Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:15 AM GMT

PDB ID	:	2Q17
Title	:	Formylglycine Generating Enzyme from Streptomyces coelicolor
Authors	:	Carlson, B.L.; Ballister, E.R.; Skordalakes, E.; King, D.S.; Breidenbach, M.A.; Gilmore, S.A.; Berger, J.M.; Bertozzi, C.R.
Deposited on	:	2007-05-23
Resolution	:	2.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

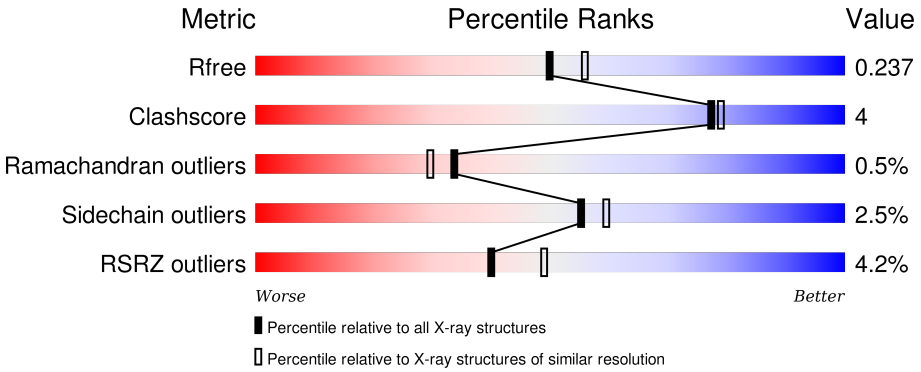
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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 <=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	346	4% 75% 8% 17%
1	B	346	3% 73% 10% • 17%
1	C	346	5% 76% 7% 17%
1	D	346	2% 74% 8% 17%
1	E	346	4% 76% 7% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12171 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 formylglycine generating enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	2	0
			2240	1396	429	407	8			
1	B	288	Total	C	N	O	S	0	2	0
			2243	1397	429	409	8			
1	C	287	Total	C	N	O	S	0	2	0
			2232	1391	425	408	8			
1	D	286	Total	C	N	O	S	0	2	0
			2224	1387	424	405	8			
1	E	289	Total	C	N	O	S	0	2	0
			2251	1403	430	410	8			

