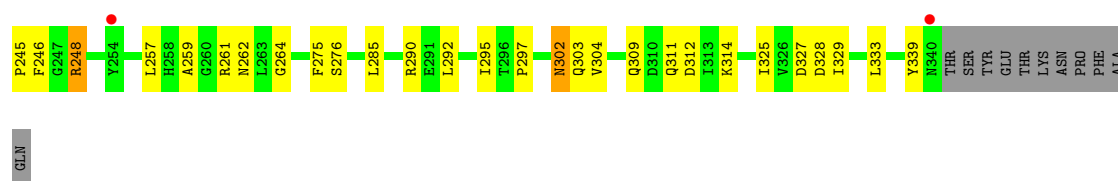


• Molecule 1: Ureidoglycolate Dehydrogenase

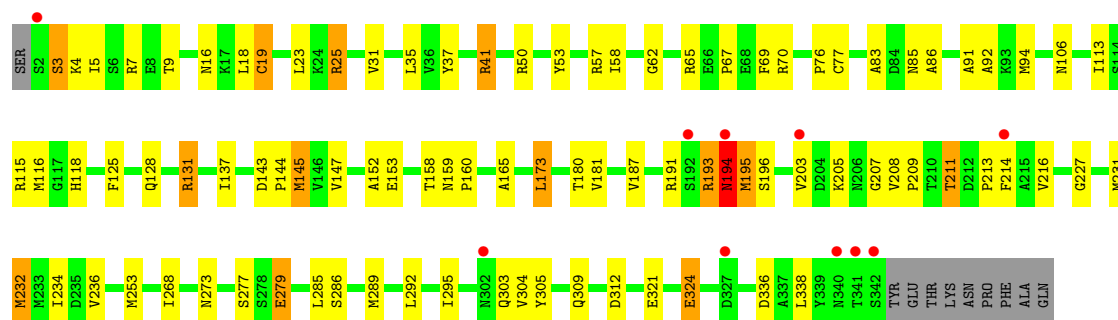


• Molecule 1: Ureidoglycolate Dehydrogenase

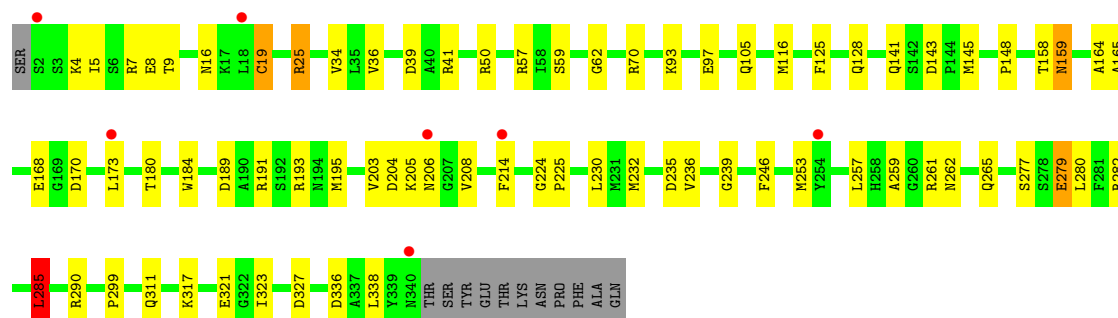
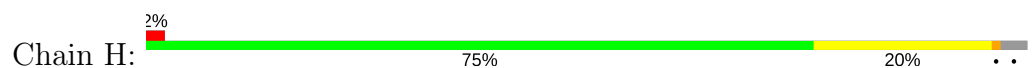




• Molecule 1: Ureidoglycolate Dehydrogenase



• Molecule 1: Ureidoglycolate Dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.72Å 129.92Å 106.47Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	19.86 – 2.25 19.85 – 2.25	Depositor EDS
% Data completeness (in resolution range)	75.6 (19.86-2.25) 90.0 (19.85-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.192 , 0.250 0.206 , 0.262	Depositor DCC
$R_{free}$ test set	5149 reflections (4.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.80	0/2660	0.83	1/3587 (0.0%)
1	B	0.88	1/2660 (0.0%)	0.90	1/3587 (0.0%)
1	C	0.82	0/2666	0.88	1/3595 (0.0%)
1	D	0.85	1/2651 (0.0%)	0.91	1/3575 (0.0%)
1	E	0.85	0/2660	0.86	2/3587 (0.1%)
1	F	0.83	0/2625	0.87	2/3539 (0.1%)
1	G	0.83	1/2638 (0.0%)	0.83	1/3557 (0.0%)
1	H	0.83	2/2625 (0.1%)	0.88	2/3539 (0.1%)
All	All	0.84	5/21185 (0.0%)	0.87	11/28566 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	G	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	19	CYS	CB-SG	-7.29	1.69	1.82
1	H	168	GLU	CG-CD	6.58	1.61	1.51
1	B	19	CYS	CB-SG	-6.14	1.71	1.82
1	D	19	CYS	CB-SG	-5.68	1.72	1.81
1	H	19	CYS	CB-SG	-5.00	1.73	1.81

