



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:22 PM UTC

PDB ID : 5G3P / pdb_00005g3p
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

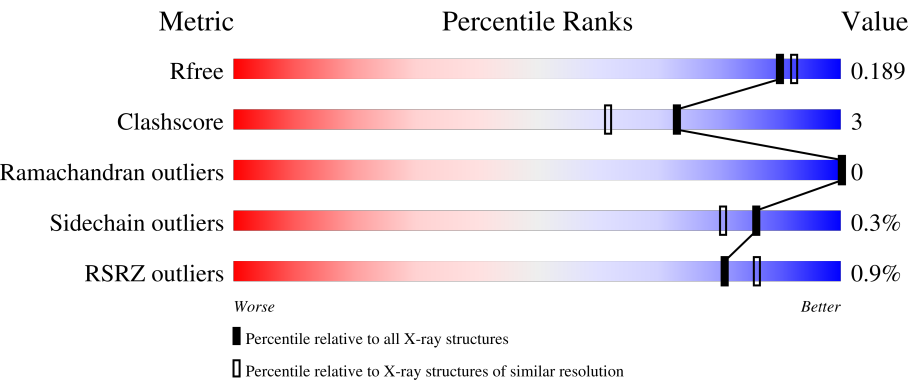
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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 of 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	88%6%5%
1	B	346	2% 88%6%6%
1	C	346	% 87%7%6%
1	D	346	87%7%6%
1	E	346	% 86%8%6%

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Mol	Chain	Length	Quality of chain
1	F	346	 87% 6% • 6%

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

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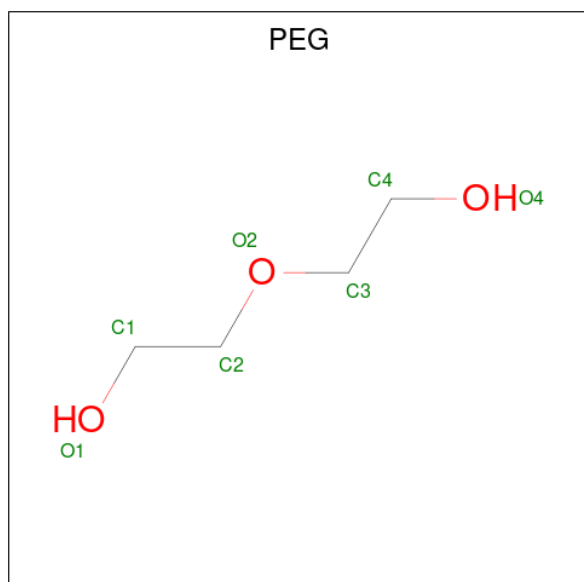
Chain	Residue	Modelled	Actual	Comment	Reference
B	336	VAL	-	expression tag	UNP E5LR94
B	337	ASP	-	expression tag	UNP E5LR94
B	338	PRO	-	expression tag	UNP E5LR94
B	339	LEU	-	expression tag	UNP E5LR94
B	340	GLU	-	expression tag	UNP E5LR94
B	341	HIS	-	expression tag	UNP E5LR94
B	342	HIS	-	expression tag	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

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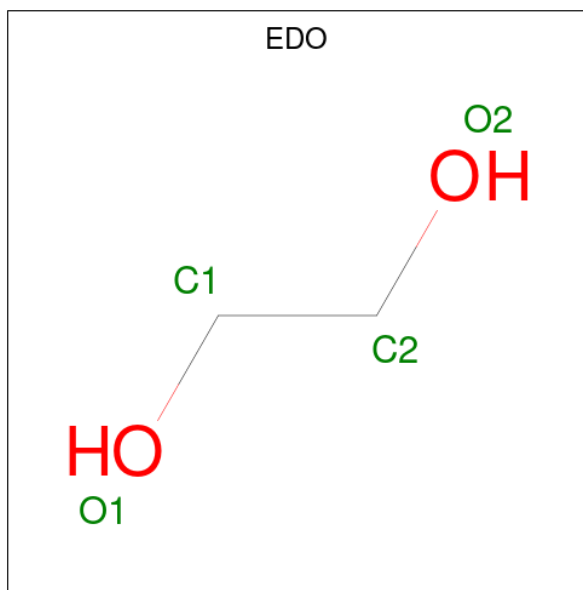
Chain	Residue	Modelled	Actual	Comment	Reference
E	336	VAL	-	expression tag	UNP E5LR94
E	337	ASP	-	expression tag	UNP E5LR94
E	338	PRO	-	expression tag	UNP E5LR94
E	339	LEU	-	expression tag	UNP E5LR94
E	340	GLU	-	expression tag	UNP E5LR94
E	341	HIS	-	expression tag	UNP E5LR94
E	342	HIS	-	expression tag	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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