There are 170 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	EXPRESSION TAG	UNP Q9F3C7
A	-30	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-29	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-28	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-27	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-26	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-25	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-24	GLY	-	EXPRESSION TAG	UNP Q9F3C7
A	-23	LYS	-	EXPRESSION TAG	UNP Q9F3C7
A	-22	PRO	-	EXPRESSION TAG	UNP Q9F3C7
A	-21	ILE	-	EXPRESSION TAG	UNP Q9F3C7
A	-20	PRO	-	EXPRESSION TAG	UNP Q9F3C7
A	-19	ASN	-	EXPRESSION TAG	UNP Q9F3C7
A	-18	PRO	-	EXPRESSION TAG	UNP Q9F3C7
A	-17	LEU	-	EXPRESSION TAG	UNP Q9F3C7
A	-16	LEU	-	EXPRESSION TAG	UNP Q9F3C7
A	-15	GLY	-	EXPRESSION TAG	UNP Q9F3C7
A	-14	LEU	-	EXPRESSION TAG	UNP Q9F3C7
A	-13	ASP	-	EXPRESSION TAG	UNP Q9F3C7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	SER	-	EXPRESSION TAG	UNP Q9F3C7
A	-11	THR	-	EXPRESSION TAG	UNP Q9F3C7
A	-10	GLU	-	EXPRESSION TAG	UNP Q9F3C7
A	-9	ASN	-	EXPRESSION TAG	UNP Q9F3C7
A	-8	LEU	-	EXPRESSION TAG	UNP Q9F3C7
A	-7	TYR	-	EXPRESSION TAG	UNP Q9F3C7
A	-6	PHE	-	EXPRESSION TAG	UNP Q9F3C7
A	-5	GLN	-	EXPRESSION TAG	UNP Q9F3C7
A	-4	GLY	-	EXPRESSION TAG	UNP Q9F3C7
A	-3	ILE	-	EXPRESSION TAG	UNP Q9F3C7
A	-2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
A	-1	PRO	-	EXPRESSION TAG	UNP Q9F3C7
A	0	PHE	-	EXPRESSION TAG	UNP Q9F3C7
A	1	THR	-	EXPRESSION TAG	UNP Q9F3C7
A	2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
B	-31	MET	-	EXPRESSION TAG	UNP Q9F3C7
B	-30	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-29	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-28	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-27	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-26	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-25	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-24	GLY	-	EXPRESSION TAG	UNP Q9F3C7
B	-23	LYS	-	EXPRESSION TAG	UNP Q9F3C7
B	-22	PRO	-	EXPRESSION TAG	UNP Q9F3C7
B	-21	ILE	-	EXPRESSION TAG	UNP Q9F3C7
B	-20	PRO	-	EXPRESSION TAG	UNP Q9F3C7
B	-19	ASN	-	EXPRESSION TAG	UNP Q9F3C7
B	-18	PRO	-	EXPRESSION TAG	UNP Q9F3C7
B	-17	LEU	-	EXPRESSION TAG	UNP Q9F3C7
B	-16	LEU	-	EXPRESSION TAG	UNP Q9F3C7
B	-15	GLY	-	EXPRESSION TAG	UNP Q9F3C7
B	-14	LEU	-	EXPRESSION TAG	UNP Q9F3C7
B	-13	ASP	-	EXPRESSION TAG	UNP Q9F3C7
B	-12	SER	-	EXPRESSION TAG	UNP Q9F3C7
B	-11	THR	-	EXPRESSION TAG	UNP Q9F3C7
B	-10	GLU	-	EXPRESSION TAG	UNP Q9F3C7
B	-9	ASN	-	EXPRESSION TAG	UNP Q9F3C7
B	-8	LEU	-	EXPRESSION TAG	UNP Q9F3C7
B	-7	TYR	-	EXPRESSION TAG	UNP Q9F3C7
B	-6	PHE	-	EXPRESSION TAG	UNP Q9F3C7
B	-5	GLN	-	EXPRESSION TAG	UNP Q9F3C7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP Q9F3C7
B	-3	ILE	-	EXPRESSION TAG	UNP Q9F3C7
B	-2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
B	-1	PRO	-	EXPRESSION TAG	UNP Q9F3C7
B	0	PHE	-	EXPRESSION TAG	UNP Q9F3C7
B	1	THR	-	EXPRESSION TAG	UNP Q9F3C7
B	2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
C	-31	MET	-	EXPRESSION TAG	UNP Q9F3C7
C	-30	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-29	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-28	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-27	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-26	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-25	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-24	GLY	-	EXPRESSION TAG	UNP Q9F3C7
C	-23	LYS	-	EXPRESSION TAG	UNP Q9F3C7
C	-22	PRO	-	EXPRESSION TAG	UNP Q9F3C7
C	-21	ILE	-	EXPRESSION TAG	UNP Q9F3C7
C	-20	PRO	-	EXPRESSION TAG	UNP Q9F3C7
C	-19	ASN	-	EXPRESSION TAG	UNP Q9F3C7
C	-18	PRO	-	EXPRESSION TAG	UNP Q9F3C7
C	-17	LEU	-	EXPRESSION TAG	UNP Q9F3C7
