



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 12:36 pm BST

PDB ID : 5G3P
Title : Bacillus cereus formamidase (BceAmiF) acetylated at the active site.
Authors : Gavira, J.A.; Conejero-Muriel, M.; Martinez-Rodriguez, S.
Deposited on : 2016-04-29
Resolution : 1.78 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

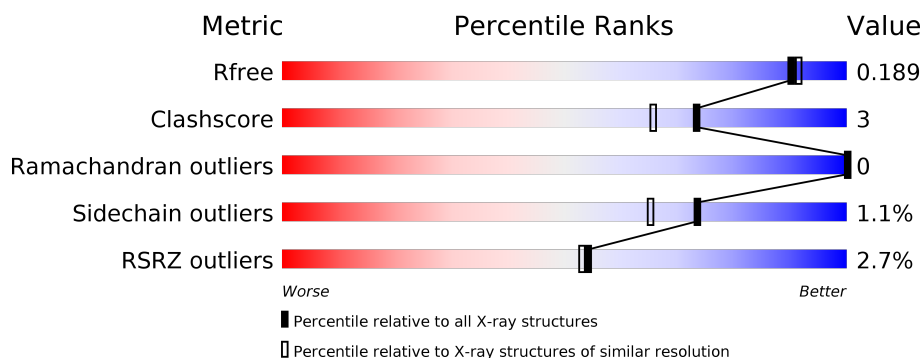
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	346	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	346	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	346	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	D	346	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	E	346	<div> <div>0%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>6%</div> </div> </div>
1	F	346	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</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
2	PEG	B	1328	-	-	X	-
2	PEG	D	1330	-	-	X	-
2	PEG	F	1328	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17882 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 FORMAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	10	0
			2618	1684	421	501	12			
1	B	326	Total	C	N	O	S	0	16	0
			2634	1702	422	498	12			
1	C	325	Total	C	N	O	S	0	14	0
			2615	1685	418	500	12			
1	D	326	Total	C	N	O	S	0	11	0
			2614	1683	419	500	12			
1	E	325	Total	C	N	O	S	0	17	0
			2637	1699	421	505	12			
1	F	325	Total	C	N	O	S	0	12	0
			2609	1679	418	500	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	TRP	-	expression tag	UNP E5LR94
A	334	PHE	-	expression tag	UNP E5LR94
A	335	ARG	-	expression tag	UNP E5LR94
A	336	VAL	-	expression tag	UNP E5LR94
A	337	ASP	-	expression tag	UNP E5LR94
A	338	PRO	-	expression tag	UNP E5LR94
A	339	LEU	-	expression tag	UNP E5LR94
A	340	GLU	-	expression tag	UNP E5LR94
A	341	HIS	-	expression tag	UNP E5LR94
A	342	HIS	-	expression tag	UNP E5LR94
A	343	HIS	-	expression tag	UNP E5LR94
A	344	HIS	-	expression tag	UNP E5LR94
A	345	HIS	-	expression tag	UNP E5LR94
A	346	HIS	-	expression tag	UNP E5LR94
B	333	TRP	-	expression tag	UNP E5LR94
B	334	PHE	-	expression tag	UNP E5LR94
B	335	ARG	-	expression tag	UNP E5LR94

Continued on next page...

Continued from previous page...