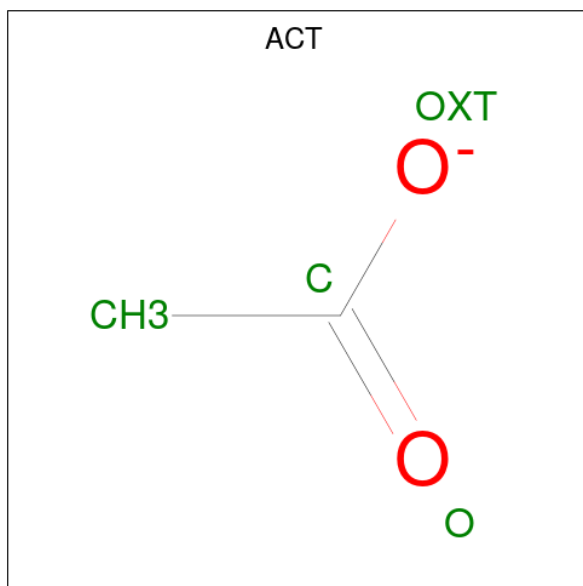
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	A	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	E	1	Total C O 7 4 3	0	0
2	E	1	Total C O 14 8 6	0	1
2	F	1	Total C O 7 4 3	0	0
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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

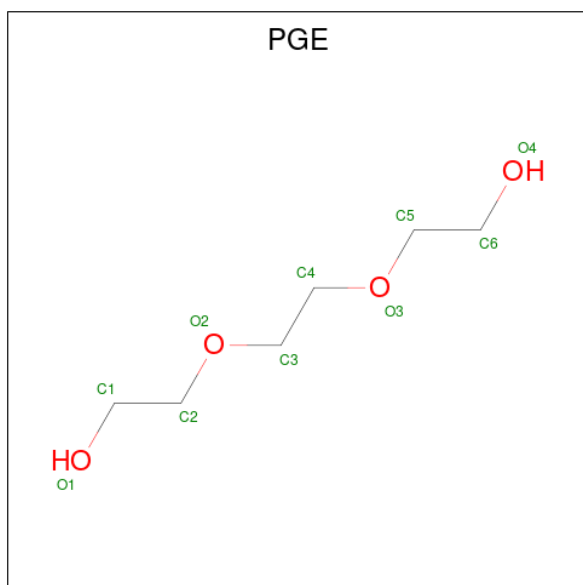
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		
5	B	4	Total	Na	0	0
			4	4		
5	C	2	Total	Na	0	0
			2	2		

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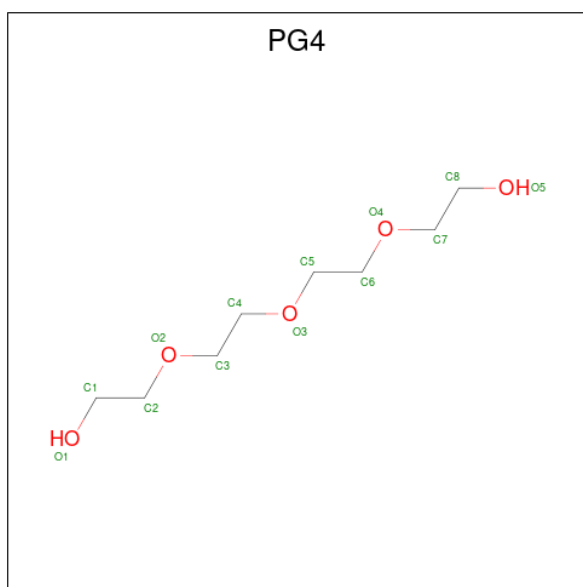
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	3	Total	Na	0	0
			3	3		
5	F	4	Total	Na	0	0
			4	4		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