C	-16	LEU	-	EXPRESSION TAG	UNP Q9F3C7
C	-15	GLY	-	EXPRESSION TAG	UNP Q9F3C7
C	-14	LEU	-	EXPRESSION TAG	UNP Q9F3C7
C	-13	ASP	-	EXPRESSION TAG	UNP Q9F3C7
C	-12	SER	-	EXPRESSION TAG	UNP Q9F3C7
C	-11	THR	-	EXPRESSION TAG	UNP Q9F3C7
C	-10	GLU	-	EXPRESSION TAG	UNP Q9F3C7
C	-9	ASN	-	EXPRESSION TAG	UNP Q9F3C7
C	-8	LEU	-	EXPRESSION TAG	UNP Q9F3C7
C	-7	TYR	-	EXPRESSION TAG	UNP Q9F3C7
C	-6	PHE	-	EXPRESSION TAG	UNP Q9F3C7
C	-5	GLN	-	EXPRESSION TAG	UNP Q9F3C7
C	-4	GLY	-	EXPRESSION TAG	UNP Q9F3C7
C	-3	ILE	-	EXPRESSION TAG	UNP Q9F3C7
C	-2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
C	-1	PRO	-	EXPRESSION TAG	UNP Q9F3C7
C	0	PHE	-	EXPRESSION TAG	UNP Q9F3C7
C	1	THR	-	EXPRESSION TAG	UNP Q9F3C7
C	2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
D	-31	MET	-	EXPRESSION TAG	UNP Q9F3C7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-29	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-28	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-27	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-26	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-25	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-24	GLY	-	EXPRESSION TAG	UNP Q9F3C7
D	-23	LYS	-	EXPRESSION TAG	UNP Q9F3C7
D	-22	PRO	-	EXPRESSION TAG	UNP Q9F3C7
D	-21	ILE	-	EXPRESSION TAG	UNP Q9F3C7
D	-20	PRO	-	EXPRESSION TAG	UNP Q9F3C7
D	-19	ASN	-	EXPRESSION TAG	UNP Q9F3C7
D	-18	PRO	-	EXPRESSION TAG	UNP Q9F3C7
D	-17	LEU	-	EXPRESSION TAG	UNP Q9F3C7
D	-16	LEU	-	EXPRESSION TAG	UNP Q9F3C7
D	-15	GLY	-	EXPRESSION TAG	UNP Q9F3C7
D	-14	LEU	-	EXPRESSION TAG	UNP Q9F3C7
D	-13	ASP	-	EXPRESSION TAG	UNP Q9F3C7
D	-12	SER	-	EXPRESSION TAG	UNP Q9F3C7
D	-11	THR	-	EXPRESSION TAG	UNP Q9F3C7
D	-10	GLU	-	EXPRESSION TAG	UNP Q9F3C7
D	-9	ASN	-	EXPRESSION TAG	UNP Q9F3C7
D	-8	LEU	-	EXPRESSION TAG	UNP Q9F3C7
D	-7	TYR	-	EXPRESSION TAG	UNP Q9F3C7
D	-6	PHE	-	EXPRESSION TAG	UNP Q9F3C7
D	-5	GLN	-	EXPRESSION TAG	UNP Q9F3C7
D	-4	GLY	-	EXPRESSION TAG	UNP Q9F3C7
D	-3	ILE	-	EXPRESSION TAG	UNP Q9F3C7
D	-2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
D	-1	PRO	-	EXPRESSION TAG	UNP Q9F3C7
D	0	PHE	-	EXPRESSION TAG	UNP Q9F3C7
D	1	THR	-	EXPRESSION TAG	UNP Q9F3C7
D	2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
E	-31	MET	-	EXPRESSION TAG	UNP Q9F3C7
E	-30	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-29	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-28	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-27	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-26	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-25	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-24	GLY	-	EXPRESSION TAG	UNP Q9F3C7
E	-23	LYS	-	EXPRESSION TAG	UNP Q9F3C7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	PRO	-	EXPRESSION TAG	UNP Q9F3C7
E	-21	ILE	-	EXPRESSION TAG	UNP Q9F3C7
E	-20	PRO	-	EXPRESSION TAG	UNP Q9F3C7
E	-19	ASN	-	EXPRESSION TAG	UNP Q9F3C7
E	-18	PRO	-	EXPRESSION TAG	UNP Q9F3C7
E	-17	LEU	-	EXPRESSION TAG	UNP Q9F3C7
E	-16	LEU	-	EXPRESSION TAG	UNP Q9F3C7
E	-15	GLY	-	EXPRESSION TAG	UNP Q9F3C7
E	-14	LEU	-	EXPRESSION TAG	UNP Q9F3C7
E	-13	ASP	-	EXPRESSION TAG	UNP Q9F3C7
E	-12	SER	-	EXPRESSION TAG	UNP Q9F3C7
E	-11	THR	-	EXPRESSION TAG	UNP Q9F3C7
E	-10	GLU	-	EXPRESSION TAG	UNP Q9F3C7
E	-9	ASN	-	EXPRESSION TAG	UNP Q9F3C7
E	-8	LEU	-	EXPRESSION TAG	UNP Q9F3C7
E	-7	TYR	-	EXPRESSION TAG	UNP Q9F3C7
E	-6	PHE	-	EXPRESSION TAG	UNP Q9F3C7
E	-5	GLN	-	EXPRESSION TAG	UNP Q9F3C7
E	-4	GLY	-	EXPRESSION TAG	UNP Q9F3C7
E	-3	ILE	-	EXPRESSION TAG	UNP Q9F3C7
E	-2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
E	-1	PRO	-	EXPRESSION TAG	UNP Q9F3C7
E	0	PHE	-	EXPRESSION TAG	UNP Q9F3C7
E	1	THR	-	EXPRESSION TAG	UNP Q9F3C7
E	2	ASP	-	EXPRESSION TAG	UNP Q9F3C7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0