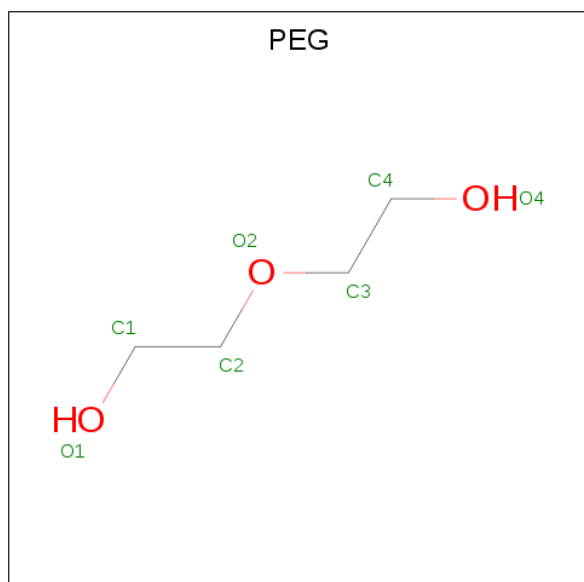
Chain	Residue	Modelled	Actual	Comment	Reference
B	336	VAL	-	expression tag	UNP E5LR94
B	337	ASP	-	expression tag	UNP E5LR94
B	338	PRO	-	expression tag	UNP E5LR94
B	339	LEU	-	expression tag	UNP E5LR94
B	340	GLU	-	expression tag	UNP E5LR94
B	341	HIS	-	expression tag	UNP E5LR94
B	342	HIS	-	expression tag	UNP E5LR94
B	343	HIS	-	expression tag	UNP E5LR94
B	344	HIS	-	expression tag	UNP E5LR94
B	345	HIS	-	expression tag	UNP E5LR94
B	346	HIS	-	expression tag	UNP E5LR94
C	333	TRP	-	expression tag	UNP E5LR94
C	334	PHE	-	expression tag	UNP E5LR94
C	335	ARG	-	expression tag	UNP E5LR94
C	336	VAL	-	expression tag	UNP E5LR94
C	337	ASP	-	expression tag	UNP E5LR94
C	338	PRO	-	expression tag	UNP E5LR94
C	339	LEU	-	expression tag	UNP E5LR94
C	340	GLU	-	expression tag	UNP E5LR94
C	341	HIS	-	expression tag	UNP E5LR94
C	342	HIS	-	expression tag	UNP E5LR94
C	343	HIS	-	expression tag	UNP E5LR94
C	344	HIS	-	expression tag	UNP E5LR94
C	345	HIS	-	expression tag	UNP E5LR94
C	346	HIS	-	expression tag	UNP E5LR94
D	333	TRP	-	expression tag	UNP E5LR94
D	334	PHE	-	expression tag	UNP E5LR94
D	335	ARG	-	expression tag	UNP E5LR94
D	336	VAL	-	expression tag	UNP E5LR94
D	337	ASP	-	expression tag	UNP E5LR94
D	338	PRO	-	expression tag	UNP E5LR94
D	339	LEU	-	expression tag	UNP E5LR94
D	340	GLU	-	expression tag	UNP E5LR94
D	341	HIS	-	expression tag	UNP E5LR94
D	342	HIS	-	expression tag	UNP E5LR94
D	343	HIS	-	expression tag	UNP E5LR94
D	344	HIS	-	expression tag	UNP E5LR94
D	345	HIS	-	expression tag	UNP E5LR94
D	346	HIS	-	expression tag	UNP E5LR94
E	333	TRP	-	expression tag	UNP E5LR94
E	334	PHE	-	expression tag	UNP E5LR94
E	335	ARG	-	expression tag	UNP E5LR94

Continued on next page...

Continued from previous page...

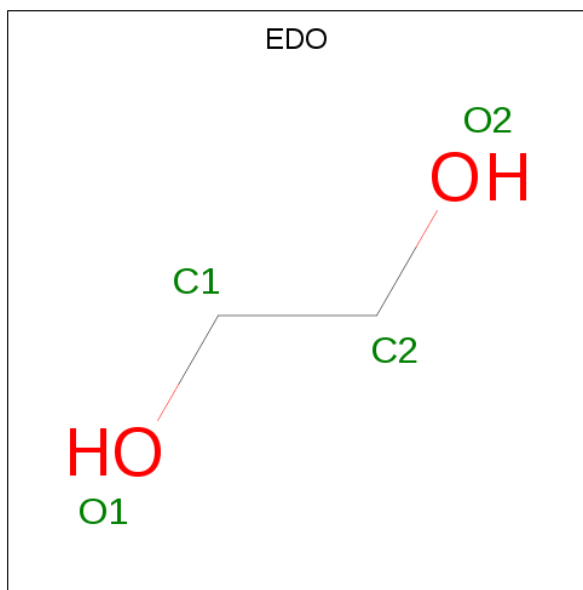
Chain	Residue	Modelled	Actual	Comment	Reference
E	336	VAL	-	expression tag	UNP E5LR94
E	337	ASP	-	expression tag	UNP E5LR94
E	338	PRO	-	expression tag	UNP E5LR94
E	339	LEU	-	expression tag	UNP E5LR94
E	340	GLU	-	expression tag	UNP E5LR94
E	341	HIS	-	expression tag	UNP E5LR94
E	342	HIS	-	expression tag	UNP E5LR94
E	343	HIS	-	expression tag	UNP E5LR94
E	344	HIS	-	expression tag	UNP E5LR94
E	345	HIS	-	expression tag	UNP E5LR94
E	346	HIS	-	expression tag	UNP E5LR94
F	333	TRP	-	expression tag	UNP E5LR94
F	334	PHE	-	expression tag	UNP E5LR94
F	335	ARG	-	expression tag	UNP E5LR94
F	336	VAL	-	expression tag	UNP E5LR94
F	337	ASP	-	expression tag	UNP E5LR94
F	338	PRO	-	expression tag	UNP E5LR94
F	339	LEU	-	expression tag	UNP E5LR94
F	340	GLU	-	expression tag	UNP E5LR94
F	341	HIS	-	expression tag	UNP E5LR94
F	342	HIS	-	expression tag	UNP E5LR94
F	343	HIS	-	expression tag	UNP E5LR94
F	344	HIS	-	expression tag	UNP E5LR94
F	345	HIS	-	expression tag	UNP E5LR94
F	346	HIS	-	expression tag	UNP E5LR94