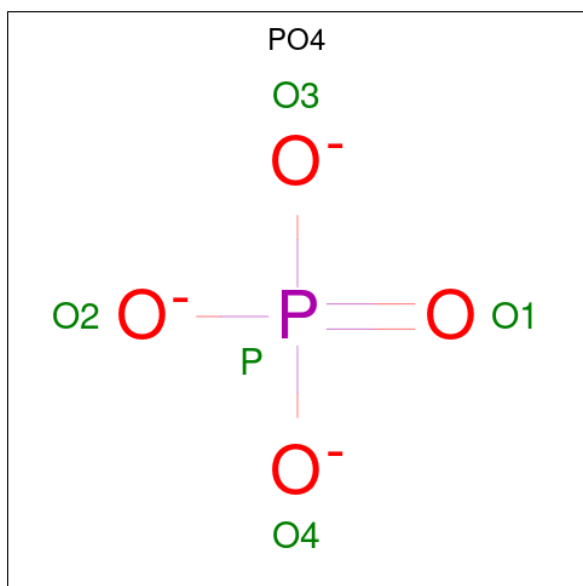
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: 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 (CCD ID: 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		

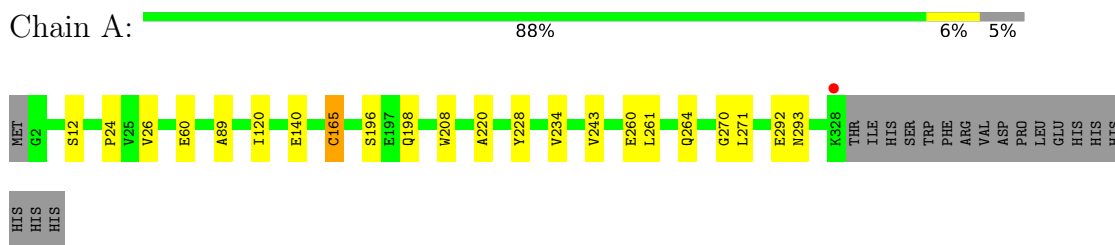
- Molecule 9 is water.

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

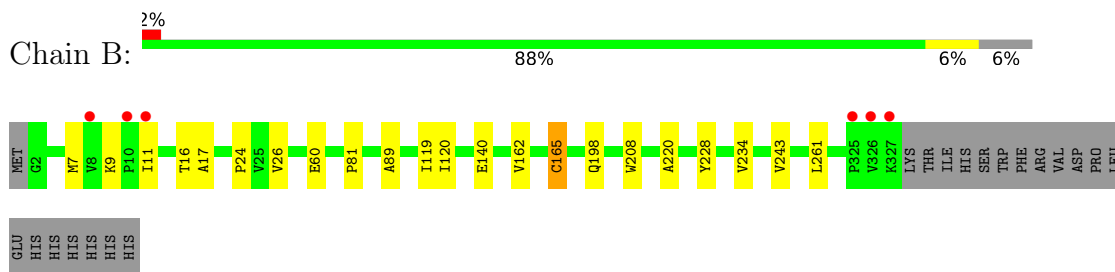
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