- Molecule 3 is water.

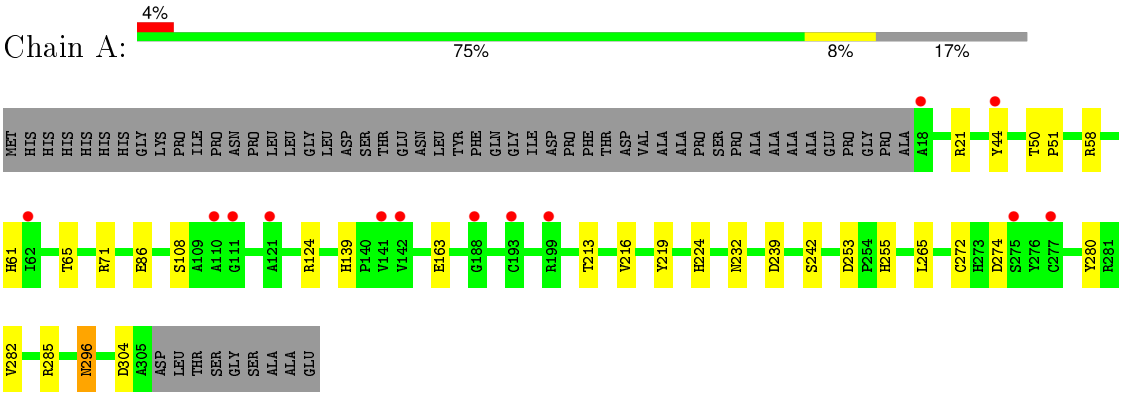
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	210	Total O 210 210	0	0
3	B	195	Total O 195 195	0	0
3	C	170	Total O 170 170	0	0
3	D	189	Total O 189 189	0	0
3	E	212	Total O 212 212	0	0

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 errors 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.

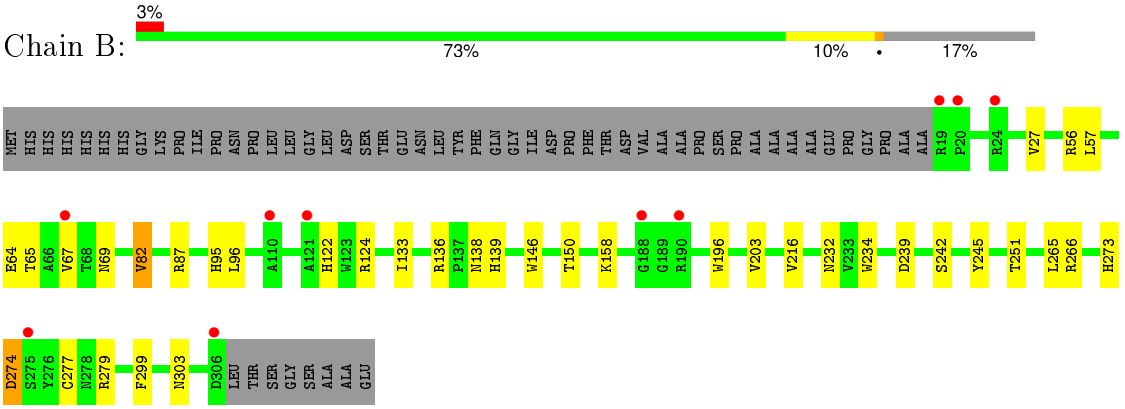
- Molecule 1: formylglycine generating enzyme

Chain A:



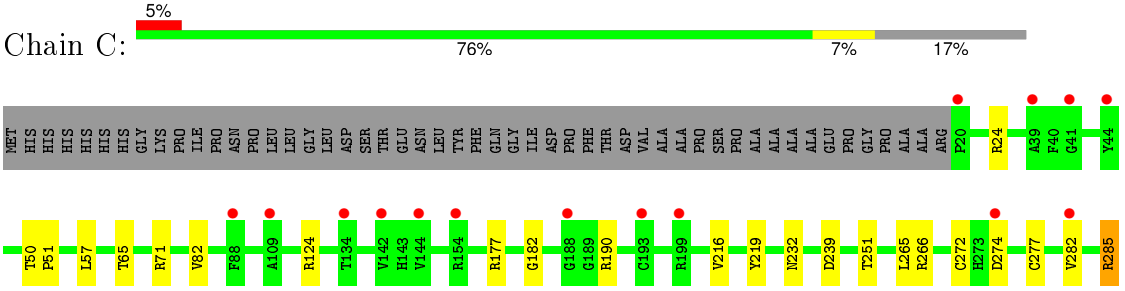
- Molecule 1: formylglycine generating enzyme

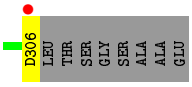
Chain B:



- Molecule 1: formylglycine generating enzyme

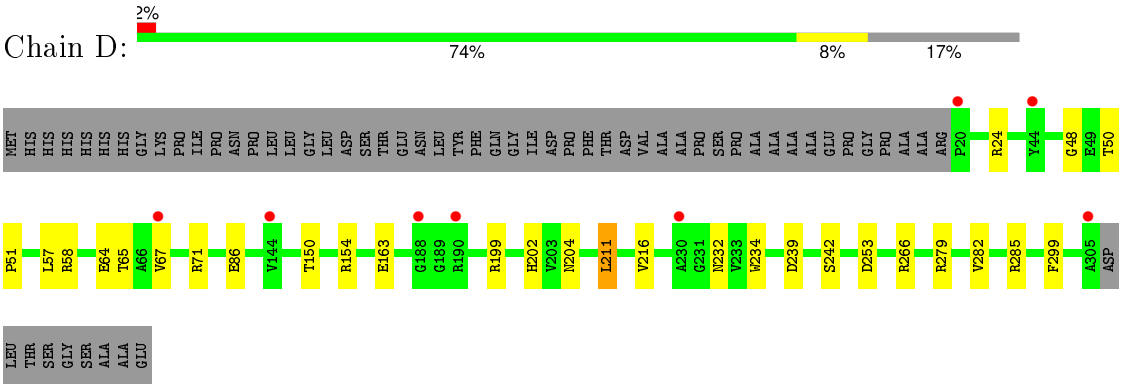
Chain C:





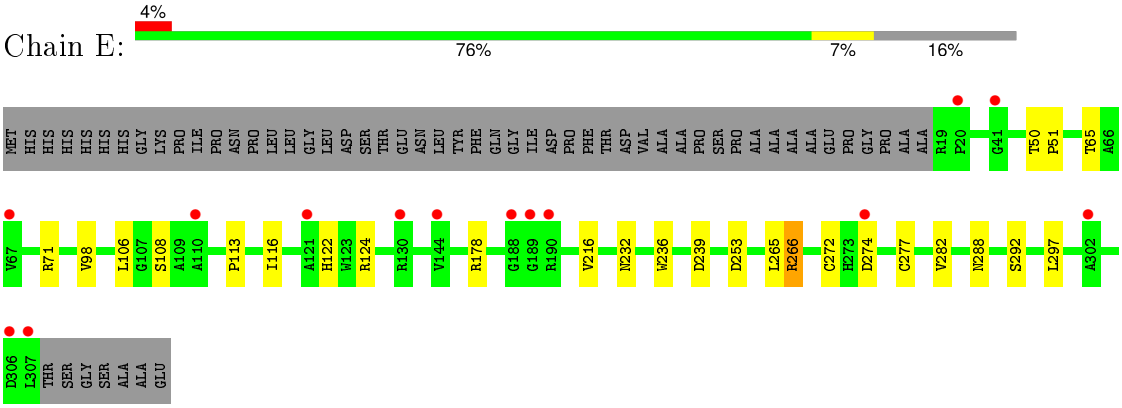
• Molecule 1: formylglycine generating enzyme

Chain D:



• Molecule 1: formylglycine generating enzyme

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.44Å 142.44Å 217.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10 17.40 – 1.95	Depositor EDS
% Data completeness (in resolution range)	83.3 (20.00-2.10) 84.4 (17.40-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.241 0.196 , 0.237	Depositor DCC
R_{free} test set	6200 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.5	EDS
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 155975 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12171	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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 23.20 % 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 4.8857e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA