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	231	MSE	CG-SE-CE	-6.16	85.34	98.90
1	E	39	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	253	MSE	CB-CG-SE	-5.58	95.95	112.70
1	F	143	ASP	CB-CG-OD2	5.55	123.29	118.30
1	C	232	MSE	CG-SE-CE	5.47	110.94	98.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	TYR	Sidechain
1	B	228	TYR	Sidechain
1	B	343	TYR	Sidechain
1	C	228	TYR	Sidechain
1	C	330	TYR	Sidechain

## 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	2616	0	2559	89	0
1	B	2616	0	2559	86	0
1	C	2622	0	2567	76	0
1	D	2607	0	2553	74	0
1	E	2616	0	2559	109	0
1	F	2582	0	2532	79	0
1	G	2595	0	2544	87	0
1	H	2582	0	2532	53	0
2	A	58	0	0	0	0
2	B	102	0	0	5	0
2	C	77	0	0	4	0
2	D	113	0	0	4	0
2	E	61	0	0	7	0
2	F	70	0	0	1	0
2	G	69	0	0	7	0
2	H	94	0	0	3	0
All	All	21480	0	20405	597	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 14.

The worst 5 of 597 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:E:50:ARG:HH21	1:E:253:MSE:HE1	1.09	1.15
1:G:232:MSE:HE2	1:G:236:VAL:HG21	1.27	1.14
1:A:153:GLU:HG3	1:B:295:ILE:HG23	1.34	1.10
1:A:232:MSE:HE3	1:B:173:LEU:HG	1.31	1.09
1:C:232:MSE:HE3	1:D:173:LEU:HD13	1.34	1.08

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	341/351 (97%)	317 (93%)	21 (6%)	3 (1%)	20	17
1	B	341/351 (97%)	323 (95%)	14 (4%)	4 (1%)	15	11
1	C	342/351 (97%)	332 (97%)	9 (3%)	1 (0%)	44	50
1	D	340/351 (97%)	329 (97%)	9 (3%)	2 (1%)	28	29
1	E	341/351 (97%)	319 (94%)	20 (6%)	2 (1%)	28	29
1	F	337/351 (96%)	321 (95%)	12 (4%)	4 (1%)	15	11
1	G	339/351 (97%)	326 (96%)	12 (4%)	1 (0%)	44	50
1	H	337/351 (96%)	325 (96%)	10 (3%)	2 (1%)	28	29
All	All	2718/2808 (97%)	2592 (95%)	107 (4%)	19 (1%)	25	25

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	MSE

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Mol	Chain	Res	Type
1	E	194	ASN
1	B	192	SER
1	B	194	ASN
1	G	194	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	A	272/267 (102%)	248 (91%)	24 (9%)	12	10
1	B	272/267 (102%)	256 (94%)	16 (6%)	23	23
1	C	273/267 (102%)	259 (95%)	14 (5%)	28	30
1	D	271/267 (102%)	249 (92%)	22 (8%)	14	12
1	E	272/267 (102%)	252 (93%)	20 (7%)	16	15
1	F	268/267 (100%)	244 (91%)	24 (9%)	11	9
1	G	270/267 (101%)	253 (94%)	17 (6%)	21	20
1	H	268/267 (100%)	256 (96%)	12 (4%)	32	36
All	All	2166/2136 (101%)	2017 (93%)	149 (7%)	18	17

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	211	THR
1	E	180	THR
1	H	25	ARG
1	D	231	MSE
1	D	326	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	267	HIS

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Mol	Chain	Res	Type
1	E	303	GLN
1	H	128	GLN
1	D	303	GLN
1	E	127	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	331/351 (94%)	0.08	10 (3%) 51 55	25, 40, 59, 75	0
1	B	331/351 (94%)	-0.07	8 (2%) 59 63	21, 33, 54, 70	0
1	C	332/351 (94%)	-0.01	11 (3%) 47 51	19, 37, 53, 68	0
1	D	330/351 (94%)	-0.14	4 (1%) 79 81	21, 34, 50, 67	0
1	E	331/351 (94%)	0.07	18 (5%) 26 31	21, 37, 59, 75	0
1	F	327/351 (93%)	-0.09	4 (1%) 79 81	24, 38, 54, 67	0
1	G	329/351 (93%)	-0.00	10 (3%) 51 55	22, 35, 58, 73	0
1	H	327/351 (93%)	-0.09	7 (2%) 64 67	19, 32, 55, 65	0
All	All	2638/2808 (93%)	-0.03	72 (2%) 55 58	19, 36, 56, 75	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	SER	6.2
1	B	341	THR	4.9
1	E	344	GLU	4.5
1	E	343	TYR	4.3
1	G	341	THR	4.2

### 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.