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



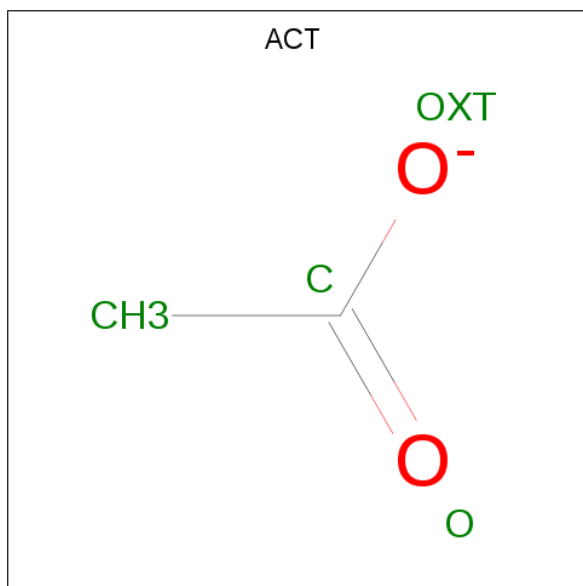
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	A	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	E	1	Total C O 7 4 3	0	0
2	E	1	Total C O 14 8 6	0	1
2	F	1	Total C O 7 4 3	0	0
2	F	1	Total C O 7 4 3	0	0
2	F	1	Total C O 7 4 3	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

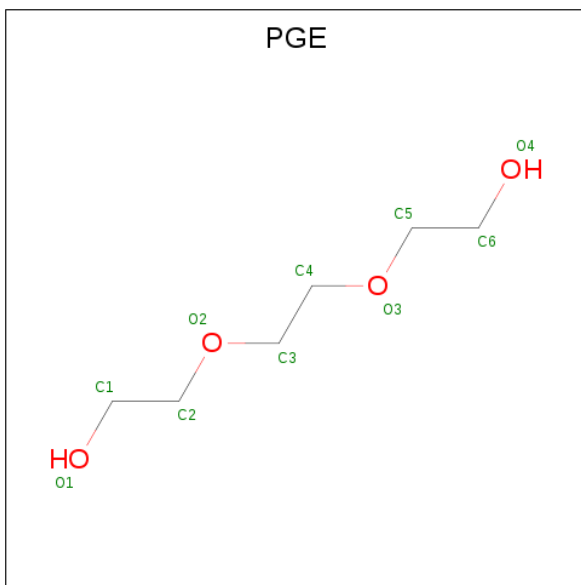
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	4	Total Na 4 4	0	0
5	A	2	Total Na 2 2	0	0
5	C	2	Total Na 2 2	0	0

Continued on next page...

Continued from previous page...

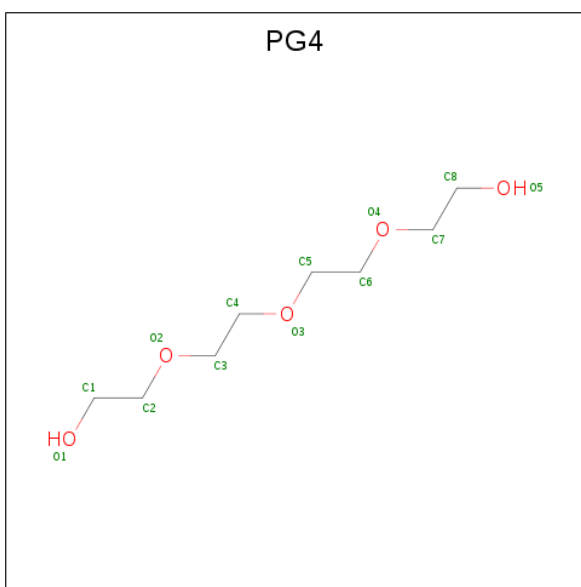
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	4	Total	Na	0	0
			4	4		
5	E	3	Total	Na	0	0
			3	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