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	0.44	0/2317	0.57	0/3166
1	B	0.45	0/2320	0.56	1/3170 (0.0%)
1	C	0.42	0/2309	0.55	0/3155
1	D	0.44	0/2301	0.56	0/3144
1	E	0.44	0/2328	0.59	2/3181 (0.1%)
All	All	0.44	0/11575	0.57	3/15816 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	266	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	E	266	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	266	ARG	NE-CZ-NH2	-5.31	117.64	120.30

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	2240	0	2069	13	0
1	B	2243	0	2068	18	0
1	C	2232	0	2056	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2224	0	2052	19	0
1	E	2251	0	2079	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	210	0	0	3	0
3	B	195	0	0	4	0
3	C	170	0	0	4	0
3	D	189	0	0	5	0
3	E	212	0	0	6	0
All	All	12171	0	10324	80	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 4.

All (80) 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:98:VAL:HG21	1:E:116:ILE:HD11	1.18	1.13
1:D:253:ASP:HB3	3:D:498:HOH:O	1.68	0.91
1:B:27:VAL:HG23	3:B:496:HOH:O	1.77	0.85
1:B:138:ASN:HB3	3:B:507:HOH:O	1.76	0.84
1:E:272[A]:CYS:SG	3:E:513:HOH:O	2.32	0.83
1:D:48:GLY:HA2	3:D:502:HOH:O	1.83	0.79
1:E:98:VAL:HG21	1:E:116:ILE:CD1	2.08	0.78
1:C:274:ASP:HA	1:C:277[B]:CYS:O	1.83	0.78
1:D:154:ARG:HD3	3:D:500:HOH:O	1.87	0.75
1:D:58:ARG:HD2	1:D:253:ASP:OD2	1.93	0.68
1:B:274:ASP:HA	1:B:277[B]:CYS:O	1.92	0.67
1:D:242:SER:O	1:D:285:ARG:NH2	2.28	0.65
1:E:98:VAL:CG2	1:E:116:ILE:HD11	2.12	0.64
1:A:242:SER:O	1:A:285:ARG:NH2	2.30	0.64
1:D:163:GLU:OE2	1:D:285:ARG:HD2	1.99	0.63
1:B:146:TRP:O	1:B:150:THR:HG23	1.97	0.63
1:E:108:SER:HB2	3:E:521:HOH:O	1.98	0.62
1:E:253:ASP:HB3	3:E:522:HOH:O	2.00	0.62
1:C:285:ARG:NH1	3:C:466:HOH:O	2.21	0.62
1:E:274:ASP:HA	1:E:277[B]:CYS:O	2.02	0.60
1:B:203:VAL:HG21	1:C:190:ARG:HH22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:HD2	3:B:458:HOH:O	2.02	0.59
1:A:163:GLU:OE2	1:A:285:ARG:HD2	2.02	0.59
1:B:196:TRP:HB3	1:B:273:HIS:HB2	1.84	0.58
1:B:65:THR:HB	1:B:216:VAL:HB	1.86	0.57
1:A:58:ARG:HD2	3:A:389:HOH:O	2.05	0.56
1:D:202:HIS:HD2	3:D:405:HOH:O	1.88	0.55
1:A:139:HIS:HD2	1:A:213:THR:OG1	1.88	0.55
1:E:50:THR:HB	1:E:51:PRO:HA	1.90	0.53