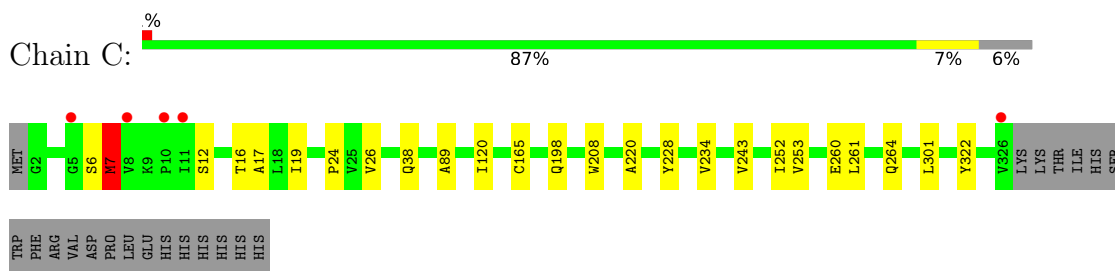
• Molecule 1: FORMAMIDASE



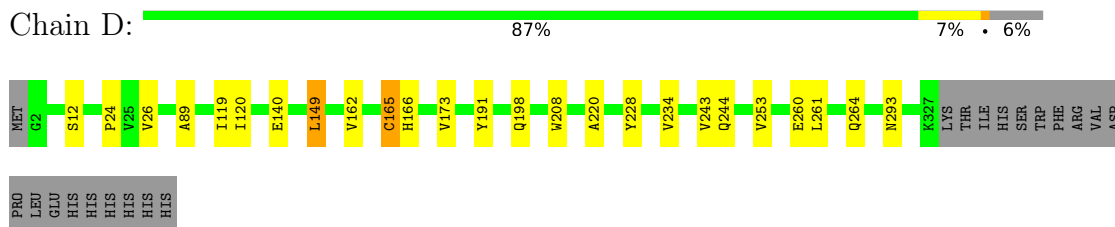
• Molecule 1: FORMAMIDASE



• Molecule 1: FORMAMIDASE



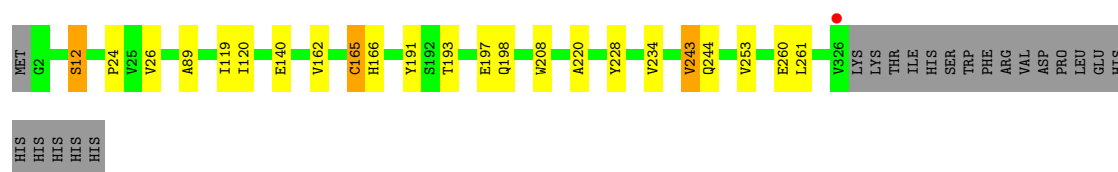
• Molecule 1: FORMAMIDASE



Chain E: 86% 8% 6%



Chain F: 87% 6% • 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.76Å 150.21Å 98.26Å 90.00° 98.68° 90.00°	Depositor
Resolution (Å)	103.23 – 1.78 103.23 – 1.78	Depositor EDS
% Data completeness (in resolution range)	93.0 (103.23-1.78) 93.0 (103.23-1.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.78Å)	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	9211 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)	0.34 , 57.7	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: PEG, ACT, PO4, SCY, NA, EDO, PGE, PG4

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	0.81	3/2689 (0.1%)	0.93	11/3657 (0.3%)
1	B	0.77	0/2727	0.83	0/3709
1	C	0.76	0/2698	0.86	4/3671 (0.1%)
1	D	0.74	0/2691	0.83	2/3662 (0.1%)
1	E	0.75	0/2723	0.83	2/3703 (0.1%)
1	F	0.73	0/2686	0.82	2/3654 (0.1%)
All	All	0.76	3/16214 (0.0%)	0.85	21/22056 (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	14.14	1.45	1.33
1	A	292[A]	GLU	C-N	6.54	1.44	1.33
1	A	292[B]	GLU	C-N	6.54	1.44	1.33

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ASN	O-C-N	18.15	137.10	121.31
1	C	7	MET	CB-CG-SD	11.31	146.65	112.70
1	A	293	ASN	CA-C-N	-9.79	109.20	121.04
1	A	293	ASN	C-N-CA	-9.79	109.20	121.04
1	D	12[A]	SER	N-CA-C	-7.13	96.89	108.52

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	15	0
1	B	2634	0	2620	18	0
1	C	2615	0	2574	22	0
1	D	2614	0	2567	18	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	1	0
9	F	262	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17882	0	15742	100	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 100 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:7:MET:HE3	1:C:7:MET:H	1.36	0.90
1:C:6:SER:OG	1:C:7:MET:HE2	1.75	0.86

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%)	284 (100%)	0	100	100
1	B	289/293 (99%)	287 (99%)	2 (1%)	76	66
1	C	286/293 (98%)	284 (99%)	2 (1%)	76	66
1	D	285/293 (97%)	283 (99%)	2 (1%)	76	66
1	E	288/293 (98%)	288 (100%)	0	100	100
1	F	284/293 (97%)	282 (99%)	2 (1%)	76	66
All	All	1716/1758 (98%)	1708 (100%)	8 (0%)	86	73

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	243[B]	VAL
1	F	243[A]	VAL
1	D	149[A]	LEU
1	C	38	GLN
1	D	149[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	244	GLN
1	F	264	GLN
1	C	244	GLN
1	C	264	GLN
1	D	244	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	C	165	1	7,8,9	0.95	0	4,9,11	1.26	1 (25%)
1	SCY	E	165	1	7,8,9	0.90	0	4,9,11	1.09	0
1	SCY	D	165	1	7,8,9	0.98	0	4,9,11	1.19	1 (25%)
1	SCY	F	165	1	7,8,9	1.01	0	4,9,11	1.31	1 (25%)
1	SCY	B	165	1	7,8,9	1.27	1 (14%)	4,9,11	0.76	0
1	SCY	A	165	1	7,8,9	1.67	2 (28%)	4,9,11	1.09	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	C	165	1	-	3/5/7/9	-
1	SCY	E	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	A	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	-3.26	1.74	1.81
1	A	165	SCY	CD-SG	-2.54	1.61	1.75
1	B	165	SCY	CD-SG	-2.22	1.63	1.75