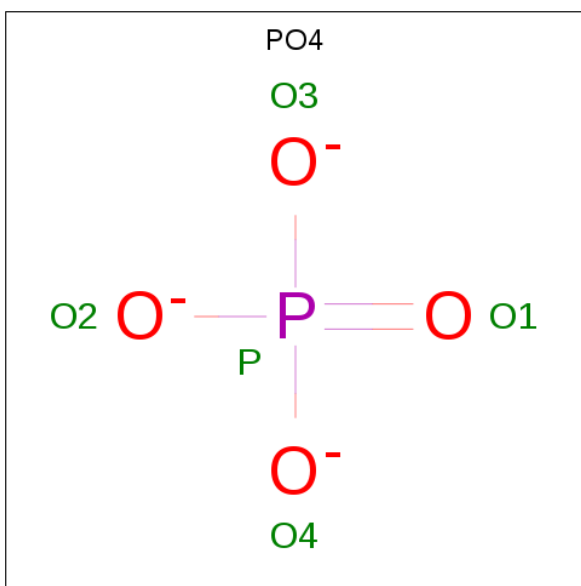
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	P	0	0
			5	4	1		
8	F	1	Total	O	P	0	0
			5	4	1		

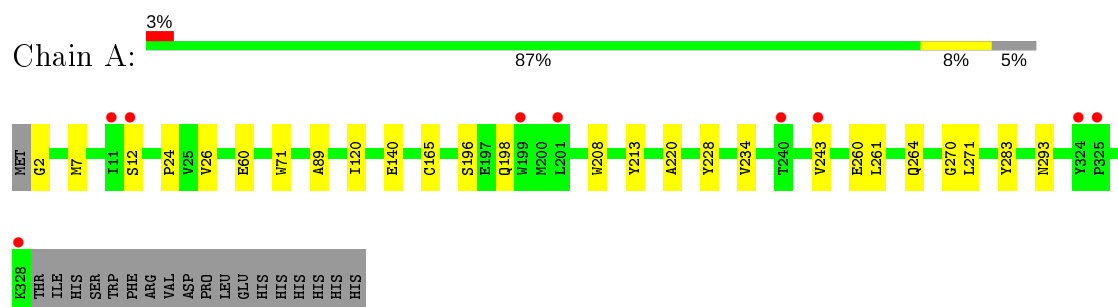
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	378	Total 378	O 378	0	0
9	B	328	Total 328	O 328	0	0
9	C	350	Total 350	O 350	0	0
9	D	304	Total 304	O 304	0	0
9	E	316	Total 316	O 316	0	0
9	F	262	Total 262	O 262	0	0

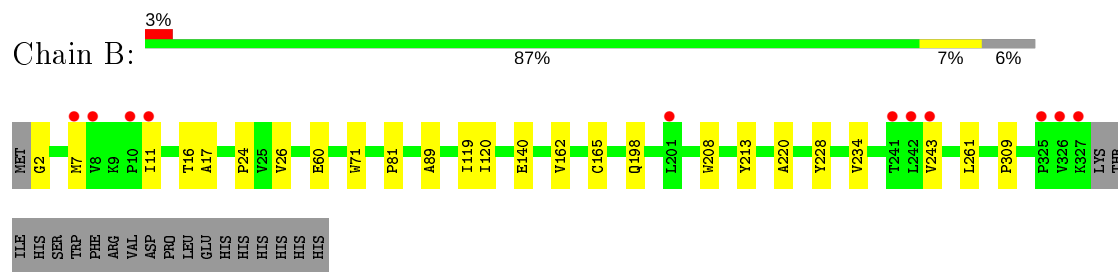
3 Residue-property plots [i](#)

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.