1:A:224:HIS:HD2	3:A:492:HOH:O	1.91	0.53
1:E:265:LEU:HD11	1:E:288:ASN:HB2	1.91	0.52
1:C:272[A]:CYS:SG	3:C:469:HOH:O	2.59	0.52
1:D:64:GLU:HG3	1:D:65:THR:HG23	1.92	0.51
1:E:71:ARG:HD3	3:E:524:HOH:O	2.09	0.51
1:B:95:HIS:CE1	1:B:96:LEU:HD13	2.46	0.50
1:A:253:ASP:OD2	1:A:255:HIS:HE1	1.94	0.50
1:B:158:LYS:NZ	3:B:504:HOH:O	2.44	0.50
1:D:199:ARG:NH1	3:D:454:HOH:O	2.44	0.50
1:C:65:THR:HB	1:C:216:VAL:HB	1.94	0.50
1:A:65:THR:HB	1:A:216:VAL:HB	1.93	0.49
1:B:64:GLU:HG3	1:B:65:THR:HG23	1.94	0.48
1:C:285:ARG:NH2	3:C:466:HOH:O	2.35	0.48
1:E:253:ASP:HB3	3:E:520:HOH:O	2.13	0.48
1:B:122:HIS:NE2	1:B:124:ARG:HB2	2.29	0.48
1:E:65:THR:HB	1:E:216:VAL:HB	1.96	0.48
1:C:50:THR:HB	1:C:51:PRO:HA	1.95	0.48
1:E:122:HIS:NE2	1:E:124:ARG:HB2	2.29	0.48
1:B:82:VAL:HG22	1:B:87:ARG:HH21	1.79	0.47
1:A:50:THR:HB	1:A:51:PRO:HA	1.95	0.47
1:B:69:ASN:HB3	1:B:133:ILE:HD12	1.97	0.46
1:A:21:ARG:NH1	1:A:304:ASP:O	2.49	0.46
1:D:266:ARG:NH2	1:D:282:VAL:O	2.49	0.45
1:D:50:THR:HB	1:D:51:PRO:HA	1.98	0.45
1:D:65:THR:HB	1:D:216:VAL:HB	1.99	0.45
1:A:86:GLU:OE1	1:A:124:ARG:NH2	2.50	0.45
1:B:67:VAL:HG21	1:B:299:PHE:CE2	2.53	0.44
1:D:204:ASN:HB3	1:D:211:LEU:HD12	2.00	0.44
1:D:234:TRP:HH2	1:D:279:ARG:HD2	1.82	0.43
1:D:67:VAL:HG21	1:D:299:PHE:CE2	2.53	0.43
1:E:266:ARG:NH2	1:E:282:VAL:O	2.51	0.43
1:D:24:ARG:HH22	1:D:71:ARG:NE	2.16	0.43
1:E:108:SER:OG	1:E:113:PRO:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:ARG:O	1:E:282:VAL:HG22	2.20	0.42
1:E:236:TRP:CH2	1:E:288:ASN:HB3	2.55	0.42
1:C:24:ARG:HH12	1:C:71:ARG:HD2	1.84	0.42
1:B:136:ARG:HB2	1:B:139:HIS:CG	2.55	0.42
1:A:272[B]:CYS:SG	1:A:280:TYR:CD2	3.13	0.42
1:C:124:ARG:HD3	3:C:434:HOH:O	2.19	0.42
1:B:234:TRP:CH2	1:B:279:ARG:HB3	2.55	0.42
1:A:61:HIS:HD2	3:A:414:HOH:O	2.03	0.41
1:E:71:ARG:HD2	1:E:71:ARG:HA	1.79	0.41
1:C:82:VAL:HG21	1:D:86:GLU:HB3	2.03	0.41
1:C:266:ARG:NH2	1:C:282:VAL:O	2.54	0.41
1:D:150:THR:HG22	1:D:154:ARG:HH12	1.85	0.41
1:C:177:ARG:HG2	1:C:182:GLY:HA2	2.03	0.41
1:E:253:ASP:CB	3:E:522:HOH:O	2.64	0.41
1:A:296:ASN:HD22	1:A:296:ASN:H	1.68	0.41
1:D:24:ARG:HH22	1:D:71:ARG:CZ	2.34	0.40
1:E:236:TRP:CZ2	1:E:297:LEU:HD21	2.56	0.40
1:B:242:SER:HB3	1:B:245:TYR:HB2	2.01	0.40