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	165	SCY	CB-CA-C	2.33	117.12	110.80
1	C	165	SCY	CB-CA-C	2.18	116.71	110.80
1	D	165	SCY	CB-CA-C	2.05	116.36	110.80

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	165	SCY	OCD-CD-SG-CB
1	A	165	SCY	CE-CD-SG-CB
1	B	165	SCY	OCD-CD-SG-CB
1	B	165	SCY	CE-CD-SG-CB
1	C	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	D	165	SCY	1	0
1	F	165	SCY	1	0
1	B	165	SCY	2	0
1	A	165	SCY	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
2	PEG	E	1327	-	6,6,6	0.51	0	5,5,5	0.25	0
4	ACT	A	1332	-	3,3,3	0.80	0	3,3,3	0.82	0
2	PEG	E	1328[B]	-	6,6,6	0.56	0	5,5,5	0.46	0
2	PEG	A	1329	-	6,6,6	0.43	0	5,5,5	0.38	0
6	PGE	E	1329	-	9,9,9	0.46	0	8,8,8	0.48	0
2	PEG	A	1330	-	6,6,6	0.50	0	5,5,5	0.80	0
2	PEG	B	1328	-	6,6,6	0.55	0	5,5,5	1.01	1 (20%)
2	PEG	F	1329	-	6,6,6	0.49	0	5,5,5	0.23	0
6	PGE	C	1328	-	9,9,9	0.47	0	8,8,8	0.24	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
4	ACT	F	1332	5	3,3,3	0.76	0	3,3,3	0.79	0
8	PO4	F	1331	-	4,4,4	1.35	0	6,6,6	1.56	0
3	EDO	E	1330	-	3,3,3	0.35	0	2,2,2	0.39	0
4	ACT	C	1330	-	3,3,3	0.85	0	3,3,3	0.67	0
6	PGE	C	1327	-	9,9,9	0.48	0	8,8,8	0.28	0
3	EDO	A	1331	-	3,3,3	0.66	0	2,2,2	0.13	0
2	PEG	F	1328	-	6,6,6	0.42	0	5,5,5	1.33	1 (20%)
2	PEG	D	1328	-	6,6,6	0.55	0	5,5,5	0.42	0
6	PGE	B	1330	-	9,9,9	0.54	0	8,8,8	0.39	0
2	PEG	D	1330	-	6,6,6	0.35	0	5,5,5	0.49	0
3	EDO	C	1329	-	3,3,3	0.43	0	2,2,2	0.35	0
6	PGE	F	1330	-	9,9,9	0.58	0	8,8,8	0.31	0
2	PEG	B	1329	-	6,6,6	0.55	0	5,5,5	0.41	0
4	ACT	B	1333	-	3,3,3	0.78	0	3,3,3	0.82	0
2	PEG	F	1327	-	6,6,6	0.37	0	5,5,5	0.30	0
8	PO4	B	1332	-	4,4,4	0.93	0	6,6,6	0.77	0
2	PEG	D	1329	-	6,6,6	0.43	0	5,5,5	0.29	0
6	PGE	D	1331	-	9,9,9	0.52	0	8,8,8	0.26	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
2	PEG	E	1327	-	-	1/4/4/4	-
2	PEG	E	1328[B]	-	-	3/4/4/4	-
2	PEG	A	1329	-	-	2/4/4/4	-
6	PGE	E	1329	-	-	4/7/7/7	-
2	PEG	A	1330	-	-	2/4/4/4	-

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

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	2.12	119.47	110.11
2	B	1328	PEG	O2-C3-C4	2.10	119.35	110.11

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	1329	PGE	O2-C3-C4-O3
2	A	1329	PEG	O2-C3-C4-O4
6	E	1329	PGE	O1-C1-C2-O2
6	F	1330	PGE	O1-C1-C2-O2
2	A	1330	PEG	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1328	PEG	7	0
2	E	1328[A]	PEG	2	0
2	F	1328	PEG	5	0
2	D	1330	PEG	5	0
4	B	1333	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.34	1 (0%) 90 93	5, 11, 19, 69	10 (3%)
1	B	325/346 (93%)	-0.27	6 (1%) 67 75	5, 10, 21, 85	16 (4%)
1	C	324/346 (93%)	-0.30	5 (1%) 72 78	5, 10, 22, 68	14 (4%)
1	D	325/346 (93%)	-0.38	0 100 100	4, 11, 20, 53	11 (3%)
1	E	324/346 (93%)	-0.33	5 (1%) 72 78	5, 10, 21, 64	17 (5%)
1	F	324/346 (93%)	-0.25	1 (0%) 90 93	5, 11, 19, 36	12 (3%)
All	All	1948/2076 (93%)	-0.31	18 (0%) 81 86	4, 10, 20, 85	80 (4%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	326	VAL	6.0
1	E	326	VAL	4.9
1	B	327	LYS	4.4
1	E	8	VAL	3.6
1	B	326	VAL	3.4