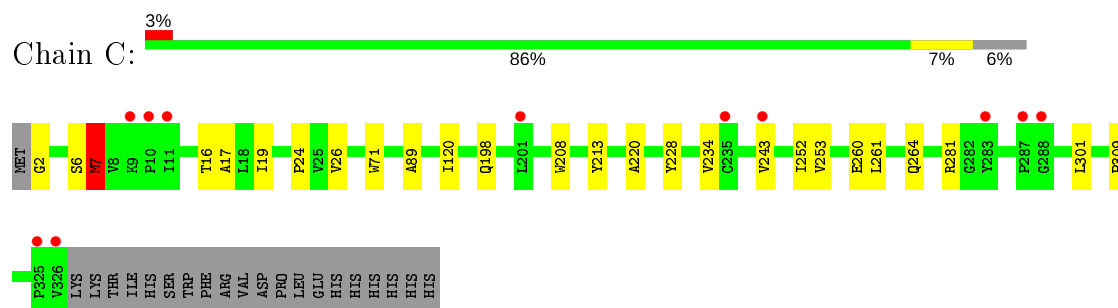
• Molecule 1: FORMAMIDASE



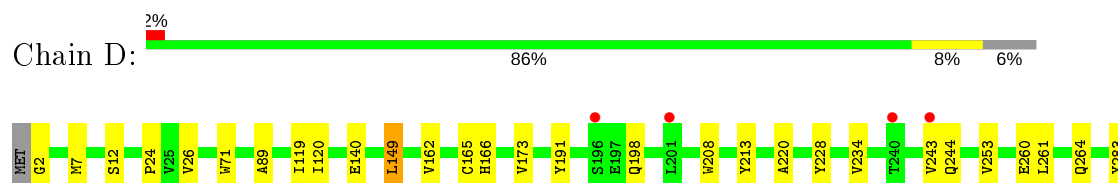
• Molecule 1: FORMAMIDASE

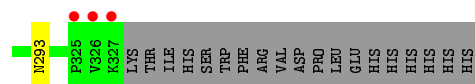


• Molecule 1: FORMAMIDASE

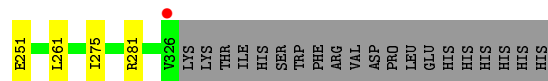
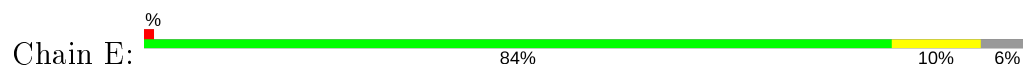


• Molecule 1: FORMAMIDASE

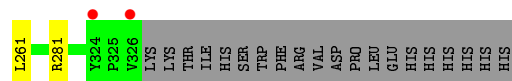
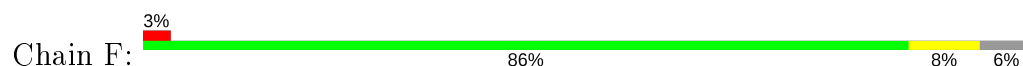




● Molecule 1: FORMAMIDASE



● Molecule 1: FORMAMIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.76 Å 150.21 Å 98.26 Å 90.00° 98.68° 90.00°	Depositor
Resolution (Å)	103.23 – 1.78 48.57 – 1.78	Depositor EDS
% Data completeness (in resolution range)	93.0 (103.23-1.78) 93.0 (48.57-1.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.78 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.164 , 0.181 0.173 , 0.189	Depositor DCC
R_{free} test set	9207 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17882	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: PGE, NA, PO4, EDO, PG4, SCY, ACT, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.64	1/2689 (0.0%)	0.78	3/3657 (0.1%)
1	B	0.63	0/2727	0.75	0/3709
1	C	0.64	0/2698	0.80	3/3671 (0.1%)
1	D	0.62	0/2691	0.79	2/3662 (0.1%)
1	E	0.64	2/2723 (0.1%)	0.78	4/3703 (0.1%)
1	F	0.62	0/2686	0.78	3/3654 (0.1%)
All	All	0.63	3/16214 (0.0%)	0.78	15/22056 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	ASN	C-N	5.80	1.45	1.34
1	E	251	GLU	CD-OE1	-5.10	1.20	1.25
1	E	251	GLU	CD-OE2	-5.01	1.20	1.25

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	MET	CB-CG-SD	11.41	146.65	112.40
1	A	293	ASN	O-C-N	8.42	137.10	121.10
1	C	7	MET	CG-SD-CE	7.33	111.92	100.20
1	E	96	LYS	CD-CE-NZ	5.79	125.02	111.70
1	C	281	ARG	NE-CZ-NH1	5.71	123.15	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	2618	0	2565	18	0
1	B	2634	0	2620	18	0
1	C	2615	0	2574	24	0
1	D	2614	0	2567	19	0
1	E	2637	0	2596	20	0
1	F	2609	0	2558	19	0
2	A	14	0	20	0	0
2	B	14	0	20	7	0
2	D	21	0	30	5	0
2	E	21	0	30	2	0
2	F	21	0	30	5	0
3	A	4	0	6	0	0
3	C	4	0	6	0	0
3	E	4	0	6	0	0
4	A	4	0	3	0	0
4	B	4	0	3	1	0
4	C	4	0	3	0	0
4	F	4	0	3	0	0
5	A	2	0	0	0	0
5	B	4	0	0	0	0
5	C	2	0	0	0	0
5	E	3	0	0	0	0
5	F	4	0	0	0	0
6	B	10	0	14	0	0
6	C	20	0	28	0	0
6	D	10	0	14	0	0
6	E	10	0	14	0	0
6	F	10	0	14	0	0
7	B	13	0	18	0	0
8	B	5	0	0	0	0
8	F	5	0	0	0	0
9	A	378	0	0	0	0
9	B	328	0	0	7	0
9	C	350	0	0	0	0
9	D	304	0	0	1	0
9	E	316	0	0	2	0
9	F	262	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17882	0	15742	106	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 3.