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	288/346 (83%)	277 (96%)	9 (3%)	2 (1%)	26	21
1	B	288/346 (83%)	279 (97%)	8 (3%)	1 (0%)	46	45
1	C	287/346 (83%)	276 (96%)	9 (3%)	2 (1%)	26	21
1	D	286/346 (83%)	273 (96%)	12 (4%)	1 (0%)	46	45
1	E	289/346 (84%)	279 (96%)	9 (3%)	1 (0%)	46	45
All	All	1438/1730 (83%)	1384 (96%)	47 (3%)	7 (0%)	34	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	219	TYR
1	A	219	TYR
1	A	232	ASN
1	B	232	ASN
1	C	232	ASN
1	D	232	ASN
1	E	232	ASN

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	219/261 (84%)	211 (96%)	8 (4%)	41	41
1	B	220/261 (84%)	213 (97%)	7 (3%)	46	48
1	C	219/261 (84%)	213 (97%)	6 (3%)	52	56
1	D	218/261 (84%)	215 (99%)	3 (1%)	74	80
1	E	221/261 (85%)	218 (99%)	3 (1%)	74	80
All	All	1097/1305 (84%)	1070 (98%)	27 (2%)	55	59

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	TYR
1	A	71	ARG
1	A	108	SER
1	A	239	ASP
1	A	265	LEU
1	A	274	ASP
1	A	282	VAL
1	A	296	ASN
1	B	57	LEU
1	B	82	VAL
1	B	239	ASP

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Mol	Chain	Res	Type
1	B	251	THR
1	B	265	LEU
1	B	274	ASP
1	B	303	ASN
1	C	57	LEU
1	C	239	ASP
1	C	251	THR
1	C	265	LEU
1	C	285	ARG
1	C	306	ASP
1	D	57	LEU
1	D	211	LEU
1	D	239	ASP
1	E	106	LEU
1	E	239	ASP
1	E	292	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	81	HIS
1	A	139	HIS
1	A	255	HIS
1	A	296	ASN
1	B	273	HIS
1	B	303	ASN
1	C	273	HIS
1	D	273	HIS
1	E	197	GLN
1	E	202	HIS
1	E	255	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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 (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, 95^{th} 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	288/346 (83%)	0.21	13 (4%)	37	46	39, 41, 42, 44	0
1	B	288/346 (83%)	0.15	10 (3%)	48	57	40, 41, 42, 44	0
1	C	287/346 (82%)	0.18	16 (5%)	28	36	40, 41, 42, 43	0
1	D	286/346 (82%)	0.15	8 (2%)	56	64	40, 41, 42, 44	0
1	E	289/346 (83%)	0.22	14 (4%)	34	43	40, 41, 42, 44	0
All	All	1438/1730 (83%)	0.18	61 (4%)	40	49	39, 41, 42, 44	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	307	LEU	7.3
1	C	306	ASP	5.2
1	C	20	PRO	4.6
1	B	306	ASP	4.0
1	A	142	VAL	3.6
1	B	188	GLY	3.5
1	A	18	ALA	3.5
1	A	277[A]	CYS	3.4
1	A	110	ALA	3.4
1	E	189	GLY	3.2
1	A	44	TYR	3.2
1	E	110	ALA	3.1
1	B	110	ALA	3.1
1	E	190	ARG	3.0
1	E	188	GLY	3.0
1	D	20	PRO	3.0
1	E	306	ASP	2.9
1	D	188	GLY	2.9
1	E	121	ALA	2.8
1	C	134	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	190	ARG	2.8
1	C	144	VAL	2.7
1	A	141	VAL	2.7
1	E	41	GLY	2.7
1	D	305	ALA	2.6
1	A	111	GLY	2.6
1	E	274	ASP	2.6
1	A	275	SER	2.6
1	C	41	GLY	2.5
1	B	121	ALA	2.5
1	A	62	ILE	2.5
1	D	144	VAL	2.5
1	A	199	ARG	2.5
1	C	88	PHE	2.4
1	E	67	VAL	2.4
1	C	39	ALA	2.4
1	C	193	CYS	2.4
1	B	20	PRO	2.4
1	D	67	VAL	2.3
1	C	188	GLY	2.3
1	C	142	VAL	2.3
1	B	275	SER	2.3
1	C	199	ARG	2.3
1	A	121	ALA	2.3
1	E	144	VAL	2.3
1	B	19	ARG	2.3
1	E	130	ARG	2.2
1	B	190	ARG	2.2
1	C	44	TYR	2.2
1	B	24	ARG	2.1
1	A	188	GLY	2.1
1	C	274	ASP	2.1
1	C	109	ALA	2.1
1	E	20	PRO	2.1
1	D	230	ALA	2.1
1	D	44	TYR	2.1
1	B	67	VAL	2.1
1	C	282	VAL	2.1
1	E	302	ALA	2.0
1	C	154	ARG	2.0
1	A	193	CYS	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	CA	A	315	1/1	1.00	0.07	-1.40	34,34,34,34	0
2	CA	E	315	1/1	0.99	0.07	-1.77	44,44,44,44	0
2	CA	C	315	1/1	0.99	0.04	-2.22	32,32,32,32	0
2	CA	D	315	1/1	1.00	0.06	-2.36	28,28,28,28	0
2	CA	B	315	1/1	0.99	0.05	-3.27	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.