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	0.95	0.08	12,13,23,25	0
1	SCY	B	165	9/10	0.95	0.08	10,11,21,22	0
1	SCY	E	165	9/10	0.96	0.07	10,11,18,20	0
1	SCY	D	165	9/10	0.97	0.06	11,12,23,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SCY	C	165	9/10	0.97	0.06	10,11,19,19	0
1	SCY	F	165	9/10	0.97	0.06	10,11,23,24	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	NA	E	1332	1/1	0.36	0.38	49,49,49,49	0
4	ACT	C	1330	4/4	0.64	0.19	46,46,48,54	0
3	EDO	A	1331	4/4	0.65	0.25	30,32,33,41	0
2	PEG	E	1328[B]	7/7	0.68	0.17	32,34,47,50	7
2	PEG	E	1328[A]	7/7	0.68	0.17	40,46,52,54	7
6	PGE	B	1330	10/10	0.72	0.21	47,59,63,63	0
2	PEG	D	1328	7/7	0.74	0.23	52,57,62,63	0
3	EDO	C	1329	4/4	0.76	0.20	55,58,59,59	0
2	PEG	F	1329	7/7	0.78	0.20	50,60,65,71	0
5	NA	A	1333	1/1	0.79	0.19	36,36,36,36	0
6	PGE	C	1327	10/10	0.80	0.17	49,53,61,68	0
2	PEG	B	1329	7/7	0.81	0.17	43,44,48,50	0
2	PEG	A	1330	7/7	0.81	0.19	37,47,52,56	0
6	PGE	D	1331	10/10	0.81	0.17	38,46,53,53	0
2	PEG	E	1327	7/7	0.82	0.15	45,50,60,67	0
2	PEG	F	1327	7/7	0.82	0.21	44,47,55,57	0
2	PEG	F	1328	7/7	0.82	0.18	34,40,45,48	0
2	PEG	A	1329	7/7	0.82	0.19	42,45,51,54	0
4	ACT	B	1333	4/4	0.83	0.13	42,48,49,50	0
6	PGE	F	1330	10/10	0.83	0.15	39,46,51,58	0
2	PEG	D	1330	7/7	0.84	0.16	32,37,42,51	0
3	EDO	E	1330	4/4	0.84	0.18	29,35,37,49	0
2	PEG	B	1328	7/7	0.84	0.16	27,37,43,57	0
5	NA	F	1335	1/1	0.84	0.13	32,32,32,32	0
4	ACT	A	1332	4/4	0.85	0.12	34,48,49,51	0
5	NA	F	1333	1/1	0.86	0.14	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	D	1329	7/7	0.86	0.17	44,44,50,50	0
6	PGE	E	1329	10/10	0.86	0.15	36,40,49,51	0
4	ACT	F	1332	4/4	0.86	0.12	38,47,52,54	0
7	PG4	B	1331	13/13	0.87	0.12	37,39,54,60	0
5	NA	F	1334	1/1	0.88	0.12	45,45,45,45	0
6	PGE	C	1328	10/10	0.88	0.12	34,35,43,44	0
5	NA	B	1336	1/1	0.89	0.11	27,27,27,27	0
5	NA	E	1340	1/1	0.89	0.10	49,49,49,49	0
5	NA	B	1335	1/1	0.90	0.10	30,30,30,30	0
5	NA	B	1337	1/1	0.90	0.13	37,37,37,37	0
5	NA	A	1340	1/1	0.91	0.10	41,41,41,41	0
5	NA	B	1334	1/1	0.92	0.13	40,40,40,40	0
5	NA	C	1331	1/1	0.95	0.10	33,33,33,33	0
5	NA	E	1331	1/1	0.96	0.07	26,26,26,26	0
5	NA	F	1336	1/1	0.97	0.06	25,25,25,25	0
5	NA	C	1332	1/1	0.97	0.11	23,23,23,23	0
8	PO4	B	1332	5/5	0.98	0.07	16,17,19,20	0
8	PO4	F	1331	5/5	0.98	0.06	18,20,21,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.