The worst 5 of 106 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)
9:B:2108:HOH:O	1:E:194:GLN:HB2	1.54	1.05
1:C:6:SER:OG	1:C:7:MET:CE	2.05	1.05
1:F:12[B]:SER:OG	1:F:260[B]:GLU:OE2	1.87	0.93
1:C:6:SER:OG	1:C:7:MET:HE2	1.67	0.92
1:C:243[B]:VAL:HG22	1:C:253:VAL:HG13	1.71	0.72

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	334/346 (96%)	323 (97%)	11 (3%)	0	100	100
1	B	340/346 (98%)	328 (96%)	12 (4%)	0	100	100
1	C	336/346 (97%)	324 (96%)	12 (4%)	0	100	100
1	D	335/346 (97%)	322 (96%)	13 (4%)	0	100	100
1	E	339/346 (98%)	329 (97%)	10 (3%)	0	100	100
1	F	334/346 (96%)	321 (96%)	13 (4%)	0	100	100
All	All	2018/2076 (97%)	1947 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	284/293 (97%)	281 (99%)	3 (1%)	73	65
1	B	289/293 (99%)	286 (99%)	3 (1%)	76	68
1	C	286/293 (98%)	283 (99%)	3 (1%)	76	68
1	D	285/293 (97%)	280 (98%)	5 (2%)	59	45
1	E	288/293 (98%)	286 (99%)	2 (1%)	84	79
1	F	284/293 (97%)	280 (99%)	4 (1%)	67	56
All	All	1716/1758 (98%)	1696 (99%)	20 (1%)	73	62

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	7	MET
1	D	71	TRP
1	F	7	MET
1	C	71	TRP
1	C	309	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	264	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	SCY	E	165	1	7,8,9	0.89	0	3,9,11	0.59	0
1	SCY	A	165	1	7,8,9	1.61	2 (28%)	3,9,11	0.47	0
1	SCY	D	165	1	7,8,9	0.92	0	3,9,11	0.64	0
1	SCY	F	165	1	7,8,9	0.96	0	3,9,11	0.62	0
1	SCY	B	165	1	7,8,9	1.23	1 (14%)	3,9,11	0.58	0
1	SCY	C	165	1	7,8,9	0.91	0	3,9,11	0.66	0

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
1	SCY	E	165	1	-	3/5/7/9	-
1	SCY	A	165	1	-	3/5/7/9	-
1	SCY	D	165	1	-	3/5/7/9	-
1	SCY	F	165	1	-	3/5/7/9	-
1	SCY	B	165	1	-	3/5/7/9	-
1	SCY	C	165	1	-	3/5/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	SCY	CB-SG	-3.22	1.74	1.81
1	A	165	SCY	CD-SG	-2.33	1.61	1.75
1	B	165	SCY	CD-SG	-2.04	1.63	1.75

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	165	SCY	CA-CB-SG-CD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	E	165	SCY	OCD-CD-SG-CB
1	E	165	SCY	CE-CD-SG-CB
1	A	165	SCY	CA-CB-SG-CD
1	A	165	SCY	OCD-CD-SG-CB

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	165	SCY	1	0
1	A	165	SCY	2	0
1	D	165	SCY	1	0
1	F	165	SCY	1	0
1	B	165	SCY	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 15 are monoatomic - leaving 29 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	$\# Z > 2$
6	PGE	C	1328	-	9,9,9	0.47	0	8,8,8	0.24	0
2	PEG	F	1327	-	6,6,6	0.36	0	5,5,5	0.30	0
2	PEG	E	1327	-	6,6,6	0.50	0	5,5,5	0.26	0
6	PGE	C	1327	-	9,9,9	0.48	0	8,8,8	0.28	0
2	PEG	A	1330	-	6,6,6	0.49	0	5,5,5	0.80	0
6	PGE	B	1330	-	9,9,9	0.54	0	8,8,8	0.40	0
4	ACT	F	1332	5	1,3,3	1.63	0	0,3,3	0.00	-
6	PGE	D	1331	-	9,9,9	0.52	0	8,8,8	0.26	0
4	ACT	A	1332	-	1,3,3	1.88	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	E	1328[B]	-	6,6,6	0.55	0	5,5,5	0.47	0
2	PEG	E	1328[A]	-	6,6,6	0.51	0	5,5,5	0.17	0
7	PG4	B	1331	-	12,12,12	0.48	0	11,11,11	0.28	0
2	PEG	D	1328	-	6,6,6	0.55	0	5,5,5	0.42	0
2	PEG	D	1329	-	6,6,6	0.43	0	5,5,5	0.29	0
3	EDO	A	1331	-	3,3,3	0.70	0	2,2,2	0.18	0
8	PO4	F	1331	-	4,4,4	1.28	0	6,6,6	1.49	0
3	EDO	E	1330	-	3,3,3	0.38	0	2,2,2	0.35	0
2	PEG	B	1328	-	6,6,6	0.55	0	5,5,5	1.01	1 (20%)
3	EDO	C	1329	-	3,3,3	0.45	0	2,2,2	0.31	0
8	PO4	B	1332	-	4,4,4	0.88	0	6,6,6	0.75	0
2	PEG	B	1329	-	6,6,6	0.54	0	5,5,5	0.42	0
6	PGE	E	1329	-	9,9,9	0.46	0	8,8,8	0.48	0
4	ACT	B	1333	-	1,3,3	1.34	0	0,3,3	0.00	-
2	PEG	D	1330	-	6,6,6	0.34	0	5,5,5	0.49	0
2	PEG	A	1329	-	6,6,6	0.43	0	5,5,5	0.39	0
2	PEG	F	1329	-	6,6,6	0.48	0	5,5,5	0.23	0
4	ACT	C	1330	-	1,3,3	1.98	0	0,3,3	0.00	-
6	PGE	F	1330	-	9,9,9	0.58	0	8,8,8	0.31	0
2	PEG	F	1328	-	6,6,6	0.41	0	5,5,5	1.34	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	C	1328	-	-	1/7/7/7	-
2	PEG	F	1327	-	-	3/4/4/4	-
2	PEG	E	1327	-	-	1/4/4/4	-
6	PGE	C	1327	-	-	2/7/7/7	-
2	PEG	A	1330	-	-	2/4/4/4	-
6	PGE	B	1330	-	-	4/7/7/7	-
6	PGE	D	1331	-	-	2/7/7/7	-
2	PEG	E	1328[B]	-	-	3/4/4/4	-
2	PEG	E	1328[A]	-	-	3/4/4/4	-
7	PG4	B	1331	-	-	1/10/10/10	-
2	PEG	D	1328	-	-	2/4/4/4	-
2	PEG	D	1329	-	-	2/4/4/4	-
3	EDO	A	1331	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	E	1330	-	-	1/1/1/1	-
2	PEG	B	1328	-	-	3/4/4/4	-
3	EDO	C	1329	-	-	0/1/1/1	-
2	PEG	B	1329	-	-	1/4/4/4	-
6	PGE	E	1329	-	-	4/7/7/7	-
2	PEG	D	1330	-	-	3/4/4/4	-
2	PEG	A	1329	-	-	2/4/4/4	-
2	PEG	F	1329	-	-	2/4/4/4	-
6	PGE	F	1330	-	-	1/7/7/7	-
2	PEG	F	1328	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1328	PEG	O2-C3-C4	2.14	119.47	110.07
2	B	1328	PEG	O2-C3-C4	2.11	119.35	110.07

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	1329	PGE	O2-C3-C4-O3
2	F	1327	PEG	O2-C3-C4-O4
2	D	1328	PEG	O2-C3-C4-O4
6	E	1329	PGE	O1-C1-C2-O2
6	E	1329	PGE	O3-C5-C6-O4

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1328[A]	PEG	2	0
2	B	1328	PEG	7	0
4	B	1333	ACT	1	0
2	D	1330	PEG	5	0
2	F	1328	PEG	5	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 [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, 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	326/346 (94%)	-0.01	9 (2%) 53 51	7, 11, 19, 69	0
1	B	325/346 (93%)	-0.13	11 (3%) 45 44	7, 10, 22, 85	0
1	C	324/346 (93%)	-0.09	11 (3%) 45 44	6, 10, 22, 68	0
1	D	325/346 (93%)	-0.04	7 (2%) 62 61	8, 11, 20, 53	0
1	E	324/346 (93%)	-0.20	4 (1%) 79 79	7, 10, 21, 64	0
1	F	324/346 (93%)	0.10	11 (3%) 45 44	7, 11, 19, 36	0
All	All	1948/2076 (93%)	-0.06	53 (2%) 54 53	6, 11, 21, 85	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	326	VAL	7.0
1	B	327	LYS	5.2
1	B	11[A]	ILE	4.4
1	D	326	VAL	4.1
1	C	11	ILE	4.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SCY	A	165	9/10	0.94	0.10	12,13,23,25	0
1	SCY	B	165	9/10	0.95	0.11	10,11,21,22	0
1	SCY	D	165	9/10	0.97	0.08	11,12,23,24	0
1	SCY	F	165	9/10	0.97	0.07	10,11,23,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SCY	E	165	9/10	0.97	0.11	10,11,18,20	0
1	SCY	C	165	9/10	0.97	0.09	10,11,19,19	0

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. 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(\AA^2)	Q<0.9
5	NA	E	1332	1/1	0.29	0.36	49,49,49,49	0
3	EDO	C	1329	4/4	0.55	0.20	55,58,59,59	0
4	ACT	C	1330	4/4	0.61	0.21	46,46,48,54	0
3	EDO	A	1331	4/4	0.64	0.38	30,32,33,41	0
2	PEG	F	1329	7/7	0.65	0.27	50,60,65,71	0
2	PEG	D	1328	7/7	0.70	0.29	52,57,62,63	0
2	PEG	A	1330	7/7	0.73	0.19	37,47,52,56	0
6	PGE	B	1330	10/10	0.73	0.23	47,59,63,63	0
2	PEG	B	1329	7/7	0.75	0.21	43,44,48,50	0
6	PGE	C	1327	10/10	0.77	0.22	49,53,61,68	0
2	PEG	E	1327	7/7	0.77	0.13	45,50,60,67	0
2	PEG	E	1328[A]	7/7	0.79	0.20	40,46,52,54	7
2	PEG	E	1328[B]	7/7	0.79	0.20	32,34,47,50	7
6	PGE	D	1331	10/10	0.80	0.15	38,46,53,53	0
3	EDO	E	1330	4/4	0.81	0.25	29,35,37,49	0
5	NA	E	1340	1/1	0.81	0.14	49,49,49,49	0
5	NA	F	1334	1/1	0.81	0.17	45,45,45,45	0
6	PGE	F	1330	10/10	0.81	0.14	39,46,51,58	0
2	PEG	F	1328	7/7	0.83	0.29	34,40,45,48	0
5	NA	A	1333	1/1	0.84	0.20	36,36,36,36	0
2	PEG	D	1330	7/7	0.86	0.28	32,37,42,51	0
6	PGE	C	1328	10/10	0.86	0.12	34,35,43,44	0
2	PEG	B	1328	7/7	0.87	0.28	27,37,43,57	0
2	PEG	A	1329	7/7	0.87	0.21	42,45,51,54	0
4	ACT	B	1333	4/4	0.88	0.11	42,48,49,50	0
5	NA	F	1333	1/1	0.88	0.22	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEG	D	1329	7/7	0.88	0.18	44,44,50,50	0
4	ACT	A	1332	4/4	0.88	0.12	34,48,49,51	0
2	PEG	F	1327	7/7	0.89	0.23	44,47,55,57	0
6	PGE	E	1329	10/10	0.89	0.14	36,40,49,51	0
5	NA	B	1335	1/1	0.89	0.16	30,30,30,30	0
5	NA	B	1336	1/1	0.89	0.14	27,27,27,27	0
5	NA	A	1340	1/1	0.91	0.10	41,41,41,41	0
7	PG4	B	1331	13/13	0.91	0.12	37,39,54,60	0
4	ACT	F	1332	4/4	0.91	0.15	38,47,52,54	0
5	NA	B	1334	1/1	0.92	0.17	40,40,40,40	0
5	NA	F	1335	1/1	0.92	0.19	32,32,32,32	0
5	NA	C	1331	1/1	0.95	0.12	33,33,33,33	0
5	NA	B	1337	1/1	0.96	0.14	37,37,37,37	0
5	NA	E	1331	1/1	0.97	0.12	26,26,26,26	0
5	NA	C	1332	1/1	0.98	0.23	23,23,23,23	0
5	NA	F	1336	1/1	0.98	0.11	25,25,25,25	0
8	PO4	B	1332	5/5	0.99	0.16	16,17,19,20	0
8	PO4	F	1331	5/5	0.99	0.15	18,20,21,24	0

6.5 Other polymers

There are no such residues in this